

HF CALCULATION ON Ia and Ic

Job WF28131 started on DESKTOP-T7TL8TH at Thu Mar 09 16:30:51 2023
Jaguar version 3.5, release 42

Job name: Ia
Task: Geometry optimization

Stoichiometry: C9NH7
Molecular weight: 129.06 amu
Molecular charge: 0
Spin multiplicity: 1
Point Group: Cs

SCF method: RHF
Basis set: 6-31G**
Basis functions: 185

Total electrons: 68
Alpha electrons: 34
Beta electrons: 34
Total orbitals: 185
Core orbitals: 34
Open-shell orbitals: 0
Occupied orbitals: 34
Shells: 1

Non-default options chosen:

Geometry will be optimized in redundant internal coordinates
Initial Hessian: from previous calculation

WARNING: Hessian has too many zero eigenvalues
Some coordinates may be inadvertently frozen

Iter	Energy	Gmax	Grms	Dmax	Drms
1	-399.285542 *	0.05414 .	0.01394 .	0.06946 .	0.02646 .
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
2	-399.295677 .	0.01196 .	0.00388 .	0.02854 .	0.00917 .
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
3	-399.296460 .	0.00681 .	0.00159 .	0.01376 .	0.00375 .
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
4	-399.296540 .	0.00214 .	0.00058 .	0.00379 .	0.00122 .
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
5	-399.296559 *	0.00039 *	0.00011 *	0.00079 *	0.00033 *

** Geometry optimization complete **

Final energy -399.29655875068

Job WF28131 completed on DESKTOP-T7TL8TH at Thu Mar 09 16:31:58 2023

Wall Time: 000:01:07

CPU Time: 000:00:00

TITAN Properties Program: (PC/x86)

Release 6.0.2

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-15.53909	-11.27106	-11.26094	-11.24910	-11.24814
(ev):		-422.84044	-306.70126	-306.42581	-306.10379	-306.07750
		A	A	A	A	A
1	H1 S	-0.00005	-0.00006	0.00008	0.00000	-0.00006
2	H1 S	-0.00035	-0.00056	0.00066	0.00003	-0.00076
3	H1 PX	0.00000	0.00000	-0.00001	0.00000	0.00000
4	H1 PY	0.00000	0.00004	-0.00002	0.00000	-0.00002
5	H1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1 S	0.00002	0.00077	-0.00006	0.00007	-0.00833
7	C1 S	0.00010	0.00030	-0.00015	-0.00005	0.00015
8	C1 PX	-0.00003	-0.00010	0.00005	0.00000	-0.00005
9	C1 PY	-0.00001	-0.00004	0.00003	0.00000	0.00003
10	C1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1 S	-0.00114	-0.00198	0.00172	0.00041	-0.00364
12	C1 PX	0.00106	0.00145	-0.00190	-0.00019	0.00231
13	C1 PY	-0.00015	0.00003	0.00072	-0.00010	0.00025
14	C1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1 DXX	0.00000	-0.00004	-0.00001	-0.00001	-0.00006
16	C1 DYY	0.00002	-0.00006	-0.00006	0.00001	-0.00009
17	C1 DZZ	0.00005	0.00013	-0.00007	-0.00002	0.00015
18	C1 DXY	0.00000	0.00000	-0.00001	0.00000	0.00004
19	C1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2 S	-0.00002	-0.01105	0.00015	0.00003	-0.05698
22	C2 S	-0.00004	-0.00053	0.00013	0.00000	-0.00147
23	C2 PX	0.00000	0.00014	0.00001	0.00001	0.00008
24	C2 PY	0.00005	-0.00005	-0.00007	-0.00002	0.00013
25	C2 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2 S	0.00041	-0.00160	-0.00068	-0.00003	-0.00082
27	C2 PX	0.00003	-0.00109	-0.00103	-0.00013	0.00037
28	C2 PY	-0.00076	-0.00088	-0.00039	-0.00020	-0.00124
29	C2 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2 DXX	-0.00013	0.00042	0.00001	0.00000	0.00051
31	C2 DYY	0.00002	0.00066	0.00002	0.00002	0.00046
32	C2 DZZ	-0.00002	0.00010	0.00006	0.00001	0.00016
33	C2 DXY	0.00003	-0.00022	0.00004	-0.00001	-0.00004

34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00001	-0.01158	0.00000	0.00041	0.00038
37	C3	S	0.00003	-0.00025	0.00010	0.00007	0.00000
38	C3	PX	-0.00004	-0.00006	-0.00006	0.00002	-0.00001
39	C3	PY	-0.00002	0.00000	-0.00003	0.00004	-0.00004
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00002	-0.00764	-0.00269	-0.00153	-0.00001
42	C3	PX	-0.00080	0.00282	0.00300	-0.00004	-0.00020
43	C3	PY	0.00101	0.00218	-0.00071	0.00043	0.00387
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00056	-0.00004	0.00000	0.00003
46	C3	DYY	-0.00007	0.00028	0.00021	-0.00004	0.00002
47	C3	DZZ	0.00001	0.00019	0.00008	0.00000	0.00002
48	C3	DXY	0.00002	0.00013	0.00000	-0.00001	0.00002
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00001	0.00013	0.00007	-0.00001	-0.07202
52	C4	S	-0.00005	-0.00011	0.00012	0.00004	-0.00224
53	C4	PX	0.00000	-0.00004	0.00000	-0.00001	-0.00005
54	C4	PY	-0.00002	-0.00006	0.00002	-0.00001	-0.00001
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00141	0.00238	-0.00255	-0.00032	-0.00020
57	C4	PX	-0.00027	-0.00057	0.00021	0.00013	0.00083
58	C4	PY	-0.00054	-0.00101	0.00133	0.00027	-0.00116
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00001	0.00005	0.00000	0.00000	0.00081
61	C4	DYY	0.00000	0.00004	0.00000	0.00000	0.00041
62	C4	DZZ	-0.00001	-0.00001	0.00004	0.00002	0.00024
63	C4	DXY	0.00000	0.00001	0.00000	0.00000	-0.00005
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00002	0.00143	-0.00011	-0.00046	-0.99130
67	C5	S	0.00007	0.00043	-0.00016	-0.00003	-0.02725
68	C5	PX	0.00002	0.00006	-0.00001	0.00001	-0.00015
69	C5	PY	-0.00004	-0.00013	0.00005	0.00000	0.00002
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.00031	-0.00039	0.00178	0.00037	0.00998
72	C5	PX	-0.00073	-0.00156	0.00062	0.00005	0.00014
73	C5	PY	0.00039	0.00106	-0.00122	-0.00018	-0.00005
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	-0.00005	-0.00001	0.00000	0.00165
76	C5	DYY	0.00003	-0.00013	-0.00002	0.00000	0.00146
77	C5	DZZ	0.00005	0.00015	-0.00007	-0.00001	0.00245
78	C5	DXY	-0.00001	-0.00002	-0.00001	0.00000	-0.00014
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00005	-0.99556	-0.00040	-0.00004	-0.00071
82	C6	S	-0.00030	-0.02754	-0.00038	-0.00006	0.00023
83	C6	PX	-0.00005	-0.00006	-0.00007	-0.00003	0.00001
84	C6	PY	-0.00009	0.00022	-0.00007	0.00005	0.00009
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.00424	0.00877	0.00480	0.00002	-0.00015
87	C6	PX	0.00018	0.00460	0.00276	0.00037	-0.00039

88	C6	PY	0.00160	0.00281	-0.00122	-0.00010	-0.00316
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00009	0.00177	0.00006	0.00000	0.00003
91	C6	DYY	0.00059	0.00094	0.00017	-0.00002	-0.00010
92	C6	DZZ	0.00003	0.00241	-0.00009	-0.00003	0.00006
93	C6	DXY	0.00019	-0.00008	-0.00001	0.00003	0.00002
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00002	0.00154	0.02231	0.00586	-0.00010
97	C7	S	-0.00005	-0.00027	0.00078	0.00020	-0.00015
98	C7	PX	-0.00005	0.00005	0.00006	0.00002	0.00001
99	C7	PY	-0.00003	-0.00005	0.00005	-0.00006	0.00004
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00160	0.00610	0.00335	0.00129	0.00360
102	C7	PX	-0.00097	-0.00416	-0.00120	-0.00073	-0.00147
103	C7	PY	0.00105	0.00112	-0.00258	0.00063	0.00105
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00006	-0.00072	-0.00010	0.00002
106	C7	DYY	-0.00002	-0.00009	-0.00034	-0.00007	0.00001
107	C7	DZZ	-0.00001	-0.00017	-0.00015	-0.00002	-0.00005
108	C7	DXY	0.00002	0.00008	-0.00013	-0.00007	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	0.00000	-0.00001	-0.00001	0.00010
112	H3	S	0.00010	0.00023	-0.00029	-0.00010	0.00021
113	H3	PX	0.00000	0.00001	0.00001	0.00000	0.00002
114	H3	PY	0.00001	0.00002	-0.00001	0.00000	0.00006
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00006	-0.00012	0.00006	0.00000	0.00025
117	H4	S	-0.00027	-0.00079	0.00043	0.00004	-0.00186
118	H4	PX	0.00001	0.00003	0.00000	0.00000	0.00014
119	H4	PY	0.00002	0.00001	0.00000	0.00000	-0.00021
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.99524	0.00031	-0.00011	-0.00004	0.00004
122	N1	S	-0.02515	-0.00072	0.00073	0.00001	0.00015
123	N1	PX	-0.00197	0.00006	0.00002	-0.00003	-0.00001
124	N1	PY	-0.00078	-0.00009	-0.00011	-0.00003	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00731	0.00539	-0.00350	0.00086	-0.00201
127	N1	PX	0.00294	0.00164	-0.00208	0.00018	-0.00006
128	N1	PY	0.00070	0.00204	0.00046	0.00006	-0.00076
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00282	0.00015	-0.00040	-0.00010	0.00012
131	N1	DYY	0.00262	0.00013	-0.00011	-0.00016	0.00003
132	N1	DZZ	0.00306	-0.00047	0.00041	-0.00002	0.00007
133	N1	DXY	-0.00021	0.00004	0.00023	0.00009	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.00002	-0.00009	-0.00004	-0.00001	0.00001
137	H6	S	-0.00001	-0.00031	-0.00037	-0.00004	0.00017
138	H6	PX	0.00003	-0.00010	0.00000	0.00000	-0.00013
139	H6	PY	0.00004	0.00003	-0.00001	0.00000	-0.00004
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00002	-0.00036	0.99275	0.07266	-0.00008

5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.95337	0.03077	-0.27760	-0.06524	-0.00041
7	C1	S	-0.02630	0.00067	-0.00767	-0.00173	0.00029
8	C1	PX	0.00015	0.00001	0.00013	0.00014	0.00002
9	C1	PY	0.00024	-0.00007	-0.00003	0.00020	0.00007
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00840	0.00260	0.00266	0.00377	-0.00490
12	C1	PX	-0.00007	-0.00181	0.00104	-0.00069	0.00263
13	C1	PY	0.00014	-0.00002	0.00144	-0.00103	0.00079
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00158	0.00001	0.00000	-0.00040	-0.00009
16	C1	DYY	0.00160	-0.00003	0.00007	-0.00058	-0.00006
17	C1	DZZ	0.00237	-0.00011	0.00071	0.00002	0.00008
18	C1	DXY	0.00013	-0.00001	0.00002	-0.00026	-0.00002
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00327	-0.00002	-0.00995	-0.00583	0.99383
22	C2	S	-0.00003	0.00019	-0.00070	-0.00030	0.02758
23	C2	PX	0.00005	0.00001	-0.00002	-0.00004	0.00030
24	C2	PY	-0.00005	0.00003	-0.00001	0.00001	-0.00010
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00287	-0.00316	0.00463	0.00032	-0.00969
27	C2	PX	0.00126	-0.00212	0.00270	0.00016	-0.00009
28	C2	PY	-0.00069	-0.00040	-0.00073	-0.00017	-0.00049
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00002	-0.00007	0.00015	0.00008	-0.00153
31	C2	DYY	-0.00002	0.00002	0.00018	0.00010	-0.00151
32	C2	DZZ	-0.00003	0.00006	-0.00012	-0.00003	-0.00249
33	C2	DXY	-0.00002	0.00000	0.00003	-0.00003	0.00014
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06061	-0.14358	-0.03720	0.98259	0.00548
37	C3	S	-0.00163	-0.00364	-0.00118	0.02765	0.00007
38	C3	PX	0.00006	-0.00001	0.00005	-0.00014	0.00003
39	C3	PY	0.00003	-0.00019	-0.00012	-0.00002	-0.00016
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00488	-0.00538	-0.00244	-0.01646	-0.00156
42	C3	PX	0.00039	0.00017	-0.00048	0.00126	0.00053
43	C3	PY	0.00238	-0.00009	0.00563	0.00150	0.00590
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00045	0.00058	0.00021	-0.00175	0.00007
46	C3	DYY	0.00060	0.00059	0.00035	-0.00099	0.00002
47	C3	DZZ	0.00029	0.00047	0.00012	-0.00229	-0.00003
48	C3	DXY	0.00020	0.00007	0.00008	0.00012	0.00003
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.27703	0.02303	0.95303	0.02234	0.00638
52	C4	S	-0.00749	0.00084	0.02627	0.00045	-0.00011
53	C4	PX	0.00015	-0.00004	-0.00012	0.00002	0.00008
54	C4	PY	-0.00010	0.00000	-0.00012	0.00002	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00074	-0.00273	-0.01004	-0.00071	0.00211
57	C4	PX	-0.00115	0.00058	-0.00012	-0.00001	-0.00057
58	C4	PY	0.00063	0.00169	-0.00002	-0.00002	-0.00161

59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00079	-0.00004	-0.00139	0.00006	0.00014
61	C4	DYY	0.00077	-0.00010	-0.00127	0.00014	0.00006
62	C4	DZZ	0.00071	0.00001	-0.00234	-0.00010	-0.00009
63	C4	DXY	0.00007	0.00000	-0.00014	-0.00003	0.00003
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02813	-0.00194	-0.06663	-0.00035	-0.05820
67	C5	S	0.00095	-0.00016	-0.00148	-0.00001	-0.00170
68	C5	PX	0.00010	0.00000	-0.00004	-0.00002	0.00011
69	C5	PY	-0.00001	-0.00002	-0.00001	0.00003	0.00014
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.00220	0.00282	0.00110	0.00017	0.00292
72	C5	PX	-0.00099	0.00043	0.00030	0.00006	-0.00112
73	C5	PY	0.00086	-0.00137	0.00161	0.00000	-0.00065
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00004	0.00000	-0.00058	-0.00007	-0.00031
76	C5	DYY	0.00001	0.00001	-0.00021	-0.00005	-0.00035
77	C5	DZZ	0.00002	-0.00002	0.00014	-0.00003	0.00012
78	C5	DXY	0.00007	0.00000	-0.00008	0.00001	0.00001
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00004	0.00010	0.00046	-0.01203	-0.01154
82	C6	S	0.00011	-0.00009	0.00019	-0.00025	-0.00018
83	C6	PX	0.00004	-0.00001	0.00000	-0.00006	0.00008
84	C6	PY	0.00012	-0.00001	0.00009	0.00005	0.00001
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00031	0.00046	-0.00148	0.00528	0.00431
87	C6	PX	0.00115	0.00097	0.00060	0.00226	-0.00003
88	C6	PY	-0.00301	0.00322	-0.00469	-0.00096	-0.00275
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00001	-0.00008	0.00003	-0.00059	-0.00033
91	C6	DYY	0.00000	-0.00006	-0.00004	-0.00028	-0.00051
92	C6	DZZ	0.00004	-0.00005	0.00003	-0.00012	-0.00008
93	C6	DXY	0.00000	0.00003	-0.00001	0.00006	0.00018
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.02747	-0.98415	0.01912	-0.14547	-0.00065
97	C7	S	-0.00091	-0.02740	0.00025	-0.00438	-0.00024
98	C7	PX	0.00006	0.00020	0.00000	0.00016	-0.00002
99	C7	PY	0.00008	-0.00003	0.00007	-0.00021	0.00009
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00449	0.01233	0.00615	0.00820	0.00575
102	C7	PX	-0.00221	-0.00237	-0.00233	-0.00188	-0.00234
103	C7	PY	0.00081	0.00057	0.00195	0.00178	0.00158
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00004	0.00145	-0.00002	-0.00032	0.00004
106	C7	DYY	0.00003	0.00160	-0.00001	-0.00016	0.00003
107	C7	DZZ	0.00004	0.00236	-0.00014	0.00023	-0.00006
108	C7	DXY	0.00005	0.00030	0.00003	0.00024	-0.00002
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00005	-0.00005	-0.00025	-0.00001	0.00006
112	H3	S	-0.00042	-0.00045	0.00188	0.00019	0.00057

113	H3	PX	-0.00001	0.00000	0.00013	0.00002	-0.00003
114	H3	PY	0.00008	-0.00002	0.00027	0.00003	0.00003
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00004	0.00002	-0.00010	0.00001	0.00003
117	H4	S	-0.00034	0.00026	-0.00068	0.00001	-0.00028
118	H4	PX	-0.00003	0.00000	0.00004	0.00000	0.00006
119	H4	PY	0.00000	0.00001	-0.00009	-0.00002	-0.00017
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00003	-0.00011	0.00003	0.00007	0.00007
122	N1	S	0.00013	-0.00029	0.00011	0.00019	0.00014
123	N1	PX	-0.00001	-0.00002	0.00000	0.00005	0.00005
124	N1	PY	-0.00005	-0.00002	-0.00004	-0.00001	-0.00004
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.00175	0.00408	-0.00204	-0.00220	-0.00278
127	N1	PX	-0.00038	0.00092	-0.00024	-0.00075	-0.00036
128	N1	PY	-0.00019	0.00083	-0.00041	-0.00001	-0.00064
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00006	-0.00027	0.00008	0.00016	0.00018
131	N1	DYY	0.00005	-0.00017	0.00006	0.00016	0.00017
132	N1	DZZ	0.00005	-0.00019	0.00004	0.00014	0.00005
133	N1	DXY	-0.00003	0.00002	-0.00002	0.00004	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.00002	-0.00006	0.00004	0.00000	-0.00028
137	H6	S	0.00023	-0.00059	0.00078	0.00013	0.00191
138	H6	PX	-0.00001	0.00002	-0.00003	0.00000	-0.00027
139	H6	PY	0.00002	0.00001	0.00003	-0.00001	0.00002
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00066	0.02278	-0.00047	0.00339	-0.00009
142	C8	S	0.00016	0.00054	0.00015	0.00005	0.00015
143	C8	PX	-0.00004	0.00008	-0.00005	0.00001	-0.00005
144	C8	PY	0.00002	0.00001	0.00006	0.00007	0.00008
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.00155	-0.00480	-0.00138	-0.00123	-0.00118
147	C8	PX	-0.00121	-0.00094	-0.00092	-0.00158	-0.00098
148	C8	PY	-0.00148	-0.00170	-0.00207	-0.00073	-0.00168
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00001	0.00040	-0.00002	0.00014	-0.00002
151	C8	DYY	0.00002	0.00041	0.00001	0.00024	0.00005
152	C8	DZZ	0.00004	0.00007	0.00005	0.00006	0.00006
153	C8	DXY	-0.00004	0.00021	-0.00004	0.00009	-0.00002
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00008	0.00048	0.00000	0.00010	0.00001
157	H8	S	0.00059	-0.00121	0.00070	-0.00003	0.00062
158	H8	PX	-0.00001	-0.00031	0.00000	-0.00019	0.00001
159	H8	PY	0.00002	0.00009	-0.00003	0.00006	-0.00002
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00023	-0.00425	0.00005	-0.00023	0.00004
162	C10	S	-0.00001	-0.00004	0.00000	0.00001	0.00001
163	C10	PX	-0.00002	0.00006	-0.00004	-0.00002	-0.00003
164	C10	PY	-0.00002	-0.00002	-0.00004	-0.00004	-0.00004
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.00066	-0.00001	-0.00113	-0.00030	-0.00095

167	C10	PX	0.00052	-0.00029	0.00052	0.00070	0.00049
168	C10	PY	-0.00030	-0.00008	-0.00041	-0.00014	-0.00039
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00001	-0.00004	-0.00002	0.00000	-0.00001
171	C10	DYY	-0.00001	-0.00013	-0.00001	-0.00008	-0.00003
172	C10	DZZ	0.00000	0.00005	-0.00001	0.00001	0.00000
173	C10	DXY	0.00002	0.00002	0.00001	0.00005	0.00002
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.00004	0.00008	-0.00004	-0.00005	-0.00004
177	H16	S	-0.00022	0.00007	-0.00016	-0.00021	-0.00017
178	H16	PX	0.00000	-0.00001	-0.00001	-0.00001	0.00000
179	H16	PY	0.00000	0.00003	0.00000	0.00001	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00005	-0.00004	0.00007	0.00006	0.00006
182	H18	S	0.00016	-0.00024	0.00021	0.00025	0.00017
183	H18	PX	0.00000	0.00001	0.00001	0.00000	0.00000
184	H18	PY	0.00000	-0.00001	0.00000	0.00000	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	11	12	13	14	15
Eigenvalues:	-1.27357	-1.13269	-1.07025	-1.03312	-0.99958
(ev):	-34.65549	-30.82212	-29.12296	-28.11256	-27.20010

		A	A	A	A	A	
1	H1	S	0.00508	0.04286	-0.03663	0.01218	-0.06232
2	H1	S	-0.00659	0.00783	-0.01223	0.00554	-0.01052
3	H1	PX	-0.00056	-0.00474	0.00373	-0.00106	0.00637
4	H1	PY	0.00007	-0.00008	0.00052	-0.00051	-0.00063
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.01704	-0.10122	0.06278	-0.01742	0.10159
7	C1	S	0.03515	0.19254	-0.11923	0.03329	-0.19743
8	C1	PX	-0.01380	-0.06328	0.01518	0.00202	0.03112
9	C1	PY	-0.01048	0.02228	0.02771	-0.05775	-0.09198
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00014	0.12411	-0.09381	0.03294	-0.12199
12	C1	PX	0.01674	-0.00861	0.00974	-0.00553	-0.02028
13	C1	PY	-0.00405	0.00374	0.00297	-0.01056	-0.01688
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00039	0.00323	-0.00048	-0.00005	-0.00250
16	C1	DYY	0.00237	0.00761	-0.00732	0.00388	-0.00386
17	C1	DZZ	-0.00110	-0.00879	0.00572	-0.00196	0.00720
18	C1	DXY	0.00111	-0.00303	-0.00176	0.00572	0.00805
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02843	-0.08173	-0.08158	0.04291	-0.09962
22	C2	S	0.05266	0.15673	0.15473	-0.08095	0.19269
23	C2	PX	0.01858	0.05640	0.02697	-0.01484	0.03094
24	C2	PY	-0.02189	0.03667	-0.00290	-0.06621	0.02991
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.03640	0.08409	0.12102	-0.05828	0.12680
27	C2	PX	0.00244	-0.00816	0.00794	-0.00480	-0.01208
28	C2	PY	-0.01578	0.00280	-0.00156	-0.01531	0.00757
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

30	C2	DXX	-0.00008	0.00281	0.00094	-0.00032	0.00260
31	C2	DYY	0.00514	0.00528	0.00885	-0.00168	0.00556
32	C2	DZZ	-0.00308	-0.00648	-0.00684	0.00312	-0.00740
33	C2	DXY	-0.00249	0.00342	0.00015	-0.00676	0.00133
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06210	-0.06494	0.09229	-0.08166	-0.04395
37	C3	S	0.11552	0.12555	-0.17551	0.15746	0.08500
38	C3	PX	-0.03852	0.00348	-0.05756	-0.01045	-0.02326
39	C3	PY	-0.03599	0.05348	0.04817	-0.02863	-0.11117
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.05414	0.06134	-0.13372	0.10388	0.06914
42	C3	PX	-0.01472	0.00884	-0.00452	0.00197	0.00210
43	C3	PY	0.01019	0.01746	0.00622	-0.00936	-0.05975
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00731	0.00241	0.00532	0.00486	0.00152
46	C3	DYY	0.00450	0.00831	-0.01490	0.00508	0.00000
47	C3	DZZ	-0.00592	-0.00547	0.00695	-0.00623	-0.00269
48	C3	DXY	0.00217	0.00232	0.00041	0.00068	-0.00808
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.01115	-0.10899	0.01557	0.04274	0.10134
52	C4	S	0.02007	0.20724	-0.03067	-0.08134	-0.19282
53	C4	PX	-0.00247	-0.01578	-0.04421	0.04096	-0.07867
54	C4	PY	-0.01027	-0.06254	0.02813	-0.00849	0.05598
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.03508	0.12516	-0.00970	-0.06477	-0.17700
57	C4	PX	-0.00476	-0.00317	-0.00784	0.00914	-0.00326
58	C4	PY	-0.00998	-0.00379	-0.00730	0.00430	0.01316
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00103	0.00828	0.00440	-0.00741	0.00129
61	C4	DYY	0.00082	0.00483	-0.00350	0.00115	-0.00814
62	C4	DZZ	-0.00110	-0.00940	0.00076	0.00398	0.00775
63	C4	DXY	-0.00036	-0.00385	0.00367	-0.00109	0.00799
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.01295	-0.10306	-0.05186	0.07778	-0.04746
67	C5	S	0.02730	0.19488	0.10120	-0.14998	0.08939
68	C5	PX	0.00136	0.02733	-0.03222	-0.00091	-0.09624
69	C5	PY	-0.01364	-0.05246	-0.04201	0.02209	-0.06857
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00686	0.13990	0.05912	-0.10381	0.09140
72	C5	PX	-0.01354	0.01121	-0.00713	-0.00240	-0.00568
73	C5	PY	0.00881	-0.01635	0.00732	-0.00225	-0.01476
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00040	0.00859	-0.00148	-0.00467	-0.00830
76	C5	DYY	0.00108	0.00445	0.00505	-0.00322	0.00881
77	C5	DZZ	-0.00056	-0.00942	-0.00365	0.00642	-0.00340
78	C5	DXY	0.00067	0.00358	0.00388	-0.00306	0.00611
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.11142	-0.02696	-0.06497	-0.04975	-0.02426
82	C6	S	0.21497	0.05202	0.12958	0.09830	0.04650
83	C6	PX	-0.00405	0.02770	-0.10777	0.04491	0.03034

84	C6	PY	-0.10745	0.09706	-0.02603	-0.04404	0.11721
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.04237	0.05241	0.06301	0.06853	0.05741
87	C6	PX	0.01862	0.01628	-0.00106	0.02695	0.00986
88	C6	PY	0.02472	0.02468	0.01534	-0.00791	0.04176
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00004	0.00770	-0.00958	0.00803	0.00875
91	C6	DYY	0.01759	-0.00145	0.01448	-0.00183	-0.00199
92	C6	DZZ	-0.01220	-0.00247	-0.00617	-0.00484	-0.00181
93	C6	DXY	0.00446	-0.00517	0.00290	0.00358	-0.01190
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.05479	-0.00837	0.11160	-0.02793	-0.08464
97	C7	S	0.10131	0.01407	-0.21525	0.05265	0.16412
98	C7	PX	-0.05311	0.01217	0.04029	0.00294	-0.02446
99	C7	PY	0.01620	0.03771	-0.03702	0.09495	0.03157
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.06529	0.03244	-0.13974	0.04620	0.08859
102	C7	PX	-0.01327	-0.01100	-0.00470	-0.00022	0.01487
103	C7	PY	0.01731	0.00261	0.00139	0.00839	-0.01426
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00568	-0.00345	-0.00326	-0.00361	0.00222
106	C7	DYY	0.00369	0.00243	-0.00873	0.00351	0.00544
107	C7	DZZ	-0.00570	-0.00052	0.00878	-0.00198	-0.00654
108	C7	DXY	0.00036	-0.00308	-0.00003	-0.00907	-0.00348
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00307	0.04711	-0.00758	-0.02638	-0.06569
112	H3	S	0.00169	0.00817	0.00171	-0.00993	-0.02078
113	H3	PX	-0.00011	-0.00211	0.00001	0.00139	0.00189
114	H3	PY	-0.00025	-0.00476	0.00105	0.00215	0.00631
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00301	0.04505	0.02704	-0.04672	0.02899
117	H4	S	-0.00654	0.01227	0.00189	-0.01215	0.00982
118	H4	PX	0.00031	0.00241	0.00105	-0.00223	0.00050
119	H4	PY	-0.00027	-0.00431	-0.00274	0.00415	-0.00327
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.14422	0.05226	-0.06921	-0.00221	0.07083
122	N1	S	0.28540	-0.10838	0.14253	0.00393	-0.14880
123	N1	PX	0.10533	-0.03781	-0.00114	-0.00205	-0.02521
124	N1	PY	0.05565	0.01227	0.08376	0.08944	-0.00065
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.32801	-0.10545	0.17242	-0.00303	-0.16263
127	N1	PX	0.06128	-0.01864	0.00923	-0.00751	-0.01621
128	N1	PY	0.02279	0.01197	0.03252	0.03653	0.00455
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00583	-0.00405	-0.00621	-0.00293	-0.00070
131	N1	DYY	0.00608	-0.00117	0.00607	0.00102	-0.00195
132	N1	DZZ	-0.01353	0.00362	-0.00332	-0.00023	0.00361
133	N1	DXY	0.00259	0.00279	0.00627	0.01155	0.00079
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.01021	0.03125	0.04482	-0.02299	0.05826
137	H6	S	0.00074	-0.00106	0.01154	-0.00736	0.01027

138	H6	PX	0.00132	0.00352	0.00476	-0.00247	0.00581
139	H6	PY	0.00025	0.00044	0.00001	-0.00071	0.00069
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.08826	0.04637	0.06712	0.10125	-0.00594
142	C8	S	0.16846	-0.09040	-0.13103	-0.19849	0.00996
143	C8	PX	-0.04358	0.03327	-0.07860	0.02159	0.09741
144	C8	PY	0.06687	-0.00300	0.03594	0.13992	-0.00773
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.04461	-0.05447	-0.09646	-0.13342	0.02587
147	C8	PX	0.02993	-0.01586	-0.01592	-0.01459	0.01350
148	C8	PY	-0.00505	-0.00122	-0.01380	0.01365	0.01864
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00795	-0.00264	-0.00047	0.00434	-0.00079
151	C8	DYY	0.01224	-0.00436	-0.00597	-0.00822	0.00118
152	C8	DZZ	-0.00993	0.00440	0.00516	0.00721	-0.00003
153	C8	DXY	-0.00910	0.00502	-0.01305	0.00014	0.01304
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.01512	0.00456	-0.05839	0.00728	0.04888
157	H8	S	0.00498	0.00389	-0.01031	-0.00114	0.00734
158	H8	PX	-0.00146	-0.00042	0.00540	-0.00036	-0.00409
159	H8	PY	0.00025	0.00068	-0.00225	0.00136	0.00195
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.02546	0.02737	0.05883	0.13573	-0.00705
162	C10	S	0.04820	-0.05287	-0.11293	-0.26146	0.01321
163	C10	PX	-0.00158	0.00198	-0.01455	-0.00419	0.01684
164	C10	PY	0.03175	-0.02668	-0.04463	-0.08784	0.00185
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.03321	-0.03605	-0.09138	-0.20180	0.01996
167	C10	PX	-0.01366	0.00630	-0.00082	0.00029	0.00147
168	C10	PY	0.00650	-0.00198	-0.00588	-0.00783	0.00323
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00228	0.00136	0.00148	0.00274	0.00033
171	C10	DYY	0.00304	-0.00311	-0.00511	-0.01228	-0.00007
172	C10	DZZ	-0.00191	0.00210	0.00480	0.01137	-0.00057
173	C10	DXY	-0.00136	0.00059	-0.00247	-0.00090	0.00201
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00892	-0.01196	-0.03506	-0.07744	0.01033
177	H16	S	0.00489	-0.00319	-0.00814	-0.01848	0.00470
178	H16	PX	-0.00071	0.00094	0.00296	0.00625	-0.00080
179	H16	PY	0.00052	-0.00092	-0.00273	-0.00551	0.00079
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00944	-0.01359	-0.02685	-0.07738	-0.00159
182	H18	S	-0.00397	0.00043	-0.00219	-0.01651	-0.00259
183	H18	PX	0.00136	-0.00137	-0.00241	-0.00706	-0.00014
184	H18	PY	0.00078	-0.00106	-0.00146	-0.00460	-0.00037
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	16	17	18	19	20
Eigenvalues:	-0.90918	-0.80562	-0.79464	-0.75492	-0.68891
(ev):	-24.74003	-21.92213	-21.62336	-20.54253	-18.74617

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1	H1	S	-0.04160	-0.12145	0.00323	0.05688	-0.06736
2	H1	S	-0.01017	-0.05224	0.01110	0.03304	-0.04468
3	H1	PX	0.00365	0.00918	-0.00050	-0.00351	0.00419
4	H1	PY	0.00081	0.00096	0.00218	-0.00145	-0.00167
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.05775	0.08513	0.00938	-0.01010	-0.00133
7	C1	S	-0.11573	-0.17100	-0.02332	0.02053	0.00611
8	C1	PX	0.00710	-0.09298	0.01550	0.09237	-0.11945
9	C1	PY	0.06789	0.02496	0.18373	-0.06510	-0.11735
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.06845	-0.14148	0.03355	0.02456	-0.02407
12	C1	PX	-0.01697	-0.05352	-0.02600	0.03131	-0.03181
13	C1	PY	0.01212	0.00887	0.04166	-0.01756	-0.03582
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00283	-0.00463	-0.00152	0.00037	0.00039
16	C1	DYY	-0.00327	-0.00103	-0.00223	0.00204	0.00091
17	C1	DZZ	0.00460	0.00585	0.00089	-0.00070	0.00012
18	C1	DXY	-0.00724	-0.00092	-0.01249	0.00262	0.00364
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.04350	0.07420	-0.03920	0.01662	0.03760
22	C2	S	-0.08703	-0.14631	0.08207	-0.03424	-0.07515
23	C2	PX	-0.01126	0.08051	-0.03454	-0.07343	0.16026
24	C2	PY	0.12115	-0.07770	-0.16856	0.03158	-0.04769
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.06684	-0.13397	0.04277	-0.00450	-0.07966
27	C2	PX	0.00491	0.03374	-0.03445	-0.00780	0.08162
28	C2	PY	0.02475	-0.02157	-0.03089	0.01386	-0.00879
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00357	-0.00222	0.00403	-0.00315	-0.00534
31	C2	DYY	-0.00338	-0.00042	0.00156	0.00319	0.00500
32	C2	DZZ	0.00383	0.00475	-0.00276	0.00129	0.00208
33	C2	DXY	0.01108	-0.00667	-0.01027	0.00333	-0.00130
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03808	-0.03418	0.07748	-0.00916	0.01713
37	C3	S	-0.07750	0.06855	-0.15457	0.01859	-0.03461
38	C3	PX	0.03273	-0.16396	-0.01726	0.15777	0.06922
39	C3	PY	-0.13504	-0.05792	-0.08410	-0.06009	0.17632
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.05057	0.04554	-0.14254	0.03376	0.00087
42	C3	PX	-0.00081	-0.04004	-0.00716	0.05432	0.01684
43	C3	PY	-0.05841	-0.02267	-0.07335	-0.02976	0.05808
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00898	0.01101	-0.00229	-0.00553	-0.00013
46	C3	DYY	0.00177	-0.00785	-0.00301	0.00309	0.00094
47	C3	DZZ	0.00292	-0.00263	0.00521	0.00055	0.00122
48	C3	DXY	-0.00499	-0.00448	-0.00735	-0.00217	-0.00062
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.06019	-0.05636	-0.06729	0.01110	0.01646
52	C4	S	0.11904	0.11326	0.13538	-0.02204	-0.03331
53	C4	PX	-0.08377	-0.10407	0.11259	-0.02642	-0.17111
54	C4	PY	0.06968	0.08345	0.02454	0.07067	-0.11192

55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.08897	0.09334	0.09205	-0.01122	-0.02255
57	C4	PX	-0.01544	-0.02359	0.04149	-0.00810	-0.06591
58	C4	PY	0.02639	0.04149	0.04615	0.01376	-0.06440
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.01100	0.00615	-0.00428	0.00359	0.00610
61	C4	DYY	-0.00325	-0.00052	0.00496	-0.00228	-0.00487
62	C4	DZZ	-0.00498	-0.00450	-0.00405	0.00075	0.00079
63	C4	DXY	0.00355	0.00618	-0.00086	0.00038	-0.00026
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.08796	-0.01045	0.07223	-0.03450	-0.02427
67	C5	S	0.17246	0.02146	-0.14566	0.07086	0.05172
68	C5	PX	0.04460	0.15524	0.06255	-0.03717	0.13116
69	C5	PY	0.06428	0.08617	-0.02383	0.10429	-0.03240
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.15077	0.02723	-0.11528	0.05742	0.02725
72	C5	PX	0.01072	0.04103	0.03473	-0.01619	0.03684
73	C5	PY	0.02056	0.01847	-0.03962	0.05438	0.00374
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.01002	0.00931	0.00244	0.00112	0.00310
76	C5	DYY	-0.00091	-0.00463	-0.00447	0.00081	-0.00141
77	C5	DZZ	-0.00729	-0.00158	0.00490	-0.00215	-0.00145
78	C5	DXY	-0.00050	-0.00522	0.00204	-0.00245	-0.00471
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.07157	-0.07266	-0.04705	0.00784	-0.01064
82	C6	S	-0.14644	0.14981	0.09828	-0.01466	0.02337
83	C6	PX	0.01391	0.11485	-0.15118	-0.13225	-0.09436
84	C6	PY	-0.10589	-0.01234	0.04628	-0.16102	0.03599
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.12706	0.13253	0.10678	-0.02242	0.00900
87	C6	PX	-0.00951	0.04892	-0.04696	-0.03250	-0.04201
88	C6	PY	-0.03098	-0.00265	0.03807	-0.05677	0.01374
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00705	0.01075	-0.00445	-0.00643	-0.00827
91	C6	DYY	0.00048	-0.00623	0.00502	0.00169	0.00423
92	C6	DZZ	0.00497	-0.00536	-0.00334	-0.00044	-0.00040
93	C6	DXY	0.00139	0.00345	-0.00612	0.01257	0.01106
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.07287	0.02533	-0.07196	-0.03984	-0.02519
97	C7	S	0.14539	-0.05308	0.14459	0.08058	0.05014
98	C7	PX	-0.03317	-0.04423	0.03498	0.15496	0.20404
99	C7	PY	-0.01619	0.05328	-0.12489	0.09959	-0.14194
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.08401	-0.04537	0.10262	0.06671	0.06998
102	C7	PX	0.01642	-0.01871	0.03777	0.06366	0.08637
103	C7	PY	-0.01213	0.01143	-0.05470	0.00905	-0.05467
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00753	-0.00341	0.00915	-0.00603	0.00603
106	C7	DYY	-0.00034	0.00131	-0.00355	0.00415	-0.00466
107	C7	DZZ	-0.00563	0.00146	-0.00508	-0.00174	-0.00142
108	C7	DXY	0.00041	-0.00634	0.00288	-0.01012	0.00114

109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.06002	0.06581	0.09444	0.01757	-0.11496
112	H3	S	0.02149	0.02696	0.03606	0.01339	-0.06681
113	H3	PX	-0.00310	-0.00352	-0.00205	-0.00100	0.00177
114	H3	PY	-0.00404	-0.00379	-0.00729	-0.00026	0.00696
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.08449	0.00901	-0.08978	0.08953	-0.02741
117	H4	S	0.03200	0.00588	-0.03307	0.04377	-0.02477
118	H4	PX	0.00422	0.00212	-0.00314	0.00316	0.00035
119	H4	PY	-0.00588	0.00081	0.00642	-0.00505	0.00183
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.02368	0.03648	0.02404	-0.04288	-0.03197
122	N1	S	0.05000	-0.07984	-0.05061	0.09645	0.07032
123	N1	PX	0.05352	-0.00064	-0.05283	-0.08713	-0.08173
124	N1	PY	-0.04912	0.10794	0.12745	0.16277	0.02407
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.05351	-0.10848	-0.07332	0.09284	0.10369
127	N1	PX	0.02230	-0.00620	-0.02380	-0.05139	-0.04127
128	N1	PY	-0.02575	0.05482	0.04624	0.06420	0.00851
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00840	-0.00295	-0.00709	-0.01352	-0.01005
131	N1	DYY	-0.00540	0.00274	0.00606	0.00884	0.00517
132	N1	DZZ	-0.00249	0.00054	0.00186	0.00131	0.00175
133	N1	DXY	-0.00376	0.01334	0.00720	0.01260	-0.00146
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.03166	-0.10256	0.05580	0.02188	-0.12510
137	H6	S	-0.00820	-0.04558	0.01919	0.01775	-0.06567
138	H6	PX	-0.00277	-0.00812	0.00401	0.00126	-0.00776
139	H6	PY	0.00120	-0.00147	-0.00220	-0.00012	-0.00168
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.02072	0.04113	-0.00115	0.09331	-0.00193
142	C8	S	0.04332	-0.08510	0.00053	-0.19212	0.00295
143	C8	PX	0.02338	0.03998	0.16493	-0.00140	0.01329
144	C8	PY	0.15596	-0.04921	-0.00631	-0.03376	-0.08864
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.03849	-0.06912	0.01776	-0.16223	0.00794
147	C8	PX	0.02304	-0.00655	0.04675	-0.01709	0.00158
148	C8	PY	0.04305	-0.01924	0.01621	-0.01318	-0.02109
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.01268	-0.01001	0.00126	-0.00281	0.00351
151	C8	DYY	-0.00375	0.00664	-0.00150	-0.00012	-0.00750
152	C8	DZZ	-0.00307	0.00344	0.00102	0.00683	0.00063
153	C8	DXY	0.00045	0.00398	0.01079	-0.00139	-0.00295
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.04832	-0.05290	0.10594	0.09624	0.16300
157	H8	S	0.01033	-0.02615	0.04537	0.04826	0.09888
158	H8	PX	-0.00383	0.00398	-0.00761	-0.00590	-0.00987
159	H8	PY	0.00118	-0.00125	0.00149	0.00447	0.00259
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.09445	-0.05475	0.00771	-0.05990	0.01537
162	C10	S	-0.18396	0.10722	-0.01637	0.11823	-0.03042

163	C10	PX	0.00340	0.01052	0.06352	-0.00340	0.03452
164	C10	PY	0.00500	-0.07564	0.00299	-0.17732	0.08893
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.15079	0.10223	-0.00658	0.12502	-0.04243
167	C10	PX	-0.00814	0.00847	0.01621	0.00271	0.01467
168	C10	PY	0.01177	-0.02760	0.00735	-0.05955	0.03432
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00286	0.00636	-0.00019	0.01307	-0.00573
171	C10	DYY	-0.00393	-0.00262	-0.00012	-0.00695	0.00472
172	C10	DZZ	0.00814	-0.00475	0.00059	-0.00538	0.00131
173	C10	DXY	0.00015	-0.00031	0.00145	-0.00229	-0.00004
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.07487	0.07389	0.01869	0.11048	-0.02693
177	H16	S	-0.02463	0.03526	0.01412	0.06284	-0.01429
178	H16	PX	0.00557	-0.00493	-0.00053	-0.00676	0.00223
179	H16	PY	-0.00403	0.00266	0.00123	0.00288	0.00044
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.07680	0.06022	-0.03548	0.10033	-0.05492
182	H18	S	-0.03074	0.02962	-0.01838	0.05674	-0.03035
183	H18	PX	-0.00638	0.00472	-0.00203	0.00711	-0.00325
184	H18	PY	-0.00317	0.00098	-0.00161	0.00122	-0.00025
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

M0:	21	22	23	24	25
Eigenvalues:	-0.67123	-0.65389	-0.61355	-0.58253	-0.56450
(ev):	-18.26519	-17.79316	-16.69552	-15.85157	-15.36080

		A	A	A	A	A	
1	H1	S	0.09914	-0.06272	0.19193	0.05053	0.02053
2	H1	S	0.05294	-0.04437	0.13799	0.04307	0.02247
3	H1	PX	-0.00609	0.00284	-0.00983	-0.00190	-0.00053
4	H1	PY	0.00017	0.00277	-0.00023	-0.00240	-0.00197
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.04593	-0.00460	-0.00298	0.01268	-0.00418
7	C1	S	0.09435	0.00913	0.00366	-0.02752	0.00648
8	C1	PX	0.08584	-0.12195	0.29704	0.10707	0.02828
9	C1	PY	0.02406	0.16915	0.04593	-0.13632	-0.14112
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.06670	0.00498	0.00700	-0.01337	0.03634
12	C1	PX	0.06892	-0.04625	0.14247	0.03288	0.00042
13	C1	PY	0.00665	0.04849	0.01160	-0.04246	-0.05948
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00875	-0.00211	0.01300	0.00292	0.00317
16	C1	DYY	-0.00862	-0.00135	-0.01177	0.00011	-0.00041
17	C1	DZZ	-0.00273	0.00015	-0.00102	0.00000	-0.00091
18	C1	DXY	0.00058	-0.01262	0.00034	0.00393	0.01200
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.03518	-0.01448	0.00771	-0.02183	-0.00793
22	C2	S	-0.07343	0.02996	-0.01461	0.04702	0.01310
23	C2	PX	0.04273	0.07812	0.29080	0.07795	-0.04459
24	C2	PY	0.08906	0.17501	0.00365	-0.01006	-0.12356
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

26	C2	S	-0.04112	-0.00050	-0.01376	0.02979	0.04300
27	C2	PX	0.04679	0.00926	0.14261	0.01060	-0.00939
28	C2	PY	0.02599	0.04099	-0.00350	-0.01148	-0.04503
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00721	-0.00126	-0.01172	0.00163	0.00530
31	C2	DYY	0.00550	-0.00222	0.01042	-0.00217	-0.00375
32	C2	DZZ	0.00196	-0.00033	0.00107	-0.00047	-0.00127
33	C2	DXY	0.00335	0.01291	-0.00232	0.00530	-0.01005
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03549	0.02848	0.03357	-0.01322	0.01301
37	C3	S	-0.07232	-0.05906	-0.06912	0.02869	-0.02733
38	C3	PX	-0.09585	-0.03096	-0.05484	0.16789	-0.07960
39	C3	PY	0.07678	-0.07000	-0.09928	-0.06001	0.22369
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.07230	-0.08014	-0.06293	-0.00912	-0.02721
42	C3	PX	-0.03340	-0.01543	-0.03904	0.09099	-0.04637
43	C3	PY	0.04376	-0.03315	-0.03295	-0.00706	0.06729
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00591	-0.00516	0.00990	-0.01080	0.00886
46	C3	DYY	-0.00265	0.00453	-0.01144	0.00632	-0.00602
47	C3	DZZ	0.00100	0.00099	0.00134	-0.00017	-0.00024
48	C3	DXY	0.01209	-0.00395	-0.00441	0.00121	0.00712
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.04335	-0.00936	0.02374	-0.00910	0.01176
52	C4	S	-0.09009	0.01980	-0.05002	0.02044	-0.02583
53	C4	PX	0.01619	0.05530	0.01180	-0.15378	-0.02969
54	C4	PY	-0.09009	-0.22369	0.10907	0.11449	0.13738
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.06172	0.00155	-0.02427	0.01708	-0.02264
57	C4	PX	-0.00996	0.01677	0.00338	-0.05083	-0.00876
58	C4	PY	-0.07238	-0.07695	0.01919	0.05802	0.05812
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00283	-0.00225	0.00791	0.00816	-0.00182
61	C4	DYY	-0.00428	-0.00080	-0.00620	-0.00467	0.00336
62	C4	DZZ	0.00256	0.00014	0.00081	-0.00050	-0.00022
63	C4	DXY	-0.00834	-0.00520	0.00508	0.01218	0.00431
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.03934	0.00015	-0.02265	-0.00101	0.01635
67	C5	S	0.08164	-0.00133	0.04728	0.00323	-0.03466
68	C5	PX	-0.10343	-0.02773	-0.01842	0.17112	0.02088
69	C5	PY	0.05472	-0.24525	-0.09786	-0.16425	0.12537
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.05317	0.00766	0.02798	0.01805	-0.03963
72	C5	PX	-0.05362	-0.00346	-0.01269	0.08014	0.00637
73	C5	PY	0.05942	-0.10888	-0.01504	-0.09244	0.05357
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00591	-0.00138	-0.01018	0.00576	-0.00041
76	C5	DYY	0.00530	-0.00166	0.00815	-0.00652	0.00159
77	C5	DZZ	-0.00223	0.00049	-0.00093	0.00054	0.00021
78	C5	DXY	-0.00624	0.00720	0.00383	0.01226	-0.00304
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.03316	0.03487	-0.03637	0.03747	0.00118
82	C6	S	0.07362	-0.07564	0.07738	-0.08314	-0.00565
83	C6	PX	0.03259	0.04865	0.01585	-0.11372	0.08778
84	C6	PY	-0.14090	-0.06554	0.11083	0.04023	0.17581
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.03556	-0.09038	0.06001	-0.06146	-0.00679
87	C6	PX	0.02366	0.02782	-0.00086	-0.03298	0.03365
88	C6	PY	-0.05442	-0.01280	0.02745	0.01235	0.06165
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00306	-0.00569	-0.00535	-0.00638	0.00251
91	C6	DYY	0.00186	0.00678	0.00699	0.00759	0.00046
92	C6	DZZ	-0.00321	0.00095	-0.00106	0.00152	0.00104
93	C6	DXY	0.00945	0.00067	-0.00679	-0.00480	-0.01032
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01874	-0.02671	-0.01122	0.01068	0.00461
97	C7	S	-0.03881	0.05337	0.02313	-0.02043	-0.01100
98	C7	PX	-0.11690	-0.00234	0.03775	-0.12838	0.05266
99	C7	PY	-0.17279	-0.00649	0.00412	0.12769	-0.22707
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.01352	0.06399	0.01404	-0.00795	0.01358
102	C7	PX	-0.06256	-0.00190	0.03152	-0.08128	0.02098
103	C7	PY	-0.05313	-0.00477	0.00813	0.05116	-0.08427
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00722	0.00570	0.00295	-0.01004	0.01675
106	C7	DYY	-0.00406	-0.00526	-0.00221	0.00930	-0.01384
107	C7	DZZ	0.00015	-0.00194	-0.00080	0.00094	-0.00067
108	C7	DXY	0.01158	-0.00397	-0.00504	0.00682	0.00392
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.08933	-0.09744	0.03752	0.03677	0.06181
112	H3	S	-0.04488	-0.07110	0.03676	0.02372	0.05361
113	H3	PX	0.00299	0.00420	-0.00097	-0.00290	-0.00253
114	H3	PY	0.00454	0.00321	-0.00130	-0.00014	-0.00165
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.09844	-0.11972	-0.02145	-0.14894	0.04695
117	H4	S	0.05095	-0.07927	-0.02484	-0.11161	0.04145
118	H4	PX	0.00235	-0.00507	-0.00092	-0.00279	0.00223
119	H4	PY	-0.00579	0.00403	0.00024	0.00664	-0.00086
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.02667	-0.01707	0.01178	-0.02490	-0.00247
122	N1	S	-0.06010	0.03454	-0.02655	0.05571	0.00333
123	N1	PX	0.05150	0.05837	0.02204	-0.03491	0.10959
124	N1	PY	0.20152	-0.03140	-0.04329	-0.05757	-0.22395
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.10040	0.06772	-0.03141	0.08120	0.03874
127	N1	PX	0.02851	0.03286	0.01658	-0.02270	0.06800
128	N1	PY	0.09581	-0.00855	-0.02060	-0.03055	-0.10591
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00158	0.00654	0.00157	-0.00095	0.01530
131	N1	DYY	0.00137	-0.00766	-0.00049	-0.00245	-0.01468
132	N1	DZZ	-0.00200	-0.00234	-0.00009	0.00082	-0.00180
133	N1	DXY	0.01778	0.00076	-0.00306	-0.00794	-0.01428

134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.06387	-0.03403	-0.18801	-0.02272	0.04082
137	H6	S	-0.03234	-0.02935	-0.12633	-0.02433	0.03411
138	H6	PX	-0.00396	-0.00143	-0.00993	-0.00105	0.00197
139	H6	PY	0.00102	0.00262	-0.00046	-0.00053	-0.00101
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01391	0.04034	0.00296	-0.00614	-0.00422
142	C8	S	0.02944	-0.08157	-0.00652	0.01337	0.01229
143	C8	PX	0.21140	-0.01477	-0.04969	0.00946	-0.04597
144	C8	PY	0.02567	0.19287	0.01378	0.05309	0.28481
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.01456	-0.07689	0.00535	0.00509	0.03872
147	C8	PX	0.05749	-0.00846	-0.00048	-0.02436	-0.02043
148	C8	PY	0.00175	0.04255	0.00687	0.00488	0.06865
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00483	0.00989	0.00158	0.00182	0.02229
151	C8	DYY	0.00607	-0.00357	-0.00105	-0.00052	-0.01584
152	C8	DZZ	0.00011	0.00101	-0.00022	-0.00056	-0.00228
153	C8	DXY	0.00247	-0.00321	0.00355	-0.00849	-0.01187
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.04588	0.03129	0.03607	-0.12134	0.08608
157	H8	S	-0.02067	0.02127	0.02468	-0.08496	0.07630
158	H8	PX	0.00212	-0.00165	-0.00147	0.00601	-0.00420
159	H8	PY	-0.00382	0.00027	0.00116	-0.00095	-0.00182
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00015	-0.01351	-0.00073	0.00283	0.01965
162	C10	S	-0.00207	0.02536	0.00198	-0.00665	-0.04177
163	C10	PX	0.20343	-0.02694	-0.14042	0.25234	0.04706
164	C10	PY	-0.01749	-0.25779	-0.00872	-0.05388	-0.26461
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00153	0.04061	0.00419	-0.01365	-0.05492
167	C10	PX	0.08799	-0.00955	-0.07029	0.12988	0.02887
168	C10	PY	-0.00171	-0.09457	-0.00562	-0.02029	-0.11082
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00012	0.01586	0.00161	0.00043	0.01382
171	C10	DYY	-0.00022	-0.01120	-0.00147	0.00014	-0.00907
172	C10	DZZ	-0.00019	-0.00207	-0.00004	-0.00015	-0.00005
173	C10	DXY	-0.00487	-0.00247	0.00615	-0.01499	-0.00742
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.10169	0.09149	-0.06809	0.15274	0.10975
177	H16	S	0.06775	0.06634	-0.04817	0.11593	0.09676
178	H16	PX	-0.00382	-0.00535	0.00224	-0.00553	-0.00479
179	H16	PY	0.00417	-0.00012	-0.00285	0.00484	-0.00007
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.09941	0.09849	0.08001	-0.13111	0.03112
182	H18	S	-0.05999	0.06781	0.05133	-0.08794	0.03307
183	H18	PX	-0.00418	0.00589	0.00343	-0.00526	0.00204
184	H18	PY	-0.00406	-0.00071	0.00221	-0.00416	-0.00284
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:

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Eigenvalues: -0.56064 -0.55853 -0.51793 -0.49062 -0.45735
 (ev): -15.25576 -15.19827 -14.09354 -13.35042 -12.44505

		A	A	A	A	A	
1	H1	S	0.05829	0.00000	-0.00809	-0.12105	0.00000
2	H1	S	0.04003	0.00000	-0.01195	-0.10928	0.00000
3	H1	PX	-0.00266	0.00000	-0.00042	0.00439	0.00000
4	H1	PY	-0.00059	0.00000	0.00321	-0.00066	0.00000
5	H1	PZ	0.00000	0.00219	0.00000	0.00000	0.00451
6	C1	S	-0.02196	0.00000	-0.00557	-0.00958	0.00000
7	C1	S	0.04314	0.00000	0.01073	0.02144	0.00000
8	C1	PX	0.04630	0.00000	-0.02997	-0.16550	0.00000
9	C1	PY	-0.01424	0.00000	0.22327	-0.09963	0.00000
10	C1	PZ	0.00000	0.10483	0.00000	0.00000	0.21403
11	C1	S	0.06425	0.00000	-0.00771	0.03228	0.00000
12	C1	PX	0.03164	0.00000	-0.00245	-0.10987	0.00000
13	C1	PY	-0.00641	0.00000	0.09655	-0.03278	0.00000
14	C1	PZ	0.00000	0.05797	0.00000	0.00000	0.15122
15	C1	DXX	0.00901	0.00000	-0.00125	-0.01726	0.00000
16	C1	DYY	-0.00867	0.00000	-0.00287	0.01628	0.00000
17	C1	DZZ	-0.00140	0.00000	-0.00010	-0.00020	0.00000
18	C1	DXY	-0.00499	0.00000	-0.01313	0.00560	0.00000
19	C1	DXZ	0.00000	-0.00683	0.00000	0.00000	-0.01216
20	C1	DYZ	0.00000	-0.00171	0.00000	0.00000	0.01004
21	C2	S	0.00449	0.00000	0.00927	-0.00469	0.00000
22	C2	S	-0.00961	0.00000	-0.01582	0.01303	0.00000
23	C2	PX	-0.07440	0.00000	0.07198	0.18641	0.00000
24	C2	PY	-0.19696	0.00000	-0.19589	-0.00046	0.00000
25	C2	PZ	0.00000	0.11756	0.00000	0.00000	0.16070
26	C2	S	0.02005	0.00000	-0.02342	-0.00414	0.00000
27	C2	PX	-0.02488	0.00000	0.05233	0.10952	0.00000
28	C2	PY	-0.06950	0.00000	-0.08117	-0.01101	0.00000
29	C2	PZ	0.00000	0.06362	0.00000	0.00000	0.11706
30	C2	DXX	0.00596	0.00000	-0.00547	-0.01669	0.00000
31	C2	DYY	-0.00212	0.00000	0.00769	0.01495	0.00000
32	C2	DZZ	-0.00024	0.00000	0.00064	0.00027	0.00000
33	C2	DXY	-0.00606	0.00000	-0.01507	-0.00345	0.00000
34	C2	DXZ	0.00000	0.00787	0.00000	0.00000	0.00945
35	C2	DYZ	0.00000	-0.00179	0.00000	0.00000	0.01136
36	C3	S	0.02831	0.00000	0.00339	-0.00907	0.00000
37	C3	S	-0.05998	0.00000	-0.00778	0.01785	0.00000
38	C3	PX	0.08458	0.00000	-0.00741	0.17297	0.00000
39	C3	PY	-0.03965	0.00000	-0.19147	0.10262	0.00000
40	C3	PZ	0.00000	0.19514	0.00000	0.00000	0.05714
41	C3	S	-0.08891	0.00000	-0.00617	0.00576	0.00000
42	C3	PX	0.02928	0.00000	-0.00657	0.10094	0.00000
43	C3	PY	-0.01709	0.00000	-0.05574	0.05322	0.00000
44	C3	PZ	0.00000	0.11756	0.00000	0.00000	0.04332
45	C3	DXX	-0.01067	0.00000	-0.00350	-0.01682	0.00000
46	C3	DYY	0.00981	0.00000	0.00230	0.01664	0.00000
47	C3	DZZ	0.00080	0.00000	0.00055	0.00013	0.00000
48	C3	DXY	0.00436	0.00000	-0.01617	0.00526	0.00000
49	C3	DXZ	0.00000	-0.00500	0.00000	0.00000	0.00283
50	C3	DYZ	0.00000	-0.00707	0.00000	0.00000	0.01042

51	C4	S	0.00265	0.00000	0.00428	0.00931	0.00000
52	C4	S	-0.00193	0.00000	-0.00543	-0.02036	0.00000
53	C4	PX	-0.21685	0.00000	0.09085	0.19138	0.00000
54	C4	PY	-0.14112	0.00000	-0.18845	0.08258	0.00000
55	C4	PZ	0.00000	0.08454	0.00000	0.00000	0.25580
56	C4	S	-0.00716	0.00000	-0.02943	-0.04693	0.00000
57	C4	PX	-0.09783	0.00000	0.02840	0.09174	0.00000
58	C4	PY	-0.07822	0.00000	-0.08724	0.06689	0.00000
59	C4	PZ	0.00000	0.05075	0.00000	0.00000	0.18018
60	C4	DXX	0.01328	0.00000	-0.00029	-0.01578	0.00000
61	C4	DYY	-0.01359	0.00000	-0.00427	0.01573	0.00000
62	C4	DZZ	0.00094	0.00000	0.00113	0.00015	0.00000
63	C4	DXY	-0.00936	0.00000	-0.01723	0.00539	0.00000
64	C4	DXZ	0.00000	-0.00033	0.00000	0.00000	-0.00165
65	C4	DYZ	0.00000	-0.00617	0.00000	0.00000	-0.01362
66	C5	S	-0.00983	0.00000	-0.00128	0.00510	0.00000
67	C5	S	0.02117	0.00000	-0.00246	-0.01297	0.00000
68	C5	PX	0.21564	0.00000	-0.06148	-0.20592	0.00000
69	C5	PY	0.12382	0.00000	0.20056	-0.00885	0.00000
70	C5	PZ	0.00000	0.09004	0.00000	0.00000	0.22646
71	C5	S	0.02713	0.00000	0.01739	-0.01508	0.00000
72	C5	PX	0.08291	0.00000	-0.04089	-0.09978	0.00000
73	C5	PY	0.05391	0.00000	0.09943	0.00478	0.00000
74	C5	PZ	0.00000	0.05546	0.00000	0.00000	0.15770
75	C5	DXX	0.01139	0.00000	-0.00595	-0.01482	0.00000
76	C5	DYY	-0.00749	0.00000	0.01003	0.01376	0.00000
77	C5	DZZ	-0.00068	0.00000	-0.00135	-0.00020	0.00000
78	C5	DXY	-0.00966	0.00000	-0.01940	-0.00172	0.00000
79	C5	DXZ	0.00000	0.00036	0.00000	0.00000	0.00504
80	C5	DYZ	0.00000	-0.00682	0.00000	0.00000	-0.01075
81	C6	S	0.00356	0.00000	-0.00454	0.01715	0.00000
82	C6	S	-0.00613	0.00000	0.00540	-0.03986	0.00000
83	C6	PX	-0.15160	0.00000	-0.04462	-0.19586	0.00000
84	C6	PY	0.03784	0.00000	0.23242	0.07613	0.00000
85	C6	PZ	0.00000	0.24032	0.00000	0.00000	-0.02349
86	C6	S	-0.01836	0.00000	0.04079	-0.02772	0.00000
87	C6	PX	-0.06038	0.00000	-0.04129	-0.08901	0.00000
88	C6	PY	0.00422	0.00000	0.06529	0.00960	0.00000
89	C6	PZ	0.00000	0.13965	0.00000	0.00000	-0.01787
90	C6	DXX	-0.00395	0.00000	0.00491	-0.00749	0.00000
91	C6	DYY	0.00215	0.00000	-0.00378	0.00682	0.00000
92	C6	DZZ	-0.00030	0.00000	0.00185	0.00043	0.00000
93	C6	DXY	-0.00987	0.00000	-0.01398	0.00447	0.00000
94	C6	DXZ	0.00000	0.00115	0.00000	0.00000	0.00240
95	C6	DYZ	0.00000	-0.01304	0.00000	0.00000	0.01697
96	C7	S	-0.01716	0.00000	-0.01521	-0.01672	0.00000
97	C7	S	0.03965	0.00000	0.03138	0.03879	0.00000
98	C7	PX	-0.20006	0.00000	-0.00184	-0.19425	0.00000
99	C7	PY	-0.02472	0.00000	0.16704	-0.05704	0.00000
100	C7	PZ	0.00000	0.15928	0.00000	0.00000	-0.04209
101	C7	S	0.03062	0.00000	0.05772	0.06857	0.00000
102	C7	PX	-0.08877	0.00000	-0.00303	-0.11325	0.00000
103	C7	PY	0.00549	0.00000	0.06253	-0.02389	0.00000
104	C7	PZ	0.00000	0.09337	0.00000	0.00000	-0.03138

105	C7	DXX	-0.00031	0.00000	-0.00613	-0.00443	0.00000
106	C7	DYY	0.00047	0.00000	0.00464	0.00362	0.00000
107	C7	DZZ	-0.00050	0.00000	-0.00006	0.00027	0.00000
108	C7	DXY	0.01221	0.00000	-0.00732	0.01848	0.00000
109	C7	DXZ	0.00000	-0.01091	0.00000	0.00000	0.00565
110	C7	DYZ	0.00000	0.00748	0.00000	0.00000	0.00604
111	H3	S	-0.15372	0.00000	-0.10339	0.10834	0.00000
112	H3	S	-0.12257	0.00000	-0.09106	0.09730	0.00000
113	H3	PX	0.00148	0.00000	0.00389	-0.00034	0.00000
114	H3	PY	0.00718	0.00000	0.00229	-0.00443	0.00000
115	H3	PZ	0.00000	0.00164	0.00000	0.00000	0.00546
116	H4	S	0.01319	0.00000	0.15271	0.06630	0.00000
117	H4	S	0.00868	0.00000	0.13340	0.06095	0.00000
118	H4	PX	0.00308	0.00000	0.00390	-0.00051	0.00000
119	H4	PY	0.00163	0.00000	-0.00452	-0.00342	0.00000
120	H4	PZ	0.00000	0.00169	0.00000	0.00000	0.00477
121	N1	S	0.02446	0.00000	-0.02256	-0.02007	0.00000
122	N1	S	-0.05466	0.00000	0.05164	0.04389	0.00000
123	N1	PX	0.00851	0.00000	-0.11151	-0.14990	0.00000
124	N1	PY	0.04498	0.00000	-0.20840	0.02951	0.00000
125	N1	PZ	0.00000	0.25471	0.00000	0.00000	-0.15802
126	N1	S	-0.08113	0.00000	0.07619	0.07823	0.00000
127	N1	PX	0.01248	0.00000	-0.07738	-0.09635	0.00000
128	N1	PY	0.01555	0.00000	-0.11727	0.00234	0.00000
129	N1	PZ	0.00000	0.16143	0.00000	0.00000	-0.11548
130	N1	DXX	0.00263	0.00000	-0.00460	-0.00948	0.00000
131	N1	DYY	0.00097	0.00000	-0.00195	0.00154	0.00000
132	N1	DZZ	-0.00093	0.00000	0.00383	0.00307	0.00000
133	N1	DXY	-0.00065	0.00000	-0.01762	-0.00477	0.00000
134	N1	DXZ	0.00000	0.02153	0.00000	0.00000	-0.01360
135	N1	DYZ	0.00000	0.01218	0.00000	0.00000	-0.00076
136	H6	S	0.04970	0.00000	-0.05718	-0.13294	0.00000
137	H6	S	0.03908	0.00000	-0.03741	-0.10872	0.00000
138	H6	PX	0.00183	0.00000	-0.00259	-0.00497	0.00000
139	H6	PY	-0.00293	0.00000	-0.00292	-0.00061	0.00000
140	H6	PZ	0.00000	0.00248	0.00000	0.00000	0.00315
141	C8	S	-0.01855	0.00000	0.00869	-0.01342	0.00000
142	C8	S	0.03872	0.00000	-0.01937	0.02600	0.00000
143	C8	PX	0.11073	0.00000	-0.10584	0.16921	0.00000
144	C8	PY	0.13116	0.00000	0.00133	0.09508	0.00000
145	C8	PZ	0.00000	0.19254	0.00000	0.00000	-0.19895
146	C8	S	0.06815	0.00000	-0.02123	0.05862	0.00000
147	C8	PX	0.07272	0.00000	-0.07879	0.06991	0.00000
148	C8	PY	0.02958	0.00000	0.00064	0.00758	0.00000
149	C8	PZ	0.00000	0.11214	0.00000	0.00000	-0.13502
150	C8	DXX	0.00395	0.00000	0.00541	0.00837	0.00000
151	C8	DYY	-0.00086	0.00000	-0.00638	-0.00879	0.00000
152	C8	DZZ	-0.00056	0.00000	-0.00032	0.00045	0.00000
153	C8	DXY	0.01712	0.00000	-0.00701	0.01551	0.00000
154	C8	DXZ	0.00000	-0.00381	0.00000	0.00000	0.00415
155	C8	DYZ	0.00000	0.00558	0.00000	0.00000	0.00365
156	H8	S	-0.10085	0.00000	-0.02222	-0.10413	0.00000
157	H8	S	-0.08221	0.00000	-0.02230	-0.09943	0.00000
158	H8	PX	0.00390	0.00000	0.00162	0.00297	0.00000

159	H8	PY	-0.00260	0.00000	0.00176	-0.00295	0.00000
160	H8	PZ	0.00000	0.00330	0.00000	0.00000	-0.00081
161	C10	S	0.00350	0.00000	0.00396	0.00948	0.00000
162	C10	S	-0.00739	0.00000	-0.00821	-0.02022	0.00000
163	C10	PX	-0.19241	0.00000	0.14582	-0.07739	0.00000
164	C10	PY	-0.08475	0.00000	-0.02419	-0.07573	0.00000
165	C10	PZ	0.00000	0.09743	0.00000	0.00000	-0.14133
166	C10	S	-0.01034	0.00000	-0.01650	-0.04513	0.00000
167	C10	PX	-0.10955	0.00000	0.08730	-0.04752	0.00000
168	C10	PY	-0.04444	0.00000	-0.00620	-0.04258	0.00000
169	C10	PZ	0.00000	0.05719	0.00000	0.00000	-0.10163
170	C10	DXX	0.00637	0.00000	-0.00051	0.00480	0.00000
171	C10	DYY	-0.00564	0.00000	0.00131	-0.00347	0.00000
172	C10	DZZ	0.00015	0.00000	-0.00015	0.00025	0.00000
173	C10	DXY	0.01341	0.00000	-0.01258	0.00962	0.00000
174	C10	DXZ	0.00000	0.00078	0.00000	0.00000	-0.00083
175	C10	DYZ	0.00000	0.01065	0.00000	0.00000	-0.01250
176	H16	S	-0.08138	0.00000	0.09337	-0.03159	0.00000
177	H16	S	-0.06429	0.00000	0.08066	-0.02869	0.00000
178	H16	PX	0.00177	0.00000	-0.00315	0.00017	0.00000
179	H16	PY	-0.00429	0.00000	0.00273	-0.00196	0.00000
180	H16	PZ	0.00000	0.00208	0.00000	0.00000	-0.00307
181	H18	S	0.13603	0.00000	-0.08726	0.06799	0.00000
182	H18	S	0.09760	0.00000	-0.06089	0.06597	0.00000
183	H18	PX	0.00565	0.00000	-0.00360	0.00238	0.00000
184	H18	PY	0.00193	0.00000	-0.00174	0.00044	0.00000
185	H18	PZ	0.00000	0.00210	0.00000	0.00000	-0.00306

MO:	31	32	33	34	35
Eigenvalues:	-0.41260	-0.39954	-0.33330	-0.29083	0.03440
(ev):	-11.22740	-10.87203	-9.06956	-7.91387	0.93598

		A	A	A	A	A	
1	H1	S	0.06571	0.00000	0.00000	0.00000	0.00000
2	H1	S	0.07175	0.00000	0.00000	0.00000	0.00000
3	H1	PX	-0.00207	0.00000	0.00000	0.00000	0.00000
4	H1	PY	0.00015	0.00000	0.00000	0.00000	0.00000
5	H1	PZ	0.00000	0.00454	-0.00020	-0.00557	0.00466
6	C1	S	0.00887	0.00000	0.00000	0.00000	0.00000
7	C1	S	-0.02022	0.00000	0.00000	0.00000	0.00000
8	C1	PX	0.08865	0.00000	0.00000	0.00000	0.00000
9	C1	PY	0.02576	0.00000	0.00000	0.00000	0.00000
10	C1	PZ	0.00000	0.19553	-0.01614	-0.22352	0.15014
11	C1	S	-0.04265	0.00000	0.00000	0.00000	0.00000
12	C1	PX	0.05610	0.00000	0.00000	0.00000	0.00000
13	C1	PY	0.03714	0.00000	0.00000	0.00000	0.00000
14	C1	PZ	0.00000	0.14677	-0.02277	-0.20082	0.21567
15	C1	DXX	0.01015	0.00000	0.00000	0.00000	0.00000
16	C1	DYY	-0.01047	0.00000	0.00000	0.00000	0.00000
17	C1	DZZ	-0.00024	0.00000	0.00000	0.00000	0.00000
18	C1	DXY	0.00287	0.00000	0.00000	0.00000	0.00000
19	C1	DXZ	0.00000	-0.00770	0.00135	0.00775	-0.00104
20	C1	DYZ	0.00000	-0.00226	-0.01321	-0.01687	-0.01223
21	C2	S	0.01846	0.00000	0.00000	0.00000	0.00000

22	C2	S	-0.03742	0.00000	0.00000	0.00000	0.00000
23	C2	PX	-0.08753	0.00000	0.00000	0.00000	0.00000
24	C2	PY	0.10429	0.00000	0.00000	0.00000	0.00000
25	C2	PZ	0.00000	-0.23336	-0.06465	0.22514	0.13652
26	C2	S	-0.10344	0.00000	0.00000	0.00000	0.00000
27	C2	PX	-0.05512	0.00000	0.00000	0.00000	0.00000
28	C2	PY	0.04402	0.00000	0.00000	0.00000	0.00000
29	C2	PZ	0.00000	-0.17535	-0.06012	0.20282	0.20857
30	C2	DXX	0.00905	0.00000	0.00000	0.00000	0.00000
31	C2	DYY	-0.00948	0.00000	0.00000	0.00000	0.00000
32	C2	DZZ	0.00064	0.00000	0.00000	0.00000	0.00000
33	C2	DXY	0.00411	0.00000	0.00000	0.00000	0.00000
34	C2	DXZ	0.00000	-0.01004	-0.00210	0.00776	0.00263
35	C2	DYZ	0.00000	-0.00319	-0.01416	0.01156	-0.01480
36	C3	S	-0.02061	0.00000	0.00000	0.00000	0.00000
37	C3	S	0.04186	0.00000	0.00000	0.00000	0.00000
38	C3	PX	-0.22022	0.00000	0.00000	0.00000	0.00000
39	C3	PY	0.00175	0.00000	0.00000	0.00000	0.00000
40	C3	PZ	0.00000	0.21952	0.20608	0.13945	0.12177
41	C3	S	0.11754	0.00000	0.00000	0.00000	0.00000
42	C3	PX	-0.11418	0.00000	0.00000	0.00000	0.00000
43	C3	PY	0.04406	0.00000	0.00000	0.00000	0.00000
44	C3	PZ	0.00000	0.16011	0.18065	0.13713	0.15114
45	C3	DXX	0.00905	0.00000	0.00000	0.00000	0.00000
46	C3	DYY	-0.00628	0.00000	0.00000	0.00000	0.00000
47	C3	DZZ	-0.00013	0.00000	0.00000	0.00000	0.00000
48	C3	DXY	0.00046	0.00000	0.00000	0.00000	0.00000
49	C3	DXZ	0.00000	0.01200	-0.00546	0.00201	-0.00757
50	C3	DYZ	0.00000	-0.00619	-0.00757	-0.02184	0.02205
51	C4	S	0.00255	0.00000	0.00000	0.00000	0.00000
52	C4	S	-0.00474	0.00000	0.00000	0.00000	0.00000
53	C4	PX	-0.05758	0.00000	0.00000	0.00000	0.00000
54	C4	PY	0.02256	0.00000	0.00000	0.00000	0.00000
55	C4	PZ	0.00000	0.09067	-0.13757	-0.21480	-0.14883
56	C4	S	-0.01744	0.00000	0.00000	0.00000	0.00000
57	C4	PX	-0.03743	0.00000	0.00000	0.00000	0.00000
58	C4	PY	0.01236	0.00000	0.00000	0.00000	0.00000
59	C4	PZ	0.00000	0.07254	-0.11277	-0.20805	-0.19642
60	C4	DXX	0.00474	0.00000	0.00000	0.00000	0.00000
61	C4	DYY	-0.00432	0.00000	0.00000	0.00000	0.00000
62	C4	DZZ	-0.00003	0.00000	0.00000	0.00000	0.00000
63	C4	DXY	0.00128	0.00000	0.00000	0.00000	0.00000
64	C4	DXZ	0.00000	0.01122	0.00504	-0.01376	0.01263
65	C4	DYZ	0.00000	-0.00883	0.00244	0.01220	-0.00861
66	C5	S	-0.00528	0.00000	0.00000	0.00000	0.00000
67	C5	S	0.00762	0.00000	0.00000	0.00000	0.00000
68	C5	PX	0.04338	0.00000	0.00000	0.00000	0.00000
69	C5	PY	-0.03246	0.00000	0.00000	0.00000	0.00000
70	C5	PZ	0.00000	-0.16043	-0.16691	0.15793	-0.16803
71	C5	S	0.03668	0.00000	0.00000	0.00000	0.00000
72	C5	PX	0.02753	0.00000	0.00000	0.00000	0.00000
73	C5	PY	-0.04794	0.00000	0.00000	0.00000	0.00000
74	C5	PZ	0.00000	-0.12586	-0.13788	0.15760	-0.22436
75	C5	DXX	0.00518	0.00000	0.00000	0.00000	0.00000

76	C5	DYY	-0.00552	0.00000	0.00000	0.00000	0.00000
77	C5	DZZ	-0.00098	0.00000	0.00000	0.00000	0.00000
78	C5	DXY	0.00506	0.00000	0.00000	0.00000	0.00000
79	C5	DXZ	0.00000	0.00932	-0.00284	-0.01505	-0.01048
80	C5	DYZ	0.00000	0.01250	0.00449	-0.01316	-0.00895
81	C6	S	0.02069	0.00000	0.00000	0.00000	0.00000
82	C6	S	-0.05790	0.00000	0.00000	0.00000	0.00000
83	C6	PX	0.18981	0.00000	0.00000	0.00000	0.00000
84	C6	PY	0.04432	0.00000	0.00000	0.00000	0.00000
85	C6	PZ	0.00000	-0.18085	0.19332	-0.05641	0.15857
86	C6	S	0.03068	0.00000	0.00000	0.00000	0.00000
87	C6	PX	0.05040	0.00000	0.00000	0.00000	0.00000
88	C6	PY	-0.03691	0.00000	0.00000	0.00000	0.00000
89	C6	PZ	0.00000	-0.12806	0.15415	-0.06280	0.16019
90	C6	DXX	0.02499	0.00000	0.00000	0.00000	0.00000
91	C6	DYY	-0.02425	0.00000	0.00000	0.00000	0.00000
92	C6	DZZ	0.00184	0.00000	0.00000	0.00000	0.00000
93	C6	DXY	0.02102	0.00000	0.00000	0.00000	0.00000
94	C6	DXZ	0.00000	0.01726	0.00646	0.00858	0.00436
95	C6	DYZ	0.00000	0.00447	-0.00958	0.02476	0.02188
96	C7	S	-0.01306	0.00000	0.00000	0.00000	0.00000
97	C7	S	0.02640	0.00000	0.00000	0.00000	0.00000
98	C7	PX	-0.09657	0.00000	0.00000	0.00000	0.00000
99	C7	PY	-0.11827	0.00000	0.00000	0.00000	0.00000
100	C7	PZ	0.00000	0.22243	0.06792	0.24861	-0.23108
101	C7	S	0.09656	0.00000	0.00000	0.00000	0.00000
102	C7	PX	-0.05538	0.00000	0.00000	0.00000	0.00000
103	C7	PY	-0.08417	0.00000	0.00000	0.00000	0.00000
104	C7	PZ	0.00000	0.17787	0.05418	0.22947	-0.29281
105	C7	DXX	0.00302	0.00000	0.00000	0.00000	0.00000
106	C7	DYY	0.00025	0.00000	0.00000	0.00000	0.00000
107	C7	DZZ	0.00026	0.00000	0.00000	0.00000	0.00000
108	C7	DXY	0.00002	0.00000	0.00000	0.00000	0.00000
109	C7	DXZ	0.00000	-0.00739	0.00138	-0.00623	0.00492
110	C7	DYZ	0.00000	0.01117	0.01905	0.00900	0.00545
111	H3	S	-0.00821	0.00000	0.00000	0.00000	0.00000
112	H3	S	-0.00686	0.00000	0.00000	0.00000	0.00000
113	H3	PX	-0.00047	0.00000	0.00000	0.00000	0.00000
114	H3	PY	0.00042	0.00000	0.00000	0.00000	0.00000
115	H3	PZ	0.00000	0.00205	-0.00340	-0.00523	-0.00534
116	H4	S	-0.03803	0.00000	0.00000	0.00000	0.00000
117	H4	S	-0.03275	0.00000	0.00000	0.00000	0.00000
118	H4	PX	-0.00031	0.00000	0.00000	0.00000	0.00000
119	H4	PY	0.00089	0.00000	0.00000	0.00000	0.00000
120	H4	PZ	0.00000	-0.00358	-0.00402	0.00370	-0.00587
121	N1	S	-0.06370	0.00000	0.00000	0.00000	0.00000
122	N1	S	0.13749	0.00000	0.00000	0.00000	0.00000
123	N1	PX	-0.45341	0.00000	0.00000	0.00000	0.00000
124	N1	PY	-0.10426	0.00000	0.00000	0.00000	0.00000
125	N1	PZ	0.00000	-0.20217	0.08992	-0.27021	-0.17580
126	N1	S	0.24774	0.00000	0.00000	0.00000	0.00000
127	N1	PX	-0.35810	0.00000	0.00000	0.00000	0.00000
128	N1	PY	-0.08874	0.00000	0.00000	0.00000	0.00000
129	N1	PZ	0.00000	-0.16244	0.08295	-0.24417	-0.19485

130	N1	DXX	-0.02542	0.00000	0.00000	0.00000	0.00000
131	N1	DYY	-0.00297	0.00000	0.00000	0.00000	0.00000
132	N1	DZZ	0.01062	0.00000	0.00000	0.00000	0.00000
133	N1	DXY	-0.00376	0.00000	0.00000	0.00000	0.00000
134	N1	DXZ	0.00000	-0.01086	0.00311	-0.01518	-0.01141
135	N1	DYZ	0.00000	-0.01422	0.01795	-0.00886	0.00453
136	H6	S	0.05200	0.00000	0.00000	0.00000	0.00000
137	H6	S	0.07985	0.00000	0.00000	0.00000	0.00000
138	H6	PX	0.00181	0.00000	0.00000	0.00000	0.00000
139	H6	PY	0.00063	0.00000	0.00000	0.00000	0.00000
140	H6	PZ	0.00000	-0.00526	-0.00137	0.00538	0.00395
141	C8	S	0.02869	0.00000	0.00000	0.00000	0.00000
142	C8	S	-0.07019	0.00000	0.00000	0.00000	0.00000
143	C8	PX	0.17716	0.00000	0.00000	0.00000	0.00000
144	C8	PY	-0.05369	0.00000	0.00000	0.00000	0.00000
145	C8	PZ	0.00000	0.06863	-0.26226	0.00570	-0.08309
146	C8	S	-0.05674	0.00000	0.00000	0.00000	0.00000
147	C8	PX	0.02008	0.00000	0.00000	0.00000	0.00000
148	C8	PY	-0.03286	0.00000	0.00000	0.00000	0.00000
149	C8	PZ	0.00000	0.04250	-0.20817	-0.00429	-0.12808
150	C8	DXX	0.01314	0.00000	0.00000	0.00000	0.00000
151	C8	DYY	-0.01763	0.00000	0.00000	0.00000	0.00000
152	C8	DZZ	0.00175	0.00000	0.00000	0.00000	0.00000
153	C8	DXY	0.01688	0.00000	0.00000	0.00000	0.00000
154	C8	DXZ	0.00000	0.01431	-0.00113	0.01973	-0.00260
155	C8	DYZ	0.00000	-0.00522	0.02647	-0.00332	-0.02745
156	H8	S	-0.01773	0.00000	0.00000	0.00000	0.00000
157	H8	S	-0.02505	0.00000	0.00000	0.00000	0.00000
158	H8	PX	0.00065	0.00000	0.00000	0.00000	0.00000
159	H8	PY	-0.00278	0.00000	0.00000	0.00000	0.00000
160	H8	PZ	0.00000	0.00515	0.00142	0.00638	-0.00793
161	C10	S	0.00825	0.00000	0.00000	0.00000	0.00000
162	C10	S	-0.01906	0.00000	0.00000	0.00000	0.00000
163	C10	PX	-0.02188	0.00000	0.00000	0.00000	0.00000
164	C10	PY	-0.02298	0.00000	0.00000	0.00000	0.00000
165	C10	PZ	0.00000	0.06425	-0.30721	0.01696	0.26557
166	C10	S	-0.05537	0.00000	0.00000	0.00000	0.00000
167	C10	PX	0.00103	0.00000	0.00000	0.00000	0.00000
168	C10	PY	-0.00055	0.00000	0.00000	0.00000	0.00000
169	C10	PZ	0.00000	0.05398	-0.26954	0.01980	0.37242
170	C10	DXX	0.00237	0.00000	0.00000	0.00000	0.00000
171	C10	DYY	-0.00065	0.00000	0.00000	0.00000	0.00000
172	C10	DZZ	-0.00050	0.00000	0.00000	0.00000	0.00000
173	C10	DXY	0.00832	0.00000	0.00000	0.00000	0.00000
174	C10	DXZ	0.00000	0.00195	-0.00214	0.00255	-0.00001
175	C10	DYZ	0.00000	0.00488	-0.01979	0.00073	-0.00224
176	H16	S	-0.01950	0.00000	0.00000	0.00000	0.00000
177	H16	S	-0.01731	0.00000	0.00000	0.00000	0.00000
178	H16	PX	-0.00014	0.00000	0.00000	0.00000	0.00000
179	H16	PY	-0.00024	0.00000	0.00000	0.00000	0.00000
180	H16	PZ	0.00000	0.00165	-0.00720	0.00077	0.00862
181	H18	S	0.02449	0.00000	0.00000	0.00000	0.00000
182	H18	S	0.06222	0.00000	0.00000	0.00000	0.00000
183	H18	PX	0.00012	0.00000	0.00000	0.00000	0.00000

184	H18	PY	0.00119	0.00000	0.00000	0.00000	0.00000
185	H18	PZ	0.00000	0.00109	-0.00684	-0.00007	0.00838

MO:		36	37	38	39	40
Eigenvalues:		0.17203	0.19622	0.24449	0.26350	0.28437
(ev):		4.68115	5.33948	6.65287	7.17009	7.73808

			A	A	A	A	A
1	H1	S	0.00000	0.00000	-0.03010	0.00068	0.00000
2	H1	S	0.00000	0.00000	-0.94876	-0.58727	0.00000
3	H1	PX	0.00000	0.00000	0.00101	0.00327	0.00000
4	H1	PY	0.00000	0.00000	0.00147	0.00243	0.00000
5	H1	PZ	0.01169	0.00436	0.00000	0.00000	0.00356
6	C1	S	0.00000	0.00000	-0.04148	-0.01226	0.00000
7	C1	S	0.00000	0.00000	0.05493	-0.00284	0.00000
8	C1	PX	0.00000	0.00000	0.12054	0.08192	0.00000
9	C1	PY	0.00000	0.00000	0.01037	0.02457	0.00000
10	C1	PZ	0.26841	0.10644	0.00000	0.00000	0.05096
11	C1	S	0.00000	0.00000	0.65003	0.44337	0.00000
12	C1	PX	0.00000	0.00000	0.44568	0.37706	0.00000
13	C1	PY	0.00000	0.00000	-0.09971	-0.04016	0.00000
14	C1	PZ	0.51787	0.20165	0.00000	0.00000	0.20857
15	C1	DXX	0.00000	0.00000	-0.01538	-0.00116	0.00000
16	C1	DYY	0.00000	0.00000	0.00981	0.00426	0.00000
17	C1	DZZ	0.00000	0.00000	0.00026	-0.00341	0.00000
18	C1	DXY	0.00000	0.00000	0.00283	0.00034	0.00000
19	C1	DXZ	0.01067	0.00249	0.00000	0.00000	0.00846
20	C1	DYZ	0.00181	-0.03054	0.00000	0.00000	0.00404
21	C2	S	0.00000	0.00000	-0.03163	0.01228	0.00000
22	C2	S	0.00000	0.00000	0.04481	-0.01915	0.00000
23	C2	PX	0.00000	0.00000	-0.09046	0.02996	0.00000
24	C2	PY	0.00000	0.00000	0.01086	0.01322	0.00000
25	C2	PZ	0.26196	-0.11263	0.00000	0.00000	0.04203
26	C2	S	0.00000	0.00000	0.42495	-0.16914	0.00000
27	C2	PX	0.00000	0.00000	-0.34087	0.25974	0.00000
28	C2	PY	0.00000	0.00000	-0.23129	0.18440	0.00000
29	C2	PZ	0.48937	-0.22077	0.00000	0.00000	0.14706
30	C2	DXX	0.00000	0.00000	-0.01616	0.00724	0.00000
31	C2	DYY	0.00000	0.00000	0.01062	-0.00524	0.00000
32	C2	DZZ	0.00000	0.00000	0.00094	0.00010	0.00000
33	C2	DXY	0.00000	0.00000	-0.00546	-0.00402	0.00000
34	C2	DXZ	-0.00993	0.00000	0.00000	0.00000	-0.00783
35	C2	DYZ	0.00264	0.03060	0.00000	0.00000	0.00435
36	C3	S	0.00000	0.00000	-0.01492	0.01377	0.00000
37	C3	S	0.00000	0.00000	0.03500	-0.04435	0.00000
38	C3	PX	0.00000	0.00000	0.00058	0.03641	0.00000
39	C3	PY	0.00000	0.00000	-0.00421	0.04455	0.00000
40	C3	PZ	-0.17069	0.21221	0.00000	0.00000	-0.10214
41	C3	S	0.00000	0.00000	0.04757	0.33499	0.00000
42	C3	PX	0.00000	0.00000	-0.04112	-0.39441	0.00000
43	C3	PY	0.00000	0.00000	-0.03003	-0.10454	0.00000
44	C3	PZ	-0.30203	0.41076	0.00000	0.00000	-0.33004
45	C3	DXX	0.00000	0.00000	0.00639	0.01384	0.00000
46	C3	DYY	0.00000	0.00000	-0.01053	-0.00845	0.00000

47	C3	DZZ	0.00000	0.00000	0.00254	-0.00073	0.00000
48	C3	DXY	0.00000	0.00000	0.01319	-0.00908	0.00000
49	C3	DXZ	0.02012	0.01384	0.00000	0.00000	0.02455
50	C3	DYZ	0.00996	0.01399	0.00000	0.00000	-0.01056
51	C4	S	0.00000	0.00000	-0.04527	-0.00636	0.00000
52	C4	S	0.00000	0.00000	0.04531	-0.00040	0.00000
53	C4	PX	0.00000	0.00000	0.06267	0.02210	0.00000
54	C4	PY	0.00000	0.00000	0.15492	0.04076	0.00000
55	C4	PZ	-0.14126	-0.26377	0.00000	0.00000	-0.00683
56	C4	S	0.00000	0.00000	0.93033	0.25155	0.00000
57	C4	PX	0.00000	0.00000	0.21689	0.00240	0.00000
58	C4	PY	0.00000	0.00000	0.45521	0.08515	0.00000
59	C4	PZ	-0.30732	-0.53076	0.00000	0.00000	-0.09599
60	C4	DXX	0.00000	0.00000	0.00698	0.00395	0.00000
61	C4	DYY	0.00000	0.00000	-0.00913	-0.00362	0.00000
62	C4	DZZ	0.00000	0.00000	-0.00199	-0.00099	0.00000
63	C4	DXY	0.00000	0.00000	-0.01537	-0.00052	0.00000
64	C4	DXZ	0.02152	-0.01403	0.00000	0.00000	0.00431
65	C4	DYZ	-0.01436	-0.00503	0.00000	0.00000	-0.00041
66	C5	S	0.00000	0.00000	-0.04611	0.00334	0.00000
67	C5	S	0.00000	0.00000	0.04953	-0.00155	0.00000
68	C5	PX	0.00000	0.00000	-0.07073	0.02378	0.00000
69	C5	PY	0.00000	0.00000	0.14039	0.00743	0.00000
70	C5	PZ	-0.12642	0.27287	0.00000	0.00000	0.01416
71	C5	S	0.00000	0.00000	0.93920	-0.25890	0.00000
72	C5	PX	0.00000	0.00000	-0.34876	0.03922	0.00000
73	C5	PY	0.00000	0.00000	0.36817	0.02304	0.00000
74	C5	PZ	-0.27144	0.54337	0.00000	0.00000	-0.03630
75	C5	DXX	0.00000	0.00000	0.00330	-0.00258	0.00000
76	C5	DYY	0.00000	0.00000	-0.00560	-0.00029	0.00000
77	C5	DZZ	0.00000	0.00000	-0.00190	0.00011	0.00000
78	C5	DXY	0.00000	0.00000	0.01758	0.00089	0.00000
79	C5	DXZ	-0.02119	-0.01351	0.00000	0.00000	-0.00523
80	C5	DYZ	-0.01618	0.00424	0.00000	0.00000	-0.00048
81	C6	S	0.00000	0.00000	-0.01711	-0.00981	0.00000
82	C6	S	0.00000	0.00000	0.04079	0.03398	0.00000
83	C6	PX	0.00000	0.00000	0.00547	0.06968	0.00000
84	C6	PY	0.00000	0.00000	0.00365	0.03766	0.00000
85	C6	PZ	-0.17964	-0.22291	0.00000	0.00000	-0.08669
86	C6	S	0.00000	0.00000	-0.06201	-0.14026	0.00000
87	C6	PX	0.00000	0.00000	0.16129	-0.17398	0.00000
88	C6	PY	0.00000	0.00000	0.05871	0.01192	0.00000
89	C6	PZ	-0.28144	-0.39166	0.00000	0.00000	-0.24812
90	C6	DXX	0.00000	0.00000	0.00658	-0.01428	0.00000
91	C6	DYY	0.00000	0.00000	-0.01692	0.00876	0.00000
92	C6	DZZ	0.00000	0.00000	0.00419	0.00329	0.00000
93	C6	DXY	0.00000	0.00000	-0.01278	0.00722	0.00000
94	C6	DXZ	-0.02003	0.01134	0.00000	0.00000	-0.02534
95	C6	DYZ	0.00715	-0.01579	0.00000	0.00000	-0.01478
96	C7	S	0.00000	0.00000	0.00748	-0.05180	0.00000
97	C7	S	0.00000	0.00000	-0.03081	0.07741	0.00000
98	C7	PX	0.00000	0.00000	0.00183	0.17642	0.00000
99	C7	PY	0.00000	0.00000	-0.04414	-0.06416	0.00000
100	C7	PZ	0.05473	-0.16151	0.00000	0.00000	0.22002

101	C7	S	0.00000	0.00000	0.07783	0.75253	0.00000
102	C7	PX	0.00000	0.00000	-0.09838	1.16302	0.00000
103	C7	PY	0.00000	0.00000	-0.16560	-0.24931	0.00000
104	C7	PZ	0.13353	-0.33716	0.00000	0.00000	0.64657
105	C7	DXX	0.00000	0.00000	0.00003	-0.00194	0.00000
106	C7	DYY	0.00000	0.00000	0.00517	-0.00149	0.00000
107	C7	DZZ	0.00000	0.00000	-0.00257	0.00011	0.00000
108	C7	DXY	0.00000	0.00000	-0.00268	0.00528	0.00000
109	C7	DXZ	-0.00123	0.00065	0.00000	0.00000	0.02833
110	C7	DYZ	-0.01543	0.01618	0.00000	0.00000	0.00822
111	H3	S	0.00000	0.00000	-0.03340	-0.00752	0.00000
112	H3	S	0.00000	0.00000	-1.16585	-0.25400	0.00000
113	H3	PX	0.00000	0.00000	0.00046	0.00087	0.00000
114	H3	PY	0.00000	0.00000	0.00213	0.00035	0.00000
115	H3	PZ	-0.00584	-0.01161	0.00000	0.00000	0.00001
116	H4	S	0.00000	0.00000	-0.03575	-0.00049	0.00000
117	H4	S	0.00000	0.00000	-1.14216	0.07585	0.00000
118	H4	PX	0.00000	0.00000	0.00049	0.00091	0.00000
119	H4	PY	0.00000	0.00000	0.00259	-0.00103	0.00000
120	H4	PZ	-0.00527	0.01185	0.00000	0.00000	0.00094
121	N1	S	0.00000	0.00000	0.00525	-0.01629	0.00000
122	N1	S	0.00000	0.00000	-0.03111	0.06533	0.00000
123	N1	PX	0.00000	0.00000	-0.01240	0.03128	0.00000
124	N1	PY	0.00000	0.00000	-0.04365	-0.03131	0.00000
125	N1	PZ	0.04739	0.18189	0.00000	0.00000	0.24716
126	N1	S	0.00000	0.00000	0.10210	-0.11950	0.00000
127	N1	PX	0.00000	0.00000	0.01666	-0.00917	0.00000
128	N1	PY	0.00000	0.00000	0.01878	-0.01871	0.00000
129	N1	PZ	0.08609	0.28939	0.00000	0.00000	0.50240
130	N1	DXX	0.00000	0.00000	-0.00530	0.00422	0.00000
131	N1	DYY	0.00000	0.00000	0.00475	-0.00454	0.00000
132	N1	DZZ	0.00000	0.00000	-0.00459	0.00914	0.00000
133	N1	DXY	0.00000	0.00000	0.00216	0.00450	0.00000
134	N1	DXZ	0.00346	0.00820	0.00000	0.00000	-0.00880
135	N1	DYZ	-0.01225	-0.01202	0.00000	0.00000	0.01465
136	H6	S	0.00000	0.00000	-0.03185	0.02282	0.00000
137	H6	S	0.00000	0.00000	-0.72120	0.37490	0.00000
138	H6	PX	0.00000	0.00000	-0.00014	0.00083	0.00000
139	H6	PY	0.00000	0.00000	0.00232	0.00021	0.00000
140	H6	PZ	0.01111	-0.00459	0.00000	0.00000	0.00290
141	C8	S	0.00000	0.00000	0.00592	0.00830	0.00000
142	C8	S	0.00000	0.00000	-0.00159	-0.03694	0.00000
143	C8	PX	0.00000	0.00000	-0.01060	0.03977	0.00000
144	C8	PY	0.00000	0.00000	-0.01295	-0.00567	0.00000
145	C8	PZ	0.18415	0.00596	0.00000	0.00000	-0.39716
146	C8	S	0.00000	0.00000	-0.19966	0.46109	0.00000
147	C8	PX	0.00000	0.00000	-0.10987	-0.03690	0.00000
148	C8	PY	0.00000	0.00000	-0.10665	0.33345	0.00000
149	C8	PZ	0.25589	0.02083	0.00000	0.00000	-0.88173
150	C8	DXX	0.00000	0.00000	0.00254	0.00938	0.00000
151	C8	DYY	0.00000	0.00000	-0.00583	0.00012	0.00000
152	C8	DZZ	0.00000	0.00000	0.00068	-0.00168	0.00000
153	C8	DXY	0.00000	0.00000	-0.00040	-0.01096	0.00000
154	C8	DXZ	0.00157	-0.02191	0.00000	0.00000	-0.00327

155	C8	DYZ	0.00926	0.00114	0.00000	0.00000	-0.00096
156	H8	S	0.00000	0.00000	0.00909	0.00182	0.00000
157	H8	S	0.00000	0.00000	0.02025	-1.66394	0.00000
158	H8	PX	0.00000	0.00000	-0.00019	0.00712	0.00000
159	H8	PY	0.00000	0.00000	-0.00338	0.00046	0.00000
160	H8	PZ	0.00271	-0.00762	0.00000	0.00000	0.01494
161	C10	S	0.00000	0.00000	0.01620	-0.07055	0.00000
162	C10	S	0.00000	0.00000	-0.02342	0.07396	0.00000
163	C10	PX	0.00000	0.00000	-0.01004	0.09134	0.00000
164	C10	PY	0.00000	0.00000	0.01628	-0.13550	0.00000
165	C10	PZ	-0.17567	0.00443	0.00000	0.00000	0.15246
166	C10	S	0.00000	0.00000	-0.27800	1.35203	0.00000
167	C10	PX	0.00000	0.00000	0.00490	0.37851	0.00000
168	C10	PY	0.00000	0.00000	0.09909	-0.53963	0.00000
169	C10	PZ	-0.32249	-0.00444	0.00000	0.00000	0.60364
170	C10	DXX	0.00000	0.00000	0.00117	-0.00188	0.00000
171	C10	DYY	0.00000	0.00000	0.00065	-0.00058	0.00000
172	C10	DZZ	0.00000	0.00000	0.00006	-0.00553	0.00000
173	C10	DXY	0.00000	0.00000	0.00030	0.00264	0.00000
174	C10	DXZ	0.00066	-0.00511	0.00000	0.00000	-0.00091
175	C10	DYZ	0.01287	0.00050	0.00000	0.00000	-0.03100
176	H16	S	0.00000	0.00000	0.00255	-0.01071	0.00000
177	H16	S	0.00000	0.00000	0.21027	-1.38758	0.00000
178	H16	PX	0.00000	0.00000	0.00002	0.00046	0.00000
179	H16	PY	0.00000	0.00000	0.00088	-0.00607	0.00000
180	H16	PZ	-0.00779	-0.00071	0.00000	0.00000	0.01053
181	H18	S	0.00000	0.00000	0.00466	-0.01850	0.00000
182	H18	S	0.00000	0.00000	0.15677	-0.48527	0.00000
183	H18	PX	0.00000	0.00000	0.00010	-0.00008	0.00000
184	H18	PY	0.00000	0.00000	0.00078	-0.00263	0.00000
185	H18	PZ	-0.00750	0.00111	0.00000	0.00000	0.00927

MO:	41	42	43	44	45
Eigenvalues:	0.28500	0.30257	0.30727	0.32265	0.33518
(ev):	7.75532	8.23342	8.36138	8.77967	9.12063

		A	A	A	A	A	
1	H1	S	0.00799	0.00866	-0.03099	-0.00037	-0.03005
2	H1	S	1.17798	0.99575	0.44056	1.23137	-0.56069
3	H1	PX	-0.00475	-0.00306	-0.00441	-0.00508	-0.00169
4	H1	PY	0.00154	0.00169	-0.00192	0.00305	0.00326
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.03540	0.04276	0.02824	0.06147	-0.02673
7	C1	S	-0.02874	-0.05267	-0.05562	-0.09565	0.04213
8	C1	PX	-0.15265	-0.10217	-0.01008	-0.08987	0.03722
9	C1	PY	-0.00557	0.03632	0.00883	0.01148	0.02527
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.83763	-0.78626	-0.40716	-0.96621	0.02162
12	C1	PX	-0.67752	-0.59581	-0.29920	-0.69891	0.40215
13	C1	PY	-0.14190	0.13193	-0.53840	-0.32873	0.31442
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00191	0.00073	-0.01292	-0.00805	-0.00867
16	C1	DYY	-0.00217	0.00213	0.01092	0.01001	-0.00079
17	C1	DZZ	0.00305	-0.00021	-0.00076	-0.00160	-0.00152

18	C1	DXY	0.00477	0.00129	-0.00450	0.00460	0.00741
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02702	-0.02619	0.01725	0.06256	0.05613
22	C2	S	0.02331	0.02096	0.00198	-0.09402	-0.08054
23	C2	PX	-0.12607	-0.10579	0.08517	0.08277	0.11007
24	C2	PY	-0.00589	-0.01663	-0.00227	0.03404	-0.03648
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.57893	0.61987	-0.59769	-1.06597	-0.58610
27	C2	PX	-0.56078	-0.49113	0.20803	0.76586	0.98185
28	C2	PY	-0.26313	-0.05574	0.01595	0.01985	-0.40606
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00960	0.00008	0.00016	-0.00615	0.00092
31	C2	DYY	0.00828	-0.00009	-0.00411	0.00632	0.00597
32	C2	DZZ	-0.00183	-0.00133	0.00287	-0.00156	0.00173
33	C2	DXY	-0.00068	-0.00252	-0.00574	-0.00821	0.00778
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00572	-0.00822	0.00809	-0.00236	-0.00847
37	C3	S	0.04237	0.02915	0.02856	-0.01607	-0.00717
38	C3	PX	-0.08107	0.03135	0.04570	0.04318	0.02018
39	C3	PY	0.04875	0.02880	-0.00942	0.09957	-0.00697
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.61084	0.01899	-1.10983	0.00024	0.57414
42	C3	PX	-0.00101	0.41837	0.16011	-0.18569	0.11586
43	C3	PY	0.19964	-0.12814	0.16273	-0.06444	0.02935
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.01179	-0.00156	0.00749	0.00372	0.00033
46	C3	DYY	0.00421	-0.00356	-0.02218	-0.00976	0.00840
47	C3	DZZ	0.00387	0.00342	0.00268	0.00055	-0.00273
48	C3	DXY	0.00299	-0.01321	-0.00085	-0.01833	0.00029
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00381	0.00864	-0.06001	-0.04267	0.07438
52	C4	S	0.00790	0.01060	0.06702	0.03234	-0.10474
53	C4	PX	-0.02800	-0.02206	0.06570	0.05630	0.04867
54	C4	PY	-0.02871	-0.05888	0.07736	0.08485	-0.06997
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.20762	-0.52045	1.23326	0.99372	-0.96099
57	C4	PX	0.24482	0.14788	0.51336	0.52878	-0.08331
58	C4	PY	-0.12100	-0.20440	0.56097	0.38507	-0.80207
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.00675	-0.00293	-0.00086	0.00173	0.01666
61	C4	DYY	0.00584	-0.00079	0.00337	0.00272	-0.00847
62	C4	DZZ	0.00114	0.00191	-0.00270	-0.00459	-0.00068
63	C4	DXY	-0.00292	-0.00232	0.00303	0.00815	-0.00435
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02905	-0.01341	0.02101	-0.02621	-0.09455
67	C5	S	0.01073	-0.00638	-0.04052	0.01494	0.12020
68	C5	PX	-0.08554	-0.02802	-0.01063	-0.06617	-0.00075
69	C5	PY	0.09442	0.07861	-0.01870	0.06119	0.10652
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

71	C5	S	0.99007	0.55696	-0.08919	0.58773	1.39400
72	C5	PX	-0.14185	0.08983	-0.06111	-0.46232	-0.45414
73	C5	PY	0.36353	0.28858	-0.30672	0.24852	0.96058
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00866	0.00584	0.00278	0.00537	-0.01570
76	C5	DYY	-0.00259	-0.00238	0.00274	-0.00149	0.00884
77	C5	DZZ	-0.00360	-0.00259	-0.00190	-0.00431	-0.00175
78	C5	DXY	0.00007	-0.00271	-0.00048	-0.00661	-0.01199
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01593	-0.00646	-0.00535	-0.02255	0.00531
82	C6	S	-0.04478	-0.00393	-0.01803	0.04251	0.00166
83	C6	PX	-0.05883	0.01224	0.05113	-0.04062	-0.00273
84	C6	PY	0.01084	-0.01095	0.06075	0.05811	0.02304
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.13143	0.30601	0.37854	0.07653	-0.48738
87	C6	PX	0.18084	0.41041	0.16578	-0.27909	-0.00303
88	C6	PY	0.06595	0.11015	0.04905	-0.09925	-0.21228
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01588	-0.00060	-0.00206	-0.00675	-0.00336
91	C6	DYY	-0.01606	0.00218	0.01189	-0.00106	-0.00474
92	C6	DZZ	-0.00240	-0.00065	-0.00281	0.00211	0.00070
93	C6	DXY	-0.00118	0.00036	-0.00181	0.02064	0.00127
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00662	-0.01502	0.06742	-0.02984	0.02931
97	C7	S	-0.01287	-0.00308	-0.13624	0.05226	-0.01206
98	C7	PX	-0.06339	0.13039	-0.07280	0.06043	-0.02195
99	C7	PY	0.00581	0.00930	0.07957	-0.04375	0.05133
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.00441	0.44058	-0.61198	0.22009	-0.56690
102	C7	PX	-0.35485	0.41643	-0.63964	0.63772	-0.11907
103	C7	PY	0.45472	-0.37298	0.78114	0.10672	-0.09171
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.01218	-0.01266	0.00060	-0.01069	0.00311
106	C7	DYY	-0.00859	0.00986	0.01334	-0.00433	-0.00112
107	C7	DZZ	-0.00039	-0.00200	-0.00854	0.00543	0.00293
108	C7	DXY	-0.00494	0.00956	0.01318	0.00958	0.00246
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00291	-0.00956	-0.00162	0.00970	0.00622
112	H3	S	0.16063	0.35112	-1.25032	-1.01261	1.19815
113	H3	PX	-0.00235	-0.00126	0.00162	0.00450	0.00363
114	H3	PY	0.00068	-0.00216	0.00599	0.00365	-0.00644
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00441	0.00390	0.01311	0.00802	0.00534
117	H4	S	-0.88499	-0.49922	0.34001	-0.73197	-1.67065
118	H4	PX	-0.00385	-0.00266	-0.00187	-0.00558	0.00041
119	H4	PY	0.00294	0.00145	-0.00113	0.00069	0.00780
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00135	-0.01409	-0.01249	0.01606	0.00685
122	N1	S	-0.02004	0.05348	0.02271	-0.02194	-0.00947
123	N1	PX	-0.06232	0.08820	-0.00123	0.00796	0.02576
124	N1	PY	-0.00006	-0.04900	-0.02375	0.05074	-0.00605

125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.15635	-0.00162	0.14231	-0.22057	-0.20549
127	N1	PX	-0.02834	-0.00065	-0.02460	-0.01737	-0.10678
128	N1	PY	0.10153	0.05758	-0.05282	-0.03908	0.08615
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.00091	-0.00105	0.00745	-0.00223	0.00115
131	N1	DYY	0.00289	0.00049	-0.01987	0.00669	-0.00377
132	N1	DZZ	-0.00383	0.00632	0.00223	0.00334	-0.00007
133	N1	DXY	-0.00977	0.00977	-0.00069	-0.00848	-0.00024
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.02758	0.00489	-0.00228	0.00144	0.02101
137	H6	S	-0.96317	-0.80302	0.54869	1.26812	1.37537
138	H6	PX	-0.00251	-0.00313	0.00244	0.00587	0.00360
139	H6	PY	-0.00009	0.00057	0.00263	0.00304	-0.00384
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01209	0.00670	-0.02425	-0.02611	-0.00886
142	C8	S	0.01755	-0.01756	0.02883	0.02386	0.01377
143	C8	PX	-0.01920	0.07574	0.13763	-0.04581	0.00792
144	C8	PY	0.06287	-0.05238	0.06167	0.00187	0.03177
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.30986	0.00530	0.36638	0.69856	0.08620
147	C8	PX	0.06976	-0.36001	0.16273	0.31456	-0.16297
148	C8	PY	-0.17749	0.00909	-0.24374	0.01348	0.21827
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00786	0.01267	-0.00934	0.00629	-0.00191
151	C8	DYY	0.00411	-0.00456	0.00685	-0.00680	0.00463
152	C8	DZZ	0.00194	-0.00337	-0.00032	0.00018	0.00038
153	C8	DXY	0.01172	-0.03070	-0.01973	0.01503	-0.01037
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.03048	-0.04162	-0.00957	-0.04395	0.01847
157	H8	S	0.57578	-0.87748	1.32511	-0.80256	0.42538
158	H8	PX	0.00101	0.00151	-0.00121	-0.00228	0.00107
159	H8	PY	0.00344	0.00346	0.00582	0.00044	0.00229
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.07105	0.05218	-0.01587	0.03459	-0.00596
162	C10	S	0.08612	-0.06157	0.02311	-0.03009	0.00047
163	C10	PX	-0.03499	0.20167	0.17336	-0.11671	0.07068
164	C10	PY	-0.12007	0.05928	-0.04792	0.03334	-0.01196
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.98993	-0.83964	0.00876	-0.62913	0.21559
167	C10	PX	-0.24665	1.09187	0.80702	-0.71069	0.41381
168	C10	PY	-0.57969	0.19726	-0.29199	-0.01223	0.02498
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00739	0.00642	-0.00323	-0.00118	-0.00054
171	C10	DYY	-0.00199	-0.00060	-0.00495	0.00335	-0.00138
172	C10	DZZ	-0.00247	0.00148	0.00100	0.00308	0.00001
173	C10	DXY	-0.00519	0.01185	0.01227	-0.00803	0.00400
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.00265	-0.01034	-0.03875	0.02515	-0.01248
177	H16	S	-0.68886	-0.50302	-1.12812	0.99122	-0.46176
178	H16	PX	-0.00261	0.00458	0.00156	-0.00217	0.00127

179	H16	PY	-0.00261	0.00039	0.00123	-0.00114	0.00047
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.03261	0.03781	0.02639	-0.01463	0.00813
182	H18	S	-1.10230	1.68880	0.72991	-0.41110	0.36028
183	H18	PX	-0.00006	0.00258	0.00467	-0.00247	0.00155
184	H18	PY	-0.00217	0.00199	-0.00086	-0.00014	-0.00087
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	46	47	48	49	50
Eigenvalues:	0.37743	0.40578	0.43114	0.44063	0.47847
(ev):	10.27040	11.04189	11.73184	11.99020	13.01975

		A	A	A	A	A	
1	H1	S	0.00000	0.02203	-0.06158	-0.07220	0.07146
2	H1	S	0.00000	0.71283	-0.28327	0.08502	-0.05349
3	H1	PX	0.00000	-0.00276	-0.00416	-0.00524	0.00551
4	H1	PY	0.00000	0.00835	0.01169	-0.00034	0.01018
5	H1	PZ	-0.01428	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.02755	0.03317	0.04028	-0.02248
7	C1	S	0.00000	0.00717	-0.07451	-0.00932	0.01741
8	C1	PX	0.00000	-0.02354	0.08946	0.01815	-0.01263
9	C1	PY	0.00000	-0.01216	0.10950	0.05654	0.11001
10	C1	PZ	-0.19480	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.55673	-0.69026	-1.35810	1.10520
12	C1	PX	0.00000	-0.64941	0.33061	0.27918	-0.27466
13	C1	PY	0.00000	1.38673	0.22291	-0.11647	1.32139
14	C1	PZ	-0.63665	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	-0.00162	-0.02128	-0.02449	0.02217
16	C1	DYY	0.00000	0.00582	0.02345	0.01821	-0.00825
17	C1	DZZ	0.00000	0.00436	-0.00798	0.00272	-0.00162
18	C1	DXY	0.00000	0.02001	0.01645	-0.00689	0.02129
19	C1	DXZ	-0.01838	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00658	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	-0.02244	-0.02253	-0.02212	-0.00468
22	C2	S	0.00000	0.03669	0.00982	0.03383	0.02920
23	C2	PX	0.00000	0.08397	-0.04145	0.00715	0.04118
24	C2	PY	0.00000	-0.06694	-0.01439	-0.04287	0.09384
25	C2	PZ	0.21091	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	0.21522	0.71437	0.59938	0.13116
27	C2	PX	0.00000	0.21485	-0.62489	-0.03552	0.20370
28	C2	PY	0.00000	-0.67785	-0.80795	0.83916	1.32769
29	C2	PZ	0.65261	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	0.00025	0.02378	0.02850	0.00840
31	C2	DYY	0.00000	-0.00394	-0.01949	-0.02359	0.01221
32	C2	DZZ	0.00000	0.00175	-0.00008	0.00102	-0.00447
33	C2	DXY	0.00000	0.01831	0.01511	-0.00962	-0.02068
34	C2	DXZ	-0.01981	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00604	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.08716	-0.03537	-0.00414	-0.03263
37	C3	S	0.00000	0.12396	0.06332	0.00244	0.07049
38	C3	PX	0.00000	0.00108	0.01474	0.21186	0.00868
39	C3	PY	0.00000	0.03647	0.15579	-0.03466	0.03092
40	C3	PZ	0.31189	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	2.05302	-0.47711	0.33672	0.45070

42	C3	PX	0.00000	0.74814	-0.02999	0.99098	-0.00143
43	C3	PY	0.00000	0.37227	0.97884	-0.23654	0.25237
44	C3	PZ	0.74677	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.02446	0.01186	0.02544	-0.01446
46	C3	DYY	0.00000	0.03159	-0.03087	-0.01488	0.02660
47	C3	DZZ	0.00000	0.00499	0.00686	-0.00464	0.00045
48	C3	DXY	0.00000	0.00614	-0.00585	-0.00418	-0.02286
49	C3	DXZ	0.01175	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00786	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.02604	0.04491	-0.00329	0.02402
52	C4	S	0.00000	-0.02176	-0.02289	-0.00148	-0.03130
53	C4	PX	0.00000	0.08967	0.14794	0.07073	-0.09141
54	C4	PY	0.00000	0.14687	0.01491	-0.07605	0.09528
55	C4	PZ	0.19442	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-1.18641	-1.06207	0.06705	-1.08840
57	C4	PX	0.00000	0.35845	1.25299	0.55265	-1.10802
58	C4	PY	0.00000	1.02308	0.12663	-0.85952	0.69293
59	C4	PZ	0.56991	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00569	0.01884	0.01331	-0.00590
61	C4	DYY	0.00000	-0.01382	-0.02080	-0.01262	-0.00060
62	C4	DZZ	0.00000	-0.00167	0.00030	-0.00331	-0.00132
63	C4	DXY	0.00000	0.00988	0.00194	-0.00993	-0.01684
64	C4	DXZ	0.00304	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.01146	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.02520	-0.04724	0.00527	0.04578
67	C5	S	0.00000	0.02597	0.01553	0.00157	-0.02041
68	C5	PX	0.00000	0.09352	0.16933	0.10098	-0.01391
69	C5	PY	0.00000	-0.06434	-0.05679	0.10564	0.08705
70	C5	PZ	-0.19384	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.70895	1.65080	-0.29851	-1.69517
72	C5	PX	0.00000	0.48677	1.17023	0.61760	0.06408
73	C5	PY	0.00000	-0.50147	-0.53671	0.85357	0.72094
74	C5	PZ	-0.58077	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	-0.01171	-0.01063	-0.00672	-0.00248
76	C5	DYY	0.00000	0.01582	0.01797	0.00674	-0.00424
77	C5	DZZ	0.00000	0.00183	-0.00113	0.00284	0.00076
78	C5	DXY	0.00000	0.00413	-0.00099	-0.00901	0.01585
79	C5	DXZ	0.00251	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.01221	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	0.07146	0.03782	-0.02752	0.00459
82	C6	S	0.00000	-0.08511	-0.08813	0.07879	0.03061
83	C6	PX	0.00000	-0.10231	0.10608	0.17000	-0.16029
84	C6	PY	0.00000	-0.10702	-0.04346	0.03679	0.15100
85	C6	PZ	-0.33580	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.96912	-0.72554	0.66524	-0.42126
87	C6	PX	0.00000	0.10435	0.72150	0.40233	-0.33823
88	C6	PY	0.00000	-0.46621	-0.38791	0.86069	1.26540
89	C6	PZ	-0.75535	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.00945	0.00395	-0.01867	0.00208
91	C6	DYY	0.00000	0.00358	-0.00597	0.02760	0.00352
92	C6	DZZ	0.00000	-0.00689	-0.00750	0.00328	-0.00634
93	C6	DXY	0.00000	-0.00347	0.01566	-0.00283	0.01525
94	C6	DXZ	0.00347	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00282	0.00000	0.00000	0.00000	0.00000

96	C7	S	0.00000	-0.01208	0.03305	0.02804	-0.01872
97	C7	S	0.00000	0.01324	-0.07798	-0.02182	0.07032
98	C7	PX	0.00000	-0.03399	0.09746	-0.03045	-0.02235
99	C7	PY	0.00000	-0.01820	-0.01245	-0.03860	0.10874
100	C7	PZ	-0.06172	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	0.33061	0.21031	-1.14062	0.46981
102	C7	PX	0.00000	-0.78184	0.11618	-0.19394	-1.14574
103	C7	PY	0.00000	-1.36436	1.15215	-0.29771	0.30450
104	C7	PZ	-0.40299	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00615	0.00499	-0.02960	0.00405
106	C7	DYY	0.00000	0.00418	0.00128	0.02700	0.00649
107	C7	DZZ	0.00000	0.00185	-0.00308	-0.00388	0.00260
108	C7	DXY	0.00000	-0.01964	0.01486	0.02532	-0.00110
109	C7	DXZ	-0.00480	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.02932	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	-0.01380	-0.03819	-0.04047	-0.04644
112	H3	S	0.00000	-0.92326	-0.29414	0.40242	-0.01999
113	H3	PX	0.00000	0.00913	0.00821	0.00007	-0.00955
114	H3	PY	0.00000	-0.00472	-0.00476	-0.00546	-0.00057
115	H3	PZ	0.01209	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00000	0.01978	0.03208	0.02212	-0.06799
117	H4	S	0.00000	0.50977	0.63525	-0.34260	-0.28106
118	H4	PX	0.00000	0.00766	0.00663	-0.00248	0.00561
119	H4	PY	0.00000	0.00456	0.00587	0.00197	-0.00149
120	H4	PZ	-0.01205	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00000	-0.01083	-0.00927	-0.08647	-0.06256
122	N1	S	0.00000	0.05722	-0.00298	0.08401	0.06655
123	N1	PX	0.00000	0.10929	-0.05041	0.05750	-0.00731
124	N1	PY	0.00000	0.00178	0.06922	-0.07029	0.05344
125	N1	PZ	0.14631	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00000	-0.18353	0.36997	1.96341	1.73138
127	N1	PX	0.00000	0.05469	-0.07568	0.68926	0.76048
128	N1	PY	0.00000	0.11875	0.35593	-0.36110	0.51483
129	N1	PZ	0.37853	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00000	0.00634	0.00333	-0.00525	0.00241
131	N1	DYY	0.00000	0.01162	-0.00926	-0.01474	0.01063
132	N1	DZZ	0.00000	-0.00058	-0.00355	-0.02216	-0.02015
133	N1	DXY	0.00000	-0.00044	-0.00459	0.01317	-0.00325
134	N1	DXZ	-0.00018	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	-0.02202	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.00000	0.00345	0.05863	0.08373	0.01486
137	H6	S	0.00000	0.20774	-0.71393	-0.09938	0.23437
138	H6	PX	0.00000	0.00049	-0.00741	-0.00638	-0.00276
139	H6	PY	0.00000	-0.00774	-0.00806	0.00503	0.01346
140	H6	PZ	0.01474	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00000	0.07175	-0.08607	0.05805	-0.02680
142	C8	S	0.00000	-0.03215	0.08894	-0.03719	0.10276
143	C8	PX	0.00000	-0.11134	0.08893	0.21469	-0.02264
144	C8	PY	0.00000	-0.00053	-0.01737	-0.02860	-0.12113
145	C8	PZ	0.00037	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.00000	-2.26608	2.66384	-1.88145	0.95554
147	C8	PX	0.00000	-0.95066	0.52156	1.40078	-0.03361
148	C8	PY	0.00000	0.40665	-1.23174	0.04214	-2.18970
149	C8	PZ	0.00046	0.00000	0.00000	0.00000	0.00000

150	C8	DXX	0.00000	0.00642	-0.00860	0.01361	-0.00508
151	C8	DYY	0.00000	-0.00882	0.01897	-0.02485	0.01774
152	C8	DZZ	0.00000	0.00274	0.00200	-0.00566	-0.00058
153	C8	DXY	0.00000	-0.01927	0.00050	-0.00828	0.00060
154	C8	DXZ	-0.02167	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00101	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00000	0.02641	0.00819	-0.12296	0.01984
157	H8	S	0.00000	0.13141	0.15173	0.32785	0.83967
158	H8	PX	0.00000	-0.00180	0.00114	-0.01034	-0.00450
159	H8	PY	0.00000	-0.00776	0.00571	-0.00068	-0.00177
160	H8	PZ	-0.00753	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00000	-0.03805	0.05039	-0.03273	0.03781
162	C10	S	0.00000	-0.00852	0.02820	-0.01110	0.07093
163	C10	PX	0.00000	-0.00349	-0.03411	-0.14969	0.00009
164	C10	PY	0.00000	-0.02790	0.03254	-0.04840	0.05233
165	C10	PZ	0.00891	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00000	1.26674	-2.04767	0.98608	-2.15973
167	C10	PX	0.00000	0.58155	-0.51526	-1.01902	-0.06662
168	C10	PY	0.00000	0.72319	-1.39967	0.71693	-1.65225
169	C10	PZ	0.00407	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00000	0.01068	-0.01586	0.01456	-0.00945
171	C10	DYY	0.00000	-0.00219	0.00148	-0.00083	0.00795
172	C10	DZZ	0.00000	-0.00887	0.01357	-0.01194	0.01007
173	C10	DXY	0.00000	0.00272	0.00872	0.03546	0.01052
174	C10	DXZ	-0.00752	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00015	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00000	-0.00506	-0.04310	-0.07049	-0.06946
177	H16	S	0.00000	-0.48389	0.37918	0.72256	-0.17885
178	H16	PX	0.00000	0.00495	-0.00517	0.00019	-0.00105
179	H16	PY	0.00000	0.00311	-0.00365	0.01382	-0.00085
180	H16	PZ	-0.00095	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00000	0.03554	-0.02216	0.10737	-0.01146
182	H18	S	0.00000	0.19138	-0.28790	-0.95919	-0.07605
183	H18	PX	0.00000	0.00076	0.00086	-0.00240	0.00198
184	H18	PY	0.00000	0.00329	-0.00699	-0.00747	-0.00941
185	H18	PZ	0.00186	0.00000	0.00000	0.00000	0.00000

MO:	51	52	53	54	55
Eigenvalues:	0.49030	0.51970	0.54355	0.60485	0.67678
(ev):	13.34168	14.14184	14.79076	16.45886	18.41607

		A	A	A	A	A	
1	H1	S	-0.01427	-0.03883	0.10299	0.07621	0.02263
2	H1	S	0.65913	-0.05137	-0.80123	-0.26307	-0.04286
3	H1	PX	-0.00179	-0.00407	0.01031	0.00894	0.00074
4	H1	PY	-0.00558	0.00803	0.00619	-0.00094	-0.01485
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.07350	0.00307	0.01004	0.01635	0.03748
7	C1	S	0.06177	0.00404	-0.01098	-0.04092	-0.08733
8	C1	PX	-0.16840	-0.00023	0.08290	0.02372	0.09263
9	C1	PY	0.02254	0.13338	-0.07018	0.23132	0.18922
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	2.05776	-0.24854	-0.50426	0.66036	-0.57445
12	C1	PX	-1.32308	-0.00977	1.07669	0.30135	0.25775

13	C1	PY	-0.79341	1.64943	-0.63109	1.01084	-1.61620
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00152	-0.01221	0.04103	0.01635	-0.00344
16	C1	DYY	0.00678	0.00834	-0.04132	-0.00345	0.01212
17	C1	DZZ	-0.00122	-0.00082	-0.00103	-0.00645	-0.01430
18	C1	DXY	-0.01019	0.01337	0.02318	-0.00557	-0.01669
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08744	0.00462	0.01663	-0.01740	-0.01295
22	C2	S	0.06910	-0.02408	0.04397	-0.01017	0.08527
23	C2	PX	0.15913	-0.04462	-0.04015	0.02475	0.03178
24	C2	PY	0.02454	0.17089	-0.14162	0.04600	0.13851
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	2.64763	0.41942	-1.44982	0.17842	0.70070
27	C2	PX	1.45754	-0.12867	-0.95832	0.77557	-0.07870
28	C2	PY	-0.33865	1.67089	-0.64312	-1.25593	0.52442
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01871	0.00102	0.03321	-0.03486	0.04801
31	C2	DYY	-0.00943	-0.00977	-0.02164	0.02839	0.01322
32	C2	DZZ	0.00020	0.00190	-0.00322	-0.00354	-0.01474
33	C2	DXY	0.01303	-0.01263	-0.00428	0.00735	0.00139
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.07192	0.00974	0.02860	-0.07749	-0.04116
37	C3	S	-0.04278	-0.07145	0.04352	0.04383	0.01215
38	C3	PX	-0.08835	0.09417	-0.17921	-0.06520	-0.10106
39	C3	PY	-0.05524	0.19523	0.07037	-0.02752	-0.04573
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-2.04248	0.52213	-1.10102	2.83680	0.67669
42	C3	PX	-0.73525	0.78577	-1.26728	-0.28726	0.12447
43	C3	PY	-0.79744	1.39096	0.94945	-0.39230	-1.66383
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00101	-0.00962	-0.00219	0.01796	-0.00089
46	C3	DYY	0.00540	-0.00609	0.03732	-0.01097	-0.03627
47	C3	DZZ	-0.00852	0.00394	-0.00900	0.00685	0.01582
48	C3	DXY	0.00477	-0.01692	-0.01580	-0.03217	-0.03211
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.03699	0.03841	-0.00942	-0.02968	-0.02648
52	C4	S	-0.03443	-0.00534	-0.10014	0.04084	0.04666
53	C4	PX	0.15936	-0.02083	-0.03148	-0.08066	0.20663
54	C4	PY	0.03200	0.04984	0.10790	-0.04604	-0.13551
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.95524	-1.76945	1.43224	0.64331	0.96979
57	C4	PX	0.10820	-0.21702	0.21880	-2.06549	0.60266
58	C4	PY	0.92814	0.53582	-0.56872	0.29822	-1.01452
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.02993	0.00792	-0.00590	-0.00754	0.00150
61	C4	DYY	0.02134	-0.01929	0.02224	0.00372	0.00417
62	C4	DZZ	-0.00134	0.00276	-0.01317	0.00393	-0.00059
63	C4	DXY	-0.01811	-0.02396	0.02648	-0.01712	-0.01180
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02283	0.01208	-0.00672	0.03083	0.02533

67	C5	S	-0.02948	-0.01600	-0.05464	0.02177	0.03205
68	C5	PX	-0.07994	0.08867	-0.01180	-0.19944	-0.03773
69	C5	PY	0.04274	0.05465	0.06313	-0.09646	-0.00320
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.69363	-1.07104	1.14021	-1.10059	-0.51836
72	C5	PX	0.64673	1.09997	-0.68945	-1.71537	0.65675
73	C5	PY	1.22667	0.44228	-0.65265	-0.13441	1.10596
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.03924	0.00157	-0.00335	0.00191	-0.01926
76	C5	DYY	0.03056	-0.01353	0.01800	-0.00871	0.03146
77	C5	DZZ	-0.00051	0.00003	-0.00741	0.00073	-0.00420
78	C5	DXY	0.00947	0.02829	-0.03124	0.01952	-0.01177
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.05328	-0.03661	0.08129	0.05694	0.03769
82	C6	S	-0.01967	-0.04885	0.05381	-0.07916	0.09048
83	C6	PX	0.18764	-0.04425	-0.03057	0.05270	-0.03807
84	C6	PY	-0.11615	0.07881	0.07772	0.07334	0.09536
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-1.58038	2.35462	-2.60046	-1.96479	-1.81687
87	C6	PX	0.63566	-0.61256	0.06268	-0.35854	0.62264
88	C6	PY	-1.04955	-0.16344	2.01068	-0.72264	1.98262
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.01463	-0.01739	0.02101	0.01006	0.03554
91	C6	DYY	0.02560	0.01688	0.02265	-0.03002	-0.01824
92	C6	DZZ	-0.00669	0.00692	-0.01887	-0.00525	-0.01479
93	C6	DXY	-0.00171	0.02894	0.00864	0.00756	0.03761
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.01824	0.00890	-0.04585	0.08715	0.00232
97	C7	S	0.07761	-0.04465	0.09997	-0.13183	-0.23520
98	C7	PX	-0.01396	0.05493	-0.02860	0.23037	-0.03001
99	C7	PY	0.03250	0.09474	0.15516	0.15263	-0.08748
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.07545	-0.08110	1.19192	-2.39016	-0.06388
102	C7	PX	0.76496	0.41173	0.00752	1.76302	0.04354
103	C7	PY	0.61259	0.44255	1.29911	-0.43818	-1.63376
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.02123	0.00157	0.03569	-0.01865	-0.04456
106	C7	DYY	-0.01126	-0.02055	-0.00698	-0.00053	-0.01454
107	C7	DZZ	0.00088	0.00455	-0.00472	-0.01230	-0.00298
108	C7	DXY	-0.01101	0.02891	0.00265	0.01457	0.00110
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00711	-0.10122	0.11400	-0.03964	-0.00977
112	H3	S	-0.50993	-0.03714	-0.06424	0.34488	0.32379
113	H3	PX	-0.01818	-0.00403	0.00786	-0.01217	-0.00901
114	H3	PY	0.01037	-0.00687	0.00387	0.00195	0.00038
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.02602	-0.09449	0.10061	-0.04628	0.06360
117	H4	S	-0.44439	0.24494	-0.15707	-0.20638	-0.34633
118	H4	PX	0.01891	0.00824	-0.01045	0.00430	0.00587
119	H4	PY	0.01362	-0.00674	0.00305	0.00022	0.01481
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

121	N1	S	-0.02228	0.06133	-0.08276	-0.01170	0.00584
122	N1	S	0.04651	-0.02315	0.04549	0.00476	-0.01860
123	N1	PX	-0.00062	-0.07276	0.01197	0.07515	-0.14493
124	N1	PY	0.04381	0.12835	0.14395	-0.06739	0.28232
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.14259	-2.01169	2.67197	0.13945	0.58854
127	N1	PX	-0.18583	-0.73939	0.66788	-0.05580	-0.29675
128	N1	PY	-0.01099	-0.38253	0.78200	-0.00207	1.81568
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00476	-0.00067	0.00653	0.01356	-0.00056
131	N1	DYY	-0.01821	-0.01137	0.00387	-0.02093	0.04100
132	N1	DZZ	-0.00238	0.03768	-0.04988	-0.00321	-0.01273
133	N1	DXY	0.01781	-0.00948	-0.00661	-0.02618	-0.01922
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.04367	0.00382	0.07110	-0.12393	0.11181
137	H6	S	0.59411	-0.17236	-0.52972	0.39123	-0.17694
138	H6	PX	-0.00128	-0.00041	-0.00757	0.01284	-0.01239
139	H6	PY	-0.00813	0.00467	0.00335	-0.00799	0.00495
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.02609	-0.02933	0.02608	-0.04696	-0.04975
142	C8	S	-0.04201	-0.02565	0.12892	0.05560	-0.06999
143	C8	PX	0.08527	0.06016	0.02942	0.09293	-0.35871
144	C8	PY	-0.01766	0.23805	0.13554	0.15765	0.16002
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.20217	-0.87336	-1.81052	0.64377	0.68897
147	C8	PX	0.55610	-0.13349	0.76425	1.41909	-2.01277
148	C8	PY	0.13151	2.87915	0.98822	1.28746	0.28063
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00495	-0.02009	-0.00486	-0.00558	-0.02052
151	C8	DYY	0.03447	-0.03555	0.02023	-0.01773	-0.05226
152	C8	DZZ	-0.00802	0.01797	0.00051	0.01688	0.02682
153	C8	DXY	0.00745	0.00436	0.01138	-0.04858	0.01696
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.02982	0.00081	0.02173	-0.01617	-0.10895
157	H8	S	-0.43863	-0.08131	0.02113	-0.76945	-0.34375
158	H8	PX	0.00627	0.00537	0.00725	0.00138	-0.00821
159	H8	PY	0.00107	0.01832	0.00665	0.00194	-0.01240
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00872	-0.03329	-0.03234	-0.00186	0.00353
162	C10	S	0.06738	-0.10696	0.05772	-0.09036	-0.18689
163	C10	PX	0.01291	0.02814	0.02298	-0.13784	-0.08461
164	C10	PY	0.10221	-0.07966	0.09318	-0.09325	-0.16797
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.09196	2.55093	1.12400	0.93862	0.18108
167	C10	PX	-0.34665	0.23721	-0.21923	-0.54354	1.13862
168	C10	PY	0.22986	2.06353	1.52188	0.74524	0.07089
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00556	0.00709	0.02336	0.00673	-0.03029
171	C10	DYY	-0.00882	-0.00140	-0.00240	-0.00973	-0.01333
172	C10	DZZ	0.00532	-0.00772	-0.00388	-0.00467	0.00089
173	C10	DXY	0.00052	-0.01686	0.00238	0.06286	-0.03737
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.01826	0.11310	0.06227	-0.14365	0.02553
177	H16	S	0.40690	0.18864	0.56184	0.59776	-0.71765
178	H16	PX	-0.00078	0.00080	0.00418	0.00315	0.00502
179	H16	PY	0.00265	-0.00269	0.00703	0.01687	-0.00467
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.00361	0.01194	0.07839	0.19555	-0.04932
182	H18	S	-0.05706	0.32387	0.25862	-0.44740	0.65254
183	H18	PX	-0.00321	-0.00304	-0.00510	0.00127	0.01650
184	H18	PY	0.00184	0.01122	-0.00218	-0.01648	0.00925
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	56	57	58	59	60
Eigenvalues:	0.69523	0.71512	0.73307	0.74791	0.76776
(ev):	18.91831	19.45933	19.94784	20.35166	20.89194

		A	A	A	A	A	
1	H1	S	0.06892	0.05056	0.00000	0.14966	0.00000
2	H1	S	0.29864	-0.17617	0.00000	0.08336	0.00000
3	H1	PX	-0.00441	-0.00809	0.00000	0.01080	0.00000
4	H1	PY	-0.00333	-0.00225	0.00000	-0.00042	0.00000
5	H1	PZ	0.00000	0.00000	-0.00573	0.00000	0.00050
6	C1	S	-0.01403	-0.02018	0.00000	0.00099	0.00000
7	C1	S	-0.04470	-0.37082	0.00000	0.32524	0.00000
8	C1	PX	0.07418	0.14509	0.00000	-0.04744	0.00000
9	C1	PY	-0.28108	0.25823	0.00000	0.01106	0.00000
10	C1	PZ	0.00000	0.00000	-0.44924	0.00000	-0.14109
11	C1	S	0.02882	1.04424	0.00000	-0.29038	0.00000
12	C1	PX	-0.66667	-0.29101	0.00000	-0.21613	0.00000
13	C1	PY	1.41642	-0.24273	0.00000	1.16566	0.00000
14	C1	PZ	0.00000	0.00000	0.35965	0.00000	0.11240
15	C1	DXX	0.01206	-0.01105	0.00000	0.06760	0.00000
16	C1	DYY	-0.03354	-0.06484	0.00000	0.03000	0.00000
17	C1	DZZ	0.00899	-0.00591	0.00000	-0.00817	0.00000
18	C1	DXY	-0.01461	0.00522	0.00000	-0.00759	0.00000
19	C1	DXZ	0.00000	0.00000	0.02022	0.00000	0.01220
20	C1	DYZ	0.00000	0.00000	-0.01264	0.00000	-0.01092
21	C2	S	-0.03210	0.02347	0.00000	0.07388	0.00000
22	C2	S	-0.15177	-0.36041	0.00000	0.15407	0.00000
23	C2	PX	-0.05113	-0.22547	0.00000	-0.12185	0.00000
24	C2	PY	-0.09471	0.12163	0.00000	0.32697	0.00000
25	C2	PZ	0.00000	0.00000	-0.32660	0.00000	-0.30425
26	C2	S	0.65352	-0.07583	0.00000	-1.41985	0.00000
27	C2	PX	0.07358	0.02490	0.00000	-1.00155	0.00000
28	C2	PY	-1.03628	-0.14639	0.00000	-2.08684	0.00000
29	C2	PZ	0.00000	0.00000	0.23266	0.00000	0.26924
30	C2	DXX	0.01293	-0.02333	0.00000	0.07699	0.00000
31	C2	DYY	-0.07004	-0.03746	0.00000	0.05271	0.00000
32	C2	DZZ	0.00862	-0.00710	0.00000	-0.04883	0.00000
33	C2	DXY	-0.02542	0.02100	0.00000	-0.00095	0.00000
34	C2	DXZ	0.00000	0.00000	-0.01851	0.00000	-0.01468
35	C2	DYZ	0.00000	0.00000	-0.00779	0.00000	-0.02025
36	C3	S	0.05490	-0.00482	0.00000	0.06761	0.00000
37	C3	S	-0.14849	-0.45192	0.00000	0.21847	0.00000

38	C3	PX	0.32751	-0.04370	0.00000	0.17688	0.00000
39	C3	PY	-0.17304	-0.03228	0.00000	0.02240	0.00000
40	C3	PZ	0.00000	0.00000	-0.34603	0.00000	-0.04261
41	C3	S	-0.07984	-0.65097	0.00000	-2.41115	0.00000
42	C3	PX	1.95298	-0.47332	0.00000	1.43583	0.00000
43	C3	PY	0.08630	0.68031	0.00000	1.69180	0.00000
44	C3	PZ	0.00000	0.00000	0.15968	0.00000	0.05153
45	C3	DXX	-0.00797	-0.09252	0.00000	0.06114	0.00000
46	C3	DYY	0.04051	-0.07811	0.00000	0.03308	0.00000
47	C3	DZZ	-0.02855	0.01924	0.00000	-0.03093	0.00000
48	C3	DXY	-0.01516	-0.06829	0.00000	-0.03322	0.00000
49	C3	DXZ	0.00000	0.00000	-0.00453	0.00000	0.01001
50	C3	DYZ	0.00000	0.00000	0.01808	0.00000	-0.02396
51	C4	S	-0.01808	0.02570	0.00000	0.01678	0.00000
52	C4	S	-0.13015	-0.30800	0.00000	0.23331	0.00000
53	C4	PX	-0.10496	0.17869	0.00000	0.00895	0.00000
54	C4	PY	0.13259	0.09501	0.00000	-0.02082	0.00000
55	C4	PZ	0.00000	0.00000	-0.36051	0.00000	-0.32562
56	C4	S	-0.24751	-0.26206	0.00000	-0.97401	0.00000
57	C4	PX	-0.73060	-0.05359	0.00000	-0.74892	0.00000
58	C4	PY	0.29531	0.54445	0.00000	0.88838	0.00000
59	C4	PZ	0.00000	0.00000	0.24528	0.00000	0.24418
60	C4	DXX	-0.04454	-0.05579	0.00000	-0.00217	0.00000
61	C4	DYY	-0.01114	0.00241	0.00000	0.05601	0.00000
62	C4	DZZ	0.00818	-0.00683	0.00000	-0.00964	0.00000
63	C4	DXY	0.03905	0.01344	0.00000	0.02137	0.00000
64	C4	DXZ	0.00000	0.00000	-0.00517	0.00000	0.00839
65	C4	DYZ	0.00000	0.00000	0.02606	0.00000	0.01110
66	C5	S	0.02214	-0.02895	0.00000	-0.01305	0.00000
67	C5	S	-0.27542	-0.24873	0.00000	0.34811	0.00000
68	C5	PX	-0.04278	-0.15727	0.00000	-0.22806	0.00000
69	C5	PY	0.21112	0.00165	0.00000	-0.22001	0.00000
70	C5	PZ	0.00000	0.00000	-0.36154	0.00000	-0.34296
71	C5	S	0.35755	0.68699	0.00000	1.22494	0.00000
72	C5	PX	-0.87559	0.33335	0.00000	-0.49337	0.00000
73	C5	PY	-0.50887	-0.37321	0.00000	-1.24425	0.00000
74	C5	PZ	0.00000	0.00000	0.24772	0.00000	0.26389
75	C5	DXX	-0.01464	-0.06171	0.00000	0.05145	0.00000
76	C5	DYY	0.00199	-0.02451	0.00000	0.06159	0.00000
77	C5	DZZ	-0.01909	0.00915	0.00000	-0.01277	0.00000
78	C5	DXY	-0.02784	-0.01906	0.00000	-0.00284	0.00000
79	C5	DXZ	0.00000	0.00000	0.00112	0.00000	-0.00556
80	C5	DYZ	0.00000	0.00000	0.01626	0.00000	0.02354
81	C6	S	-0.00545	-0.02806	0.00000	-0.07742	0.00000
82	C6	S	-0.25122	-0.37212	0.00000	0.41437	0.00000
83	C6	PX	0.23921	-0.19009	0.00000	0.13340	0.00000
84	C6	PY	-0.00234	-0.16428	0.00000	0.09667	0.00000
85	C6	PZ	0.00000	0.00000	-0.37678	0.00000	-0.02906
86	C6	S	0.64720	1.16243	0.00000	0.38987	0.00000
87	C6	PX	2.14425	-0.47071	0.00000	1.84528	0.00000
88	C6	PY	-0.40261	-0.56908	0.00000	0.08168	0.00000
89	C6	PZ	0.00000	0.00000	0.26801	0.00000	-0.03171
90	C6	DXX	-0.08061	-0.06455	0.00000	0.01949	0.00000
91	C6	DYY	0.02771	-0.05692	0.00000	-0.01811	0.00000

92	C6	DZZ	-0.00226	0.01152	0.00000	0.03604	0.00000
93	C6	DXY	0.00708	0.05822	0.00000	0.03933	0.00000
94	C6	DXZ	0.00000	0.00000	0.00362	0.00000	-0.00944
95	C6	DYZ	0.00000	0.00000	0.00235	0.00000	-0.00790
96	C7	S	0.02385	-0.04428	0.00000	-0.03626	0.00000
97	C7	S	-0.02775	-0.19028	0.00000	0.13394	0.00000
98	C7	PX	0.19257	-0.11429	0.00000	0.01039	0.00000
99	C7	PY	0.35878	-0.01965	0.00000	0.22222	0.00000
100	C7	PZ	0.00000	0.00000	-0.38102	0.00000	0.44797
101	C7	S	-0.25804	1.31888	0.00000	1.96468	0.00000
102	C7	PX	-0.42660	-0.47791	0.00000	-1.66957	0.00000
103	C7	PY	-1.53831	0.83158	0.00000	0.46757	0.00000
104	C7	PZ	0.00000	0.00000	0.32958	0.00000	-0.36572
105	C7	DXX	-0.00045	-0.09515	0.00000	-0.00560	0.00000
106	C7	DYY	-0.00598	-0.00290	0.00000	0.03864	0.00000
107	C7	DZZ	-0.00078	0.02886	0.00000	0.00185	0.00000
108	C7	DXY	0.00448	0.02512	0.00000	0.04831	0.00000
109	C7	DXZ	0.00000	0.00000	0.02057	0.00000	-0.00896
110	C7	DYZ	0.00000	0.00000	-0.02121	0.00000	0.00369
111	H3	S	0.06727	0.08680	0.00000	0.12979	0.00000
112	H3	S	-0.09535	-0.37471	0.00000	-0.23099	0.00000
113	H3	PX	0.00731	-0.00969	0.00000	-0.00126	0.00000
114	H3	PY	-0.00761	0.00602	0.00000	0.01429	0.00000
115	H3	PZ	0.00000	0.00000	-0.00284	0.00000	-0.00423
116	H4	S	0.13939	0.00026	0.00000	0.13184	0.00000
117	H4	S	-0.23477	0.09087	0.00000	0.38212	0.00000
118	H4	PX	-0.00457	0.01121	0.00000	0.00336	0.00000
119	H4	PY	-0.00095	-0.00452	0.00000	0.01497	0.00000
120	H4	PZ	0.00000	0.00000	-0.00549	0.00000	-0.00087
121	N1	S	0.02136	0.00883	0.00000	0.00057	0.00000
122	N1	S	-0.01846	0.02293	0.00000	-0.09993	0.00000
123	N1	PX	-0.04600	0.14551	0.00000	0.03780	0.00000
124	N1	PY	0.15291	-0.08275	0.00000	-0.05563	0.00000
125	N1	PZ	0.00000	0.00000	-0.07137	0.00000	0.09813
126	N1	S	-1.13260	-0.24592	0.00000	0.78941	0.00000
127	N1	PX	-0.99834	0.28230	0.00000	0.07155	0.00000
128	N1	PY	0.91179	-0.83174	0.00000	0.35523	0.00000
129	N1	PZ	0.00000	0.00000	-0.00110	0.00000	0.01559
130	N1	DXX	-0.00846	-0.01597	0.00000	-0.03430	0.00000
131	N1	DYY	-0.05156	0.02652	0.00000	0.01989	0.00000
132	N1	DZZ	0.03709	0.02474	0.00000	-0.03030	0.00000
133	N1	DXY	0.02937	-0.01309	0.00000	-0.00167	0.00000
134	N1	DXZ	0.00000	0.00000	-0.01499	0.00000	0.00211
135	N1	DYZ	0.00000	0.00000	-0.02203	0.00000	0.00198
136	H6	S	0.05115	0.05757	0.00000	0.25880	0.00000
137	H6	S	-0.23537	-0.09977	0.00000	-0.51264	0.00000
138	H6	PX	0.00344	0.00853	0.00000	-0.02297	0.00000
139	H6	PY	0.00654	-0.00862	0.00000	-0.00749	0.00000
140	H6	PZ	0.00000	0.00000	-0.00306	0.00000	-0.00292
141	C8	S	-0.04494	0.02663	0.00000	-0.00946	0.00000
142	C8	S	-0.23694	-0.16566	0.00000	0.01794	0.00000
143	C8	PX	0.02283	-0.03799	0.00000	0.05385	0.00000
144	C8	PY	-0.00383	-0.07629	0.00000	0.06709	0.00000
145	C8	PZ	0.00000	0.00000	-0.20391	0.00000	0.34340

146	C8	S	1.28181	-0.27566	0.00000	-0.64381	0.00000
147	C8	PX	-1.73367	0.53535	0.00000	-0.62412	0.00000
148	C8	PY	0.47013	-1.16125	0.00000	-1.29958	0.00000
149	C8	PZ	0.00000	0.00000	0.07960	0.00000	-0.24746
150	C8	DXX	-0.07507	0.01844	0.00000	0.01227	0.00000
151	C8	DYY	-0.01102	-0.05602	0.00000	-0.05302	0.00000
152	C8	DZZ	0.02481	-0.00964	0.00000	0.01249	0.00000
153	C8	DXY	-0.04193	-0.00375	0.00000	-0.00765	0.00000
154	C8	DXZ	0.00000	0.00000	-0.00908	0.00000	0.00687
155	C8	DYZ	0.00000	0.00000	0.01088	0.00000	-0.03428
156	H8	S	0.05962	-0.27197	0.00000	-0.12523	0.00000
157	H8	S	-0.05290	0.46387	0.00000	0.88067	0.00000
158	H8	PX	0.00253	-0.01863	0.00000	-0.00710	0.00000
159	H8	PY	0.00156	0.00543	0.00000	0.01025	0.00000
160	H8	PZ	0.00000	0.00000	-0.00396	0.00000	0.00900
161	C10	S	0.00420	0.00110	0.00000	0.00193	0.00000
162	C10	S	-0.18237	-0.05450	0.00000	-0.12835	0.00000
163	C10	PX	-0.12790	-0.00977	0.00000	-0.00636	0.00000
164	C10	PY	-0.03164	-0.10597	0.00000	-0.19341	0.00000
165	C10	PZ	0.00000	0.00000	-0.27598	0.00000	0.68377
166	C10	S	0.23300	-0.59333	0.00000	-0.57581	0.00000
167	C10	PX	0.75928	-0.16293	0.00000	0.15531	0.00000
168	C10	PY	-0.46811	-0.28653	0.00000	-0.15194	0.00000
169	C10	PZ	0.00000	0.00000	0.25610	0.00000	-0.61444
170	C10	DXX	-0.04765	-0.00388	0.00000	-0.01726	0.00000
171	C10	DYY	-0.01909	-0.00160	0.00000	-0.00979	0.00000
172	C10	DZZ	0.01287	-0.00524	0.00000	-0.00546	0.00000
173	C10	DXY	0.02128	0.00131	0.00000	-0.00196	0.00000
174	C10	DXZ	0.00000	0.00000	0.00207	0.00000	-0.00237
175	C10	DYZ	0.00000	0.00000	-0.01807	0.00000	0.03120
176	H16	S	-0.15906	-0.02875	0.00000	0.00884	0.00000
177	H16	S	-0.44672	-0.00905	0.00000	-0.12542	0.00000
178	H16	PX	-0.00208	-0.00307	0.00000	-0.00782	0.00000
179	H16	PY	-0.00531	0.00737	0.00000	0.00230	0.00000
180	H16	PZ	0.00000	0.00000	-0.00309	0.00000	0.00971
181	H18	S	-0.04325	0.00760	0.00000	-0.01869	0.00000
182	H18	S	0.10096	-0.15283	0.00000	0.03448	0.00000
183	H18	PX	0.01341	0.00378	0.00000	0.00668	0.00000
184	H18	PY	0.00313	0.00415	0.00000	0.00689	0.00000
185	H18	PZ	0.00000	0.00000	-0.00523	0.00000	0.01258

MO: 61 62 63 64 65
Eigenvalues: 0.76851 0.78593 0.79889 0.80783 0.82464
(ev): 20.91219 21.38635 21.73883 21.98228 22.43952

			A	A	A	A	A
1	H1	S	0.05991	-0.11608	0.29890	0.00000	0.01014
2	H1	S	-0.12974	0.02067	0.14356	0.00000	0.10166
3	H1	PX	0.00120	-0.01357	0.02172	0.00000	0.00253
4	H1	PY	0.00949	-0.00180	-0.00779	0.00000	0.00281
5	H1	PZ	0.00000	0.00000	0.00000	-0.00107	0.00000
6	C1	S	0.03518	0.01230	0.05679	0.00000	0.00030
7	C1	S	-0.21685	-0.34114	0.33078	0.00000	0.24981
8	C1	PX	0.15041	0.12373	0.07385	0.00000	-0.07491

9	C1	PY	0.26805	-0.18307	0.21346	0.00000	0.18075
10	C1	PZ	0.00000	0.00000	0.00000	-0.58788	0.00000
11	C1	S	0.67258	-0.09028	-0.64051	0.00000	-0.05614
12	C1	PX	-0.17656	0.02005	-0.04877	0.00000	-0.11725
13	C1	PY	2.03758	0.24443	-0.41225	0.00000	0.69911
14	C1	PZ	0.00000	0.00000	0.00000	0.59310	0.00000
15	C1	DXX	-0.00156	-0.06352	0.09283	0.00000	0.02034
16	C1	DYY	0.01995	-0.01416	0.09836	0.00000	0.03849
17	C1	DZZ	-0.03213	0.00360	-0.04732	0.00000	-0.00515
18	C1	DXY	0.00483	-0.03832	-0.01021	0.00000	0.01545
19	C1	DXZ	0.00000	0.00000	0.00000	0.03802	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.00590	0.00000
21	C2	S	-0.02432	0.01250	-0.01235	0.00000	0.00038
22	C2	S	0.23309	-0.13136	-0.44045	0.00000	-0.00872
23	C2	PX	0.14915	-0.08899	-0.14426	0.00000	0.02245
24	C2	PY	-0.20283	0.37291	-0.04284	0.00000	0.11482
25	C2	PZ	0.00000	0.00000	0.00000	0.52192	0.00000
26	C2	S	-0.95006	0.51333	0.51529	0.00000	-0.50906
27	C2	PX	-0.26676	0.06782	0.15930	0.00000	-0.53367
28	C2	PY	-2.09369	-0.56957	0.25999	0.00000	-0.70642
29	C2	PZ	0.00000	0.00000	0.00000	-0.45809	0.00000
30	C2	DXX	0.01495	0.00506	-0.05273	0.00000	0.00287
31	C2	DYY	-0.01207	0.00797	-0.07586	0.00000	-0.03393
32	C2	DZZ	0.02464	-0.02008	0.00905	0.00000	0.00424
33	C2	DXY	0.00348	-0.01290	0.00779	0.00000	-0.03250
34	C2	DXZ	0.00000	0.00000	0.00000	0.03776	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.01545	0.00000
36	C3	S	-0.04843	0.00073	-0.02539	0.00000	0.02110
37	C3	S	0.02213	-0.11342	0.30004	0.00000	-0.34889
38	C3	PX	0.15506	0.22695	0.32955	0.00000	0.16207
39	C3	PY	0.21968	-0.13916	-0.00934	0.00000	0.26772
40	C3	PZ	0.00000	0.00000	0.00000	-0.17567	0.00000
41	C3	S	-0.13548	0.83370	0.37374	0.00000	-0.37391
42	C3	PX	2.01321	0.46891	-0.22206	0.00000	0.79824
43	C3	PY	0.65258	-0.32778	-0.28075	0.00000	0.51970
44	C3	PZ	0.00000	0.00000	0.00000	0.05192	0.00000
45	C3	DXX	-0.01428	0.03113	0.04425	0.00000	-0.03397
46	C3	DYY	-0.06752	-0.02452	0.00152	0.00000	-0.03018
47	C3	DZZ	0.03503	-0.01532	0.00423	0.00000	-0.00536
48	C3	DXY	-0.00181	0.00882	-0.02496	0.00000	-0.00983
49	C3	DXZ	0.00000	0.00000	0.00000	-0.00633	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.00382	0.00000
51	C4	S	-0.03276	-0.06260	0.02417	0.00000	0.03767
52	C4	S	0.14778	-0.21561	0.16713	0.00000	0.36071
53	C4	PX	-0.17058	-0.10221	0.47489	0.00000	-0.05910
54	C4	PY	-0.06217	-0.05891	-0.15641	0.00000	0.00090
55	C4	PZ	0.00000	0.00000	0.00000	-0.13304	0.00000
56	C4	S	-0.23467	0.48432	-0.01888	0.00000	-0.94272
57	C4	PX	-2.25359	0.10827	-0.43034	0.00000	-0.53566
58	C4	PY	0.87726	-0.26304	0.08399	0.00000	0.56644
59	C4	PZ	0.00000	0.00000	0.00000	0.15664	0.00000
60	C4	DXX	-0.00410	-0.09848	0.05014	0.00000	0.08308
61	C4	DYY	-0.01067	-0.08195	0.03831	0.00000	0.06555
62	C4	DZZ	0.02544	0.05163	-0.03002	0.00000	-0.02827

63	C4	DXY	-0.00859	-0.00233	0.02950	0.00000	-0.01393
64	C4	DXZ	0.00000	0.00000	0.00000	-0.02396	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.04343	0.00000
66	C5	S	0.03643	0.03050	-0.03962	0.00000	0.00419
67	C5	S	-0.11399	-0.20239	-0.17951	0.00000	0.21878
68	C5	PX	-0.18873	-0.35786	0.19478	0.00000	0.18830
69	C5	PY	0.03706	-0.07840	0.09287	0.00000	0.09043
70	C5	PZ	0.00000	0.00000	0.00000	0.34910	0.00000
71	C5	S	0.31822	0.18796	0.00758	0.00000	0.20500
72	C5	PX	-2.17471	0.26392	-0.09872	0.00000	-0.58656
73	C5	PY	-1.09997	0.38681	-0.10993	0.00000	-0.82696
74	C5	PZ	0.00000	0.00000	0.00000	-0.36986	0.00000
75	C5	DXX	0.01048	0.01401	-0.08805	0.00000	0.04865
76	C5	DYY	0.02344	-0.01159	-0.03673	0.00000	0.04422
77	C5	DZZ	-0.02968	-0.02197	0.03535	0.00000	-0.01261
78	C5	DXY	-0.01620	0.01461	-0.01332	0.00000	0.02549
79	C5	DXZ	0.00000	0.00000	0.00000	-0.00789	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.04401	0.00000
81	C6	S	0.04094	-0.03681	-0.01770	0.00000	-0.01616
82	C6	S	0.02709	-0.07084	-0.21298	0.00000	-0.31150
83	C6	PX	0.10103	0.16601	0.08935	0.00000	0.21875
84	C6	PY	-0.23438	0.17793	-0.06928	0.00000	0.27008
85	C6	PZ	0.00000	0.00000	0.00000	0.19291	0.00000
86	C6	S	-0.35749	-0.21110	0.39940	0.00000	0.56985
87	C6	PX	2.16678	0.35271	-0.29014	0.00000	0.75836
88	C6	PY	0.06968	0.05423	-0.06311	0.00000	0.00004
89	C6	PZ	0.00000	0.00000	0.00000	-0.16094	0.00000
90	C6	DXX	0.00014	-0.04478	-0.04952	0.00000	-0.07967
91	C6	DYY	0.06388	-0.03907	-0.02456	0.00000	-0.00960
92	C6	DZZ	-0.02595	0.02545	0.00944	0.00000	0.01055
93	C6	DXY	-0.00708	0.03447	0.01812	0.00000	0.00545
94	C6	DXZ	0.00000	0.00000	0.00000	-0.01418	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00633	0.00000
96	C7	S	-0.00847	0.02062	0.04291	0.00000	-0.07327
97	C7	S	-0.02395	0.32289	0.31458	0.00000	-0.21496
98	C7	PX	-0.08102	-0.12998	-0.00519	0.00000	-0.09502
99	C7	PY	-0.37477	-0.16599	-0.03836	0.00000	-0.09360
100	C7	PZ	0.00000	0.00000	0.00000	-0.37253	0.00000
101	C7	S	0.45781	-0.96314	-0.93216	0.00000	1.37585
102	C7	PX	-1.12290	0.09062	0.17322	0.00000	-0.83369
103	C7	PY	-0.05217	-0.66754	-0.44091	0.00000	-0.02639
104	C7	PZ	0.00000	0.00000	0.00000	0.45915	0.00000
105	C7	DXX	-0.01951	0.06174	0.06971	0.00000	-0.08984
106	C7	DYY	0.01966	0.04396	0.06946	0.00000	-0.07757
107	C7	DZZ	0.01182	-0.00930	-0.02655	0.00000	0.05414
108	C7	DXY	0.02986	-0.01744	-0.00031	0.00000	-0.00523
109	C7	DXZ	0.00000	0.00000	0.00000	0.02397	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.00462	0.00000
111	H3	S	-0.07233	-0.26365	0.20688	0.00000	0.12707
112	H3	S	0.28680	0.10060	0.01279	0.00000	0.01806
113	H3	PX	-0.01079	-0.01072	0.00341	0.00000	0.00650
114	H3	PY	0.00062	-0.01843	0.01285	0.00000	0.01273
115	H3	PZ	0.00000	0.00000	0.00000	0.00736	0.00000
116	H4	S	0.10487	0.03775	-0.10384	0.00000	0.02256

117	H4	S	-0.29569	-0.12719	-0.01740	0.00000	0.26542
118	H4	PX	-0.01109	0.00634	0.01296	0.00000	-0.00227
119	H4	PY	0.00297	0.00551	-0.00784	0.00000	0.00004
120	H4	PZ	0.00000	0.00000	0.00000	-0.00496	0.00000
121	N1	S	-0.00680	-0.00637	0.00814	0.00000	-0.01573
122	N1	S	0.03420	-0.01260	-0.03536	0.00000	0.06548
123	N1	PX	0.11476	0.00270	0.00582	0.00000	0.04804
124	N1	PY	0.17776	-0.07229	0.02057	0.00000	-0.08110
125	N1	PZ	0.00000	0.00000	0.00000	0.13991	0.00000
126	N1	S	0.25704	0.28200	-0.24964	0.00000	-0.12299
127	N1	PX	-0.42401	-0.01856	-0.04361	0.00000	-0.27302
128	N1	PY	0.45209	0.36673	-0.13182	0.00000	0.57814
129	N1	PZ	0.00000	0.00000	0.00000	-0.04811	0.00000
130	N1	DXX	-0.01365	0.01799	-0.00087	0.00000	0.03370
131	N1	DYY	-0.00675	-0.00684	-0.01325	0.00000	-0.05185
132	N1	DZZ	-0.00883	-0.01702	-0.00446	0.00000	0.03299
133	N1	DXY	0.04645	-0.02843	-0.00342	0.00000	-0.01304
134	N1	DXZ	0.00000	0.00000	0.00000	0.02228	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.01015	0.00000
136	H6	S	-0.01219	0.04159	-0.05781	0.00000	-0.03581
137	H6	S	-0.00984	-0.08132	-0.11236	0.00000	-0.32330
138	H6	PX	-0.00139	-0.00239	0.01533	0.00000	0.00079
139	H6	PY	-0.00615	-0.00417	0.00364	0.00000	0.00101
140	H6	PZ	0.00000	0.00000	0.00000	0.00086	0.00000
141	C8	S	0.02530	0.03682	0.00070	0.00000	0.06703
142	C8	S	-0.05389	0.50258	0.34689	0.00000	-0.13366
143	C8	PX	0.15586	-0.12928	0.09555	0.00000	-0.36102
144	C8	PY	-0.05744	0.04710	0.04662	0.00000	-0.08220
145	C8	PZ	0.00000	0.00000	0.00000	0.16039	0.00000
146	C8	S	-0.18596	-1.02517	-0.47459	0.00000	-0.51090
147	C8	PX	-1.09166	-0.19790	-0.10899	0.00000	-0.66399
148	C8	PY	-0.34133	0.33978	0.26550	0.00000	0.13407
149	C8	PZ	0.00000	0.00000	0.00000	-0.22468	0.00000
150	C8	DXX	0.02613	0.06572	0.03360	0.00000	-0.01821
151	C8	DYY	0.01399	0.09046	0.03951	0.00000	0.06569
152	C8	DZZ	-0.01855	-0.01671	0.00292	0.00000	-0.03456
153	C8	DXY	0.01417	0.02237	0.00703	0.00000	-0.00203
154	C8	DXZ	0.00000	0.00000	0.00000	-0.02153	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	-0.03083	0.00000
156	H8	S	-0.03991	0.14197	0.21492	0.00000	-0.23416
157	H8	S	0.67699	-0.08312	-0.08339	0.00000	0.36346
158	H8	PX	-0.00998	0.00958	0.01275	0.00000	-0.02520
159	H8	PY	0.00609	-0.01824	-0.01772	0.00000	0.00061
160	H8	PZ	0.00000	0.00000	0.00000	-0.00007	0.00000
161	C10	S	-0.00641	0.00398	0.00904	0.00000	-0.02119
162	C10	S	0.04377	0.39121	0.17676	0.00000	0.27140
163	C10	PX	0.13453	0.00494	0.04535	0.00000	-0.16104
164	C10	PY	0.02747	0.19926	0.02907	0.00000	0.37758
165	C10	PZ	0.00000	0.00000	0.00000	0.34115	0.00000
166	C10	S	-0.24455	-0.17521	-0.04456	0.00000	-0.05458
167	C10	PX	-0.03174	0.17312	-0.08448	0.00000	0.83573
168	C10	PY	-0.20942	0.17637	0.15154	0.00000	-0.30384
169	C10	PZ	0.00000	0.00000	0.00000	-0.30962	0.00000
170	C10	DXX	-0.01142	0.06902	0.03575	0.00000	0.01958

171	C10	DYY	0.00155	0.03582	0.02595	0.00000	-0.00213
172	C10	DZZ	0.00465	-0.00774	-0.00954	0.00000	0.02194
173	C10	DXY	-0.05385	-0.01824	-0.01393	0.00000	-0.00442
174	C10	DXZ	0.00000	0.00000	0.00000	0.00760	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.01940	0.00000
176	H16	S	0.16347	0.14141	0.12804	0.00000	-0.11169
177	H16	S	-0.15679	-0.03245	0.04932	0.00000	-0.38744
178	H16	PX	-0.01158	0.01554	0.00217	0.00000	0.02350
179	H16	PY	-0.01642	-0.00629	-0.00842	0.00000	-0.00004
180	H16	PZ	0.00000	0.00000	0.00000	0.00567	0.00000
181	H18	S	-0.21554	0.10435	0.02761	0.00000	0.05325
182	H18	S	0.08728	0.25657	0.03090	0.00000	0.42769
183	H18	PX	-0.00379	-0.01009	-0.00833	0.00000	0.00776
184	H18	PY	0.01935	-0.00598	0.00054	0.00000	-0.00079
185	H18	PZ	0.00000	0.00000	0.00000	0.00229	0.00000

MO:	66	67	68	69	70
Eigenvalues:	0.83599	0.83701	0.87468	0.88089	0.89452
(ev):	22.74835	22.77633	23.80135	23.97035	24.34108

		A	A	A	A	A	
1	H1	S	0.00000	0.20055	0.00000	0.14232	0.00000
2	H1	S	0.00000	-0.11086	0.00000	-0.14291	0.00000
3	H1	PX	0.00000	0.00531	0.00000	0.01066	0.00000
4	H1	PY	0.00000	0.00166	0.00000	-0.00683	0.00000
5	H1	PZ	-0.00546	0.00000	0.00406	0.00000	-0.00071
6	C1	S	0.00000	0.02281	0.00000	0.05224	0.00000
7	C1	S	0.00000	-0.10687	0.00000	-0.02612	0.00000
8	C1	PX	0.00000	0.15149	0.00000	0.11407	0.00000
9	C1	PY	0.00000	0.07182	0.00000	-0.09651	0.00000
10	C1	PZ	0.16669	0.00000	-0.01395	0.00000	0.52113
11	C1	S	0.00000	-0.28064	0.00000	-0.50442	0.00000
12	C1	PX	0.00000	-0.00263	0.00000	0.27558	0.00000
13	C1	PY	0.00000	-0.99505	0.00000	-0.31963	0.00000
14	C1	PZ	-0.15049	0.00000	-0.07650	0.00000	-0.73907
15	C1	DXX	0.00000	0.03634	0.00000	0.03473	0.00000
16	C1	DYY	0.00000	-0.02185	0.00000	0.06406	0.00000
17	C1	DZZ	0.00000	-0.02489	0.00000	-0.04050	0.00000
18	C1	DXY	0.00000	0.01447	0.00000	-0.01660	0.00000
19	C1	DXZ	-0.02963	0.00000	0.01591	0.00000	-0.01003
20	C1	DYZ	0.03202	0.00000	0.00543	0.00000	-0.01361
21	C2	S	0.00000	-0.00282	0.00000	0.05035	0.00000
22	C2	S	0.00000	0.32734	0.00000	0.04501	0.00000
23	C2	PX	0.00000	-0.02360	0.00000	-0.09239	0.00000
24	C2	PY	0.00000	0.20807	0.00000	-0.10213	0.00000
25	C2	PZ	-0.27576	0.00000	0.17101	0.00000	0.55619
26	C2	S	0.00000	0.54544	0.00000	-0.33323	0.00000
27	C2	PX	0.00000	0.83284	0.00000	-0.17832	0.00000
28	C2	PY	0.00000	1.53212	0.00000	0.20514	0.00000
29	C2	PZ	0.26295	0.00000	-0.27645	0.00000	-0.80710
30	C2	DXX	0.00000	0.06294	0.00000	0.03290	0.00000
31	C2	DYY	0.00000	0.03194	0.00000	0.08164	0.00000
32	C2	DZZ	0.00000	-0.00554	0.00000	-0.03814	0.00000
33	C2	DXY	0.00000	-0.01728	0.00000	0.01187	0.00000

34	C2	DXZ	-0.01613	0.00000	0.03340	0.00000	0.00266
35	C2	DYZ	0.02251	0.00000	0.03468	0.00000	-0.01284
36	C3	S	0.00000	-0.06709	0.00000	-0.01104	0.00000
37	C3	S	0.00000	-0.15839	0.00000	0.09521	0.00000
38	C3	PX	0.00000	0.11752	0.00000	0.06427	0.00000
39	C3	PY	0.00000	-0.04420	0.00000	0.21209	0.00000
40	C3	PZ	-0.30209	0.00000	-0.12239	0.00000	-0.07142
41	C3	S	0.00000	1.54306	0.00000	0.02160	0.00000
42	C3	PX	0.00000	-1.32054	0.00000	-0.34329	0.00000
43	C3	PY	0.00000	-0.84248	0.00000	-0.17328	0.00000
44	C3	PZ	0.26232	0.00000	0.09488	0.00000	0.16903
45	C3	DXX	0.00000	-0.09110	0.00000	-0.00772	0.00000
46	C3	DYY	0.00000	-0.04627	0.00000	0.02279	0.00000
47	C3	DZZ	0.00000	0.04646	0.00000	0.00729	0.00000
48	C3	DXY	0.00000	-0.00364	0.00000	-0.00348	0.00000
49	C3	DXZ	0.01060	0.00000	0.00603	0.00000	-0.00662
50	C3	DYZ	0.02013	0.00000	-0.04260	0.00000	0.02935
51	C4	S	0.00000	-0.00608	0.00000	-0.04227	0.00000
52	C4	S	0.00000	0.38371	0.00000	-0.11712	0.00000
53	C4	PX	0.00000	-0.16223	0.00000	0.26490	0.00000
54	C4	PY	0.00000	0.02338	0.00000	-0.19198	0.00000
55	C4	PZ	0.57755	0.00000	-0.32873	0.00000	-0.33756
56	C4	S	0.00000	-0.36671	0.00000	0.61047	0.00000
57	C4	PX	0.00000	1.00015	0.00000	0.07520	0.00000
58	C4	PY	0.00000	-0.86988	0.00000	-0.19017	0.00000
59	C4	PZ	-0.61064	0.00000	0.52083	0.00000	0.42013
60	C4	DXX	0.00000	0.02924	0.00000	-0.05101	0.00000
61	C4	DYY	0.00000	0.07328	0.00000	-0.07426	0.00000
62	C4	DZZ	0.00000	0.00036	0.00000	0.03522	0.00000
63	C4	DXY	0.00000	0.03448	0.00000	0.01735	0.00000
64	C4	DXZ	-0.01772	0.00000	-0.01448	0.00000	0.04242
65	C4	DYZ	-0.03650	0.00000	-0.00259	0.00000	-0.00950
66	C5	S	0.00000	0.06061	0.00000	-0.03861	0.00000
67	C5	S	0.00000	0.37205	0.00000	-0.11149	0.00000
68	C5	PX	0.00000	-0.07039	0.00000	-0.24202	0.00000
69	C5	PY	0.00000	0.10652	0.00000	-0.19766	0.00000
70	C5	PZ	0.18310	0.00000	0.53025	0.00000	-0.49041
71	C5	S	0.00000	-1.70309	0.00000	0.43218	0.00000
72	C5	PX	0.00000	1.29060	0.00000	0.40601	0.00000
73	C5	PY	0.00000	1.01284	0.00000	0.14072	0.00000
74	C5	PZ	-0.12685	0.00000	-0.67911	0.00000	0.65708
75	C5	DXX	0.00000	0.09289	0.00000	-0.04702	0.00000
76	C5	DYY	0.00000	0.10681	0.00000	-0.07467	0.00000
77	C5	DZZ	0.00000	-0.05648	0.00000	0.03144	0.00000
78	C5	DXY	0.00000	-0.04313	0.00000	-0.01582	0.00000
79	C5	DXZ	0.03430	0.00000	0.00367	0.00000	-0.04153
80	C5	DYZ	0.00457	0.00000	-0.03828	0.00000	-0.01207
81	C6	S	0.00000	-0.00495	0.00000	0.00123	0.00000
82	C6	S	0.00000	-0.35410	0.00000	0.02761	0.00000
83	C6	PX	0.00000	-0.43917	0.00000	-0.19788	0.00000
84	C6	PY	0.00000	0.01311	0.00000	0.24924	0.00000
85	C6	PZ	-0.39316	0.00000	-0.56031	0.00000	-0.04509
86	C6	S	0.00000	0.71989	0.00000	0.00188	0.00000
87	C6	PX	0.00000	-1.30302	0.00000	0.00726	0.00000

88	C6	PY	0.00000	-0.41065	0.00000	-0.08424	0.00000
89	C6	PZ	0.33809	0.00000	0.79605	0.00000	0.17120
90	C6	DXX	0.00000	-0.07410	0.00000	0.00325	0.00000
91	C6	DYY	0.00000	-0.03062	0.00000	0.02403	0.00000
92	C6	DZZ	0.00000	0.00703	0.00000	-0.00430	0.00000
93	C6	DXY	0.00000	0.00666	0.00000	-0.00514	0.00000
94	C6	DXZ	-0.00328	0.00000	-0.00138	0.00000	0.00345
95	C6	DYZ	-0.02061	0.00000	0.02021	0.00000	0.00633
96	C7	S	0.00000	0.05248	0.00000	-0.00212	0.00000
97	C7	S	0.00000	-0.05708	0.00000	-0.00320	0.00000
98	C7	PX	0.00000	0.06606	0.00000	-0.04018	0.00000
99	C7	PY	0.00000	-0.04466	0.00000	0.01517	0.00000
100	C7	PZ	-0.36241	0.00000	0.52867	0.00000	-0.21095
101	C7	S	0.00000	-1.42772	0.00000	-0.01715	0.00000
102	C7	PX	0.00000	1.13778	0.00000	0.27458	0.00000
103	C7	PY	0.00000	-0.19293	0.00000	-0.00754	0.00000
104	C7	PZ	0.33142	0.00000	-0.79236	0.00000	0.07472
105	C7	DXX	0.00000	0.02924	0.00000	0.03616	0.00000
106	C7	DYY	0.00000	0.00599	0.00000	-0.04151	0.00000
107	C7	DZZ	0.00000	-0.01575	0.00000	0.00180	0.00000
108	C7	DXY	0.00000	-0.02913	0.00000	-0.01761	0.00000
109	C7	DXZ	0.01769	0.00000	-0.03219	0.00000	0.00798
110	C7	DYZ	-0.00664	0.00000	0.00908	0.00000	-0.00156
111	H3	S	0.00000	0.19336	0.00000	-0.17011	0.00000
112	H3	S	0.00000	0.19096	0.00000	0.05687	0.00000
113	H3	PX	0.00000	0.00694	0.00000	-0.00434	0.00000
114	H3	PY	0.00000	0.00892	0.00000	-0.01328	0.00000
115	H3	PZ	-0.00246	0.00000	-0.00398	0.00000	-0.00016
116	H4	S	0.00000	0.40178	0.00000	-0.16205	0.00000
117	H4	S	0.00000	-0.08079	0.00000	0.04049	0.00000
118	H4	PX	0.00000	-0.00888	0.00000	0.00756	0.00000
119	H4	PY	0.00000	0.02242	0.00000	-0.01093	0.00000
120	H4	PZ	0.00048	0.00000	-0.00492	0.00000	-0.00082
121	N1	S	0.00000	0.00915	0.00000	-0.01488	0.00000
122	N1	S	0.00000	0.00693	0.00000	0.04598	0.00000
123	N1	PX	0.00000	-0.00587	0.00000	0.07943	0.00000
124	N1	PY	0.00000	-0.04256	0.00000	-0.07013	0.00000
125	N1	PZ	-0.06538	0.00000	-0.18773	0.00000	0.06906
126	N1	S	0.00000	-0.86845	0.00000	-0.15173	0.00000
127	N1	PX	0.00000	0.00823	0.00000	-0.08686	0.00000
128	N1	PY	0.00000	-0.74596	0.00000	0.06801	0.00000
129	N1	PZ	-0.01559	0.00000	-0.06651	0.00000	-0.21476
130	N1	DXX	0.00000	-0.02254	0.00000	0.00381	0.00000
131	N1	DYY	0.00000	-0.01756	0.00000	-0.04320	0.00000
132	N1	DZZ	0.00000	0.03827	0.00000	0.02264	0.00000
133	N1	DXY	0.00000	0.01318	0.00000	0.01978	0.00000
134	N1	DXZ	-0.01319	0.00000	-0.03617	0.00000	0.00032
135	N1	DYZ	-0.00618	0.00000	-0.02831	0.00000	0.00497
136	H6	S	0.00000	0.19945	0.00000	0.13078	0.00000
137	H6	S	0.00000	0.43021	0.00000	-0.07836	0.00000
138	H6	PX	0.00000	-0.00596	0.00000	-0.00886	0.00000
139	H6	PY	0.00000	0.00543	0.00000	-0.00277	0.00000
140	H6	PZ	-0.00085	0.00000	-0.00928	0.00000	0.00251
141	C8	S	0.00000	-0.00031	0.00000	0.05529	0.00000

142	C8	S	0.00000	-0.01722	0.00000	-0.44679	0.00000
143	C8	PX	0.00000	0.22020	0.00000	0.13866	0.00000
144	C8	PY	0.00000	-0.07494	0.00000	0.22849	0.00000
145	C8	PZ	-0.11181	0.00000	-0.35690	0.00000	-0.44388
146	C8	S	0.00000	0.35443	0.00000	0.26802	0.00000
147	C8	PX	0.00000	0.62351	0.00000	-0.09761	0.00000
148	C8	PY	0.00000	0.81283	0.00000	0.24928	0.00000
149	C8	PZ	0.11319	0.00000	0.59988	0.00000	0.65560
150	C8	DXX	0.00000	-0.01768	0.00000	-0.06711	0.00000
151	C8	DYY	0.00000	0.01161	0.00000	0.08250	0.00000
152	C8	DZZ	0.00000	0.00022	0.00000	-0.03830	0.00000
153	C8	DXY	0.00000	-0.01543	0.00000	-0.01328	0.00000
154	C8	DXZ	-0.00999	0.00000	0.02066	0.00000	-0.00872
155	C8	DYZ	-0.04163	0.00000	0.01911	0.00000	-0.01519
156	H8	S	0.00000	0.24636	0.00000	0.10738	0.00000
157	H8	S	0.00000	-0.59047	0.00000	-0.25350	0.00000
158	H8	PX	0.00000	0.01609	0.00000	0.01113	0.00000
159	H8	PY	0.00000	-0.00899	0.00000	-0.00444	0.00000
160	H8	PZ	-0.00262	0.00000	-0.00824	0.00000	-0.00383
161	C10	S	0.00000	0.00397	0.00000	-0.07419	0.00000
162	C10	S	0.00000	0.08857	0.00000	-0.27981	0.00000
163	C10	PX	0.00000	0.06888	0.00000	0.03772	0.00000
164	C10	PY	0.00000	0.08145	0.00000	0.43199	0.00000
165	C10	PZ	0.56387	0.00000	0.08735	0.00000	0.34323
166	C10	S	0.00000	0.34978	0.00000	1.25121	0.00000
167	C10	PX	0.00000	-0.43675	0.00000	-0.06015	0.00000
168	C10	PY	0.00000	0.13665	0.00000	-0.37254	0.00000
169	C10	PZ	-0.60810	0.00000	-0.20054	0.00000	-0.52027
170	C10	DXX	0.00000	0.02057	0.00000	-0.09628	0.00000
171	C10	DYY	0.00000	0.01595	0.00000	-0.13795	0.00000
172	C10	DZZ	0.00000	-0.00171	0.00000	0.07351	0.00000
173	C10	DXY	0.00000	0.02671	0.00000	0.02246	0.00000
174	C10	DXZ	0.00511	0.00000	-0.01296	0.00000	0.00410
175	C10	DYZ	0.00615	0.00000	-0.02530	0.00000	-0.01495
176	H16	S	0.00000	0.00356	0.00000	-0.39026	0.00000
177	H16	S	0.00000	0.29143	0.00000	-0.03889	0.00000
178	H16	PX	0.00000	-0.00251	0.00000	-0.00818	0.00000
179	H16	PY	0.00000	0.00043	0.00000	0.01575	0.00000
180	H16	PZ	0.00959	0.00000	0.00064	0.00000	0.00519
181	H18	S	0.00000	0.04317	0.00000	-0.31767	0.00000
182	H18	S	0.00000	-0.27906	0.00000	-0.22393	0.00000
183	H18	PX	0.00000	-0.01317	0.00000	0.00337	0.00000
184	H18	PY	0.00000	-0.00511	0.00000	0.01219	0.00000
185	H18	PZ	0.00749	0.00000	0.00713	0.00000	0.00333

MO:	71	72	73	74	75
Eigenvalues:	0.90242	0.91918	0.94821	0.98293	0.98712
(ev):	24.55622	25.01221	25.80209	26.74691	26.86081

		A	A	A	A	A	
1	H1	S	0.10876	-0.32127	0.00000	0.00000	-0.04656
2	H1	S	-0.28532	0.23389	0.00000	0.00000	-0.02970
3	H1	PX	0.00962	-0.02198	0.00000	0.00000	-0.00526
4	H1	PY	-0.00034	0.00576	0.00000	0.00000	-0.01844

5	H1	PZ	0.00000	0.00000	0.00500	-0.01694	0.00000
6	C1	S	0.02685	-0.07254	0.00000	0.00000	-0.00510
7	C1	S	0.04034	-0.14989	0.00000	0.00000	-0.01351
8	C1	PX	0.06391	-0.15448	0.00000	0.00000	-0.00016
9	C1	PY	-0.09683	0.34820	0.00000	0.00000	0.04053
10	C1	PZ	0.00000	0.00000	0.26789	0.47586	0.00000
11	C1	S	-0.61499	0.97571	0.00000	0.00000	-0.48385
12	C1	PX	0.34426	-0.20229	0.00000	0.00000	0.21290
13	C1	PY	-1.27150	0.25796	0.00000	0.00000	-0.59206
14	C1	PZ	0.00000	0.00000	-0.35703	-0.93196	0.00000
15	C1	DXX	0.05916	-0.11926	0.00000	0.00000	-0.01577
16	C1	DYY	0.00392	-0.08383	0.00000	0.00000	-0.02170
17	C1	DZZ	-0.03984	0.07316	0.00000	0.00000	0.01120
18	C1	DXY	0.01299	0.01594	0.00000	0.00000	-0.01380
19	C1	DXZ	0.00000	0.00000	0.01649	-0.02479	0.00000
20	C1	DYZ	0.00000	0.00000	-0.03827	-0.01701	0.00000
21	C2	S	-0.07530	0.00593	0.00000	0.00000	0.02445
22	C2	S	-0.13280	-0.15014	0.00000	0.00000	0.17521
23	C2	PX	0.12504	-0.07795	0.00000	0.00000	0.00212
24	C2	PY	0.41878	0.09689	0.00000	0.00000	0.02661
25	C2	PZ	0.00000	0.00000	-0.41350	0.13724	0.00000
26	C2	S	0.99729	0.33617	0.00000	0.00000	-0.38110
27	C2	PX	0.17678	0.16989	0.00000	0.00000	-0.43104
28	C2	PY	0.78658	-0.98130	0.00000	0.00000	0.19883
29	C2	PZ	0.00000	0.00000	0.74379	-0.22262	0.00000
30	C2	DXX	-0.11837	0.02052	0.00000	0.00000	0.04397
31	C2	DYY	-0.08868	-0.02198	0.00000	0.00000	0.03057
32	C2	DZZ	0.07305	-0.02951	0.00000	0.00000	-0.02539
33	C2	DXY	-0.02516	-0.02191	0.00000	0.00000	-0.04152
34	C2	DXZ	0.00000	0.00000	-0.01556	0.02452	0.00000
35	C2	DYZ	0.00000	0.00000	0.01489	0.00025	0.00000
36	C3	S	0.01512	-0.01762	0.00000	0.00000	0.00224
37	C3	S	0.28245	-0.09035	0.00000	0.00000	0.16469
38	C3	PX	-0.11123	0.01728	0.00000	0.00000	-0.16227
39	C3	PY	0.14009	-0.43986	0.00000	0.00000	-0.15604
40	C3	PZ	0.00000	0.00000	0.56025	-0.43775	0.00000
41	C3	S	-0.19674	0.39895	0.00000	0.00000	-0.00414
42	C3	PX	-1.20394	0.43716	0.00000	0.00000	-0.11136
43	C3	PY	-0.53668	0.20398	0.00000	0.00000	0.41881
44	C3	PZ	0.00000	0.00000	-0.81917	0.70397	0.00000
45	C3	DXX	0.05673	-0.00966	0.00000	0.00000	-0.00774
46	C3	DYY	0.06572	-0.04906	0.00000	0.00000	0.02983
47	C3	DZZ	-0.02209	0.00401	0.00000	0.00000	0.00131
48	C3	DXY	-0.03233	-0.00198	0.00000	0.00000	-0.05777
49	C3	DXZ	0.00000	0.00000	-0.00520	0.03007	0.00000
50	C3	DYZ	0.00000	0.00000	0.04364	0.04918	0.00000
51	C4	S	-0.02588	0.06250	0.00000	0.00000	0.00060
52	C4	S	0.30672	-0.13451	0.00000	0.00000	-0.03888
53	C4	PX	-0.20928	-0.11462	0.00000	0.00000	0.08053
54	C4	PY	-0.06920	0.27754	0.00000	0.00000	-0.00945
55	C4	PZ	0.00000	0.00000	-0.54962	-0.25052	0.00000
56	C4	S	0.06395	-0.10772	0.00000	0.00000	0.22574
57	C4	PX	1.53652	-0.71437	0.00000	0.00000	0.51758
58	C4	PY	-0.85746	0.34225	0.00000	0.00000	-0.14771

59	C4	PZ	0.00000	0.00000	0.96411	0.57750	0.00000
60	C4	DXX	0.01262	0.06173	0.00000	0.00000	0.00302
61	C4	DYY	0.00886	0.05909	0.00000	0.00000	-0.02407
62	C4	DZZ	0.02673	-0.06353	0.00000	0.00000	0.00289
63	C4	DXY	-0.01612	-0.04124	0.00000	0.00000	-0.03349
64	C4	DXZ	0.00000	0.00000	0.01263	-0.00172	0.00000
65	C4	DYZ	0.00000	0.00000	0.01893	-0.02192	0.00000
66	C5	S	0.06101	-0.00271	0.00000	0.00000	-0.02373
67	C5	S	-0.20009	0.28110	0.00000	0.00000	0.06868
68	C5	PX	0.03816	0.26816	0.00000	0.00000	-0.01188
69	C5	PY	0.29835	0.01844	0.00000	0.00000	0.10344
70	C5	PZ	0.00000	0.00000	0.44202	0.11930	0.00000
71	C5	S	-0.16770	-0.34542	0.00000	0.00000	0.35500
72	C5	PX	1.18343	-1.06551	0.00000	0.00000	0.50113
73	C5	PY	0.71700	-0.44402	0.00000	0.00000	-0.43942
74	C5	PZ	0.00000	0.00000	-0.90052	-0.23238	0.00000
75	C5	DXX	0.05139	0.02704	0.00000	0.00000	0.00478
76	C5	DYY	0.04365	0.03569	0.00000	0.00000	-0.03185
77	C5	DZZ	-0.06117	0.01035	0.00000	0.00000	0.01357
78	C5	DXY	0.06183	0.01568	0.00000	0.00000	0.04977
79	C5	DXZ	0.00000	0.00000	-0.00787	0.00596	0.00000
80	C5	DYZ	0.00000	0.00000	0.02149	-0.01645	0.00000
81	C6	S	0.00840	-0.00476	0.00000	0.00000	0.05463
82	C6	S	-0.18320	0.07920	0.00000	0.00000	-0.08835
83	C6	PX	0.19225	0.01231	0.00000	0.00000	0.02517
84	C6	PY	-0.22361	0.13923	0.00000	0.00000	0.48162
85	C6	PZ	0.00000	0.00000	0.03324	-0.30240	0.00000
86	C6	S	-0.06381	-0.64071	0.00000	0.00000	0.32353
87	C6	PX	-1.36787	0.75741	0.00000	0.00000	-0.20264
88	C6	PY	0.45952	-0.55305	0.00000	0.00000	-0.55792
89	C6	PZ	0.00000	0.00000	-0.07166	0.35246	0.00000
90	C6	DXX	-0.02636	0.01159	0.00000	0.00000	-0.02266
91	C6	DYY	-0.00654	0.00916	0.00000	0.00000	0.15849
92	C6	DZZ	-0.01113	0.00224	0.00000	0.00000	-0.05903
93	C6	DXY	0.03932	0.01856	0.00000	0.00000	0.06370
94	C6	DXZ	0.00000	0.00000	0.01467	-0.03138	0.00000
95	C6	DYZ	0.00000	0.00000	-0.02461	0.01161	0.00000
96	C7	S	-0.01634	0.05513	0.00000	0.00000	-0.00059
97	C7	S	0.31477	0.21456	0.00000	0.00000	0.08812
98	C7	PX	-0.18936	-0.11211	0.00000	0.00000	-0.12482
99	C7	PY	0.08389	-0.14982	0.00000	0.00000	0.10342
100	C7	PZ	0.00000	0.00000	-0.48330	-0.09699	0.00000
101	C7	S	-0.65194	-0.42519	0.00000	0.00000	0.09534
102	C7	PX	0.76867	0.30553	0.00000	0.00000	0.49429
103	C7	PY	0.42592	-0.45872	0.00000	0.00000	-0.51400
104	C7	PZ	0.00000	0.00000	0.82834	0.24976	0.00000
105	C7	DXX	0.00153	0.09548	0.00000	0.00000	-0.04978
106	C7	DYY	0.01528	0.09186	0.00000	0.00000	0.04103
107	C7	DZZ	0.01912	-0.06404	0.00000	0.00000	0.00785
108	C7	DXY	0.02422	-0.02579	0.00000	0.00000	-0.01177
109	C7	DXZ	0.00000	0.00000	0.01569	-0.00171	0.00000
110	C7	DYZ	0.00000	0.00000	0.00983	-0.03151	0.00000
111	H3	S	-0.09476	0.19325	0.00000	0.00000	-0.05742
112	H3	S	0.22203	-0.07424	0.00000	0.00000	0.00563

113	H3	PX	0.00867	-0.00491	0.00000	0.00000	0.00521
114	H3	PY	-0.00722	0.01400	0.00000	0.00000	-0.01027
115	H3	PZ	0.00000	0.00000	0.01013	0.00047	0.00000
116	H4	S	0.13370	-0.00784	0.00000	0.00000	-0.18100
117	H4	S	-0.02701	0.09486	0.00000	0.00000	0.50607
118	H4	PX	0.01020	-0.00592	0.00000	0.00000	0.01753
119	H4	PY	0.00835	0.00330	0.00000	0.00000	-0.02376
120	H4	PZ	0.00000	0.00000	0.00089	-0.00639	0.00000
121	N1	S	-0.00097	-0.00443	0.00000	0.00000	-0.02681
122	N1	S	-0.04128	0.01058	0.00000	0.00000	0.04286
123	N1	PX	0.22851	0.08362	0.00000	0.00000	0.66019
124	N1	PY	0.01241	0.04346	0.00000	0.00000	0.21896
125	N1	PZ	0.00000	0.00000	-0.05079	0.12473	0.00000
126	N1	S	0.34193	0.10500	0.00000	0.00000	-1.12902
127	N1	PX	0.21058	-0.11400	0.00000	0.00000	-0.91734
128	N1	PY	-0.42210	0.26459	0.00000	0.00000	0.10142
129	N1	PZ	0.00000	0.00000	0.09342	0.03610	0.00000
130	N1	DXX	-0.01695	0.01643	0.00000	0.00000	-0.09168
131	N1	DYY	-0.00195	-0.00648	0.00000	0.00000	-0.18552
132	N1	DZZ	-0.02445	-0.02003	0.00000	0.00000	0.05889
133	N1	DXY	-0.01086	-0.01825	0.00000	0.00000	0.00280
134	N1	DXZ	0.00000	0.00000	-0.01540	0.03098	0.00000
135	N1	DYZ	0.00000	0.00000	0.01779	-0.03103	0.00000
136	H6	S	-0.35328	0.03459	0.00000	0.00000	0.02741
137	H6	S	0.20375	-0.12044	0.00000	0.00000	-0.27696
138	H6	PX	0.02639	-0.00343	0.00000	0.00000	-0.00210
139	H6	PY	0.00272	0.00770	0.00000	0.00000	0.00221
140	H6	PZ	0.00000	0.00000	0.00707	-0.00849	0.00000
141	C8	S	0.01811	0.02930	0.00000	0.00000	0.00747
142	C8	S	-0.14889	0.12998	0.00000	0.00000	-0.25959
143	C8	PX	-0.01884	0.11789	0.00000	0.00000	0.26527
144	C8	PY	0.14152	0.39160	0.00000	0.00000	-0.39673
145	C8	PZ	0.00000	0.00000	0.01280	0.75053	0.00000
146	C8	S	0.29980	-0.28144	0.00000	0.00000	1.07337
147	C8	PX	0.87934	-0.31771	0.00000	0.00000	-0.86084
148	C8	PY	-0.10697	-0.37678	0.00000	0.00000	1.10883
149	C8	PZ	0.00000	0.00000	-0.14284	-1.30499	0.00000
150	C8	DXX	0.03114	0.02333	0.00000	0.00000	0.03093
151	C8	DYY	0.00887	0.08287	0.00000	0.00000	-0.00947
152	C8	DZZ	-0.02792	-0.02111	0.00000	0.00000	-0.02704
153	C8	DXY	0.00873	0.00676	0.00000	0.00000	-0.09493
154	C8	DXZ	0.00000	0.00000	-0.00081	-0.00825	0.00000
155	C8	DYZ	0.00000	0.00000	-0.04355	0.04624	0.00000
156	H8	S	-0.13030	0.19321	0.00000	0.00000	-0.03565
157	H8	S	-0.07093	-0.37859	0.00000	0.00000	-0.28333
158	H8	PX	0.00216	0.02285	0.00000	0.00000	0.00664
159	H8	PY	0.00321	-0.02446	0.00000	0.00000	-0.01140
160	H8	PZ	0.00000	0.00000	0.00994	0.00877	0.00000
161	C10	S	-0.03410	-0.04966	0.00000	0.00000	0.02875
162	C10	S	-0.32541	-0.23891	0.00000	0.00000	0.19323
163	C10	PX	0.09463	0.03345	0.00000	0.00000	-0.01351
164	C10	PY	0.01622	0.18530	0.00000	0.00000	-0.11536
165	C10	PZ	0.00000	0.00000	0.14498	-0.28426	0.00000
166	C10	S	0.74055	0.66318	0.00000	0.00000	-0.13044

167	C10	PX	-0.51956	-0.05211	0.00000	0.00000	0.13273
168	C10	PY	-0.04689	-0.20170	0.00000	0.00000	0.08102
169	C10	PZ	0.00000	0.00000	-0.16222	0.68871	0.00000
170	C10	DXX	-0.07177	-0.06723	0.00000	0.00000	0.02556
171	C10	DYY	-0.07487	-0.11138	0.00000	0.00000	0.07436
172	C10	DZZ	0.02591	0.04635	0.00000	0.00000	-0.02854
173	C10	DXY	-0.00591	-0.01468	0.00000	0.00000	0.00824
174	C10	DXZ	0.00000	0.00000	0.01515	0.00298	0.00000
175	C10	DYZ	0.00000	0.00000	0.01647	0.00050	0.00000
176	H16	S	-0.18744	-0.18747	0.00000	0.00000	0.13453
177	H16	S	0.13517	-0.08214	0.00000	0.00000	0.01928
178	H16	PX	-0.01526	-0.00799	0.00000	0.00000	-0.00931
179	H16	PY	0.01347	0.00554	0.00000	0.00000	-0.02469
180	H16	PZ	0.00000	0.00000	0.00164	0.00890	0.00000
181	H18	S	-0.22753	-0.28233	0.00000	0.00000	0.05411
182	H18	S	-0.30220	-0.08322	0.00000	0.00000	0.02499
183	H18	PX	0.00450	0.00525	0.00000	0.00000	0.00110
184	H18	PY	0.00309	0.01662	0.00000	0.00000	0.00837
185	H18	PZ	0.00000	0.00000	-0.00564	0.00552	0.00000

MO:	76	77	78	79	80
Eigenvalues:	1.04060	1.04963	1.05374	1.07556	1.08597
(ev):	28.31629	28.56182	28.67377	29.26760	29.55087

		A	A	A	A	A	
1	H1	S	0.00000	-0.00292	0.15600	-0.30413	0.13931
2	H1	S	0.00000	-0.41857	-0.87875	1.12984	-1.35907
3	H1	PX	0.00000	0.01999	0.05019	-0.07865	0.07335
4	H1	PY	0.00000	0.00757	0.01953	-0.01905	0.00279
5	H1	PZ	-0.02346	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.00543	0.01659	-0.01993	0.01890
7	C1	S	0.00000	0.04194	-0.15595	0.25187	-0.12598
8	C1	PX	0.00000	-0.17775	-0.27197	0.41358	-0.49004
9	C1	PY	0.00000	0.00103	0.07902	0.03971	-0.03986
10	C1	PZ	0.22148	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.05828	0.39462	-0.59413	-0.13261
12	C1	PX	0.00000	0.64702	1.03340	-1.02902	2.12878
13	C1	PY	0.00000	0.16296	0.00997	-0.05122	0.29149
14	C1	PZ	-0.86851	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.02417	0.05959	-0.13673	0.02891
16	C1	DYY	0.00000	-0.00668	-0.03426	0.08672	-0.02578
17	C1	DZZ	0.00000	-0.00968	-0.04410	0.05072	-0.02431
18	C1	DXY	0.00000	-0.01236	0.05243	0.03485	0.02720
19	C1	DXZ	-0.01280	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00761	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.00363	-0.00079	0.01019	0.02132
22	C2	S	0.00000	-0.21087	0.13334	-0.18399	-0.27640
23	C2	PX	0.00000	0.08826	-0.09186	0.14129	0.42885
24	C2	PY	0.00000	0.01332	-0.08303	0.05888	0.10374
25	C2	PZ	-0.36201	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.32410	0.00976	0.59425	-0.02360
27	C2	PX	0.00000	-0.55732	0.48233	-0.10193	-1.61724
28	C2	PY	0.00000	-0.05588	-0.05342	-0.26611	-0.62472
29	C2	PZ	1.06059	0.00000	0.00000	0.00000	0.00000

30	C2	DXX	0.00000	-0.01994	-0.00147	0.07489	0.09449
31	C2	DYY	0.00000	-0.02400	0.01734	-0.04759	-0.08746
32	C2	DZZ	0.00000	0.00891	0.00637	-0.02981	-0.04093
33	C2	DXY	0.00000	0.00884	0.00754	0.04927	-0.00718
34	C2	DXZ	-0.01199	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02713	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.00338	0.01577	0.01986	0.00218
37	C3	S	0.00000	0.11493	0.15901	0.17243	-0.09792
38	C3	PX	0.00000	0.02665	0.06770	-0.14665	0.18548
39	C3	PY	0.00000	-0.12569	0.12425	0.19534	-0.03448
40	C3	PZ	-0.67347	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	0.08420	1.05724	-0.48209	1.01177
42	C3	PX	0.00000	-0.38081	-0.46521	0.96597	-0.57250
43	C3	PY	0.00000	0.71516	-0.58062	-1.16437	0.26419
44	C3	PZ	1.66304	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.01881	-0.01210	-0.00823	-0.03483
46	C3	DYY	0.00000	0.00919	0.11848	0.03341	0.05837
47	C3	DZZ	0.00000	0.00272	-0.03184	0.00029	-0.01050
48	C3	DXY	0.00000	0.03562	-0.00803	-0.01703	0.03391
49	C3	DXZ	-0.00579	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00238	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00659	-0.00381	-0.03161	-0.01620
52	C4	S	0.00000	0.08223	-0.05131	0.24131	0.13485
53	C4	PX	0.00000	-0.11422	-0.00500	0.24575	0.21497
54	C4	PY	0.00000	-0.08485	0.15762	0.47874	0.33304
55	C4	PZ	-0.20681	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.18554	0.45395	0.00572	0.51882
57	C4	PX	0.00000	0.20723	-0.38304	-1.16762	-1.11907
58	C4	PY	0.00000	0.36863	-0.59825	-1.58387	-1.35344
59	C4	PZ	0.67088	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	-0.01775	-0.00803	0.08179	0.00269
61	C4	DYY	0.00000	0.03849	0.01386	-0.12242	-0.00868
62	C4	DZZ	0.00000	-0.00358	-0.00701	0.05256	0.01997
63	C4	DXY	0.00000	-0.00626	-0.02245	-0.07318	-0.08021
64	C4	DXZ	-0.00732	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.01247	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.00609	-0.00493	0.03089	-0.00226
67	C5	S	0.00000	0.02494	-0.00585	-0.12044	-0.04054
68	C5	PX	0.00000	-0.15534	-0.06666	0.28921	0.00443
69	C5	PY	0.00000	0.03821	0.03329	-0.43447	0.03574
70	C5	PZ	0.28920	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.35622	-0.40394	-0.26468	0.24348
72	C5	PX	0.00000	0.36488	-0.16407	-1.44039	-0.52317
73	C5	PY	0.00000	-0.51410	0.00240	1.56288	-0.41099
74	C5	PZ	-0.81008	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.01898	-0.01374	-0.03520	-0.04995
76	C5	DYY	0.00000	-0.01167	-0.02147	0.07843	0.04517
77	C5	DZZ	0.00000	0.00641	0.00797	-0.04114	-0.00109
78	C5	DXY	0.00000	0.01851	0.01052	-0.06472	0.04273
79	C5	DXZ	0.00040	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00108	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00158	-0.01207	-0.01499	-0.00987
82	C6	S	0.00000	-0.46520	0.19854	-0.29100	0.01396
83	C6	PX	0.00000	0.21487	-0.13046	-0.04744	-0.02449

84	C6	PY	0.00000	0.26060	-0.24335	-0.04298	-0.04573
85	C6	PZ	0.60710	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.37785	-0.04720	0.78329	-0.53699
87	C6	PX	0.00000	-0.50055	0.17336	0.70101	0.30592
88	C6	PY	0.00000	0.53555	-0.43840	0.56820	0.77449
89	C6	PZ	-1.50926	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.04827	0.00183	-0.00045	-0.05102
91	C6	DYY	0.00000	-0.09797	0.02840	-0.03807	0.02269
92	C6	DZZ	0.00000	0.01257	0.00551	-0.00600	0.01207
93	C6	DXY	0.00000	0.02404	-0.01848	0.03192	-0.00866
94	C6	DXZ	0.00988	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.04068	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.01705	0.03073	-0.00116	0.00434
97	C7	S	0.00000	-0.04724	-0.17405	0.23066	-0.22457
98	C7	PX	0.00000	-0.26351	-0.69643	-0.05664	-0.21872
99	C7	PY	0.00000	-0.13748	0.23162	0.15994	0.02934
100	C7	PZ	0.17540	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	1.01338	-0.27457	-0.87469	-0.33183
102	C7	PX	0.00000	0.37399	2.99524	0.17570	1.12445
103	C7	PY	0.00000	0.31218	-1.07381	-0.82528	-0.01212
104	C7	PZ	-0.76773	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.02933	0.06232	0.03632	-0.00665
106	C7	DYY	0.00000	0.03443	-0.04882	-0.02131	-0.04802
107	C7	DZZ	0.00000	-0.02477	-0.05588	0.01289	-0.00492
108	C7	DXY	0.00000	-0.02746	-0.01497	0.01574	-0.06104
109	C7	DXZ	0.01379	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.01014	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	-0.00050	-0.02529	-0.34993	-0.21613
112	H3	S	0.00000	-0.25523	0.35238	1.60489	1.15311
113	H3	PX	0.00000	0.00155	-0.00906	-0.05828	-0.02771
114	H3	PY	0.00000	0.01406	-0.01411	-0.08045	-0.06042
115	H3	PZ	0.00835	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00000	-0.06388	-0.01063	0.28597	-0.03449
117	H4	S	0.00000	0.37141	0.06907	-1.50467	0.04550
118	H4	PX	0.00000	0.00248	0.00109	-0.05996	-0.00658
119	H4	PY	0.00000	-0.02094	-0.01023	0.06721	-0.01084
120	H4	PZ	-0.01437	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00000	-0.05899	0.02618	-0.00756	0.00128
122	N1	S	0.00000	0.19496	-0.03495	-0.01027	-0.09316
123	N1	PX	0.00000	-0.33052	0.04979	0.01787	-0.02739
124	N1	PY	0.00000	-0.09679	-0.01945	-0.07736	0.01329
125	N1	PZ	0.15618	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00000	0.04733	-1.15100	-0.09080	0.96336
127	N1	PX	0.00000	1.10857	-0.65455	-0.06290	0.07650
128	N1	PY	0.00000	0.86752	-0.31978	0.35801	0.06942
129	N1	PZ	-0.02934	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00000	-0.06451	-0.01592	-0.04778	-0.01471
131	N1	DYY	0.00000	0.01589	0.01844	-0.00534	0.03521
132	N1	DZZ	0.00000	0.14205	-0.02863	0.03045	-0.03703
133	N1	DXY	0.00000	0.00885	0.03511	0.01310	-0.01560
134	N1	DXZ	0.02978	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.02788	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.00000	-0.01992	0.04772	0.13148	0.25655
137	H6	S	0.00000	-0.26884	0.29450	-0.39754	-1.33941

138	H6	PX	0.00000	-0.01315	0.01173	-0.03384	-0.07898
139	H6	PY	0.00000	-0.02703	0.00139	0.00221	-0.00365
140	H6	PZ	0.02368	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00000	-0.01605	0.00991	0.00287	-0.00979
142	C8	S	0.00000	-0.62849	0.18592	-0.09794	-0.08721
143	C8	PX	0.00000	0.36073	-0.01674	0.16841	-0.21767
144	C8	PY	0.00000	-0.22155	-0.06427	-0.08656	-0.11087
145	C8	PZ	-0.33331	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.00000	1.03465	0.70384	0.29666	0.34647
147	C8	PX	0.00000	-1.01452	-0.44399	-0.83294	1.32921
148	C8	PY	0.00000	-0.23962	1.79620	0.25406	0.77057
149	C8	PZ	0.73537	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00000	-0.01407	0.05448	0.00692	-0.01785
151	C8	DYY	0.00000	-0.13345	0.06652	-0.01231	-0.00584
152	C8	DZZ	0.00000	0.00677	-0.03101	-0.00619	0.00314
153	C8	DXY	0.00000	0.04833	0.07996	0.00806	-0.02037
154	C8	DXZ	-0.01745	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00666	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00000	0.14922	0.10201	0.01647	0.12393
157	H8	S	0.00000	-0.38804	-2.04629	-0.15472	-0.73552
158	H8	PX	0.00000	0.03901	0.09678	0.00880	0.03029
159	H8	PY	0.00000	-0.00882	-0.02662	0.01268	-0.02855
160	H8	PZ	-0.01768	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00000	0.01261	0.00604	0.00592	0.00442
162	C10	S	0.00000	-0.33528	-0.02067	-0.00126	-0.09432
163	C10	PX	0.00000	-0.14997	-0.56117	-0.17838	0.61225
164	C10	PY	0.00000	-0.04869	0.09502	0.01281	-0.07303
165	C10	PZ	0.01851	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00000	-0.10202	1.16414	0.02233	0.62218
167	C10	PX	0.00000	0.64467	1.67132	0.70579	-1.92821
168	C10	PY	0.00000	-0.02942	0.10134	-0.08733	0.37926
169	C10	PZ	-0.21116	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00000	0.00524	0.00146	0.00558	0.00590
171	C10	DYY	0.00000	-0.01758	0.02641	0.00979	0.00635
172	C10	DZZ	0.00000	-0.01209	-0.03074	-0.00737	-0.01408
173	C10	DXY	0.00000	-0.04492	-0.07147	-0.01219	0.09604
174	C10	DXZ	-0.01628	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	-0.00334	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00000	0.26803	0.08931	0.05859	-0.15123
177	H16	S	0.00000	-0.49691	-1.08310	-0.41878	1.15281
178	H16	PX	0.00000	0.02865	0.05419	0.01728	-0.05284
179	H16	PY	0.00000	-0.02415	-0.04465	-0.01403	0.04434
180	H16	PZ	-0.00891	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00000	0.00147	-0.07430	-0.00213	0.17075
182	H18	S	0.00000	0.37281	0.85007	0.34030	-1.16968
183	H18	PX	0.00000	-0.00871	0.05060	0.01294	-0.06077
184	H18	PY	0.00000	0.02763	0.01497	0.01047	-0.05048
185	H18	PZ	0.00048	0.00000	0.00000	0.00000	0.00000

MO:	81	82	83	84	85
Eigenvalues:	1.10437	1.12072	1.12717	1.13890	1.16081
(ev):	30.05141	30.49639	30.67181	30.99115	31.58731

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1	H1	S	0.17054	-0.06642	0.00000	-0.26320	0.05922
2	H1	S	-0.74859	-0.20358	0.00000	1.56623	-0.39589
3	H1	PX	0.04873	0.01274	0.00000	-0.10272	0.00736
4	H1	PY	-0.01804	-0.02592	0.00000	0.00110	0.01658
5	H1	PZ	0.00000	0.00000	0.00361	0.00000	0.00000
6	C1	S	0.01103	-0.00156	0.00000	0.00048	0.00237
7	C1	S	-0.22353	-0.24102	0.00000	0.76989	0.09874
8	C1	PX	-0.24835	-0.04153	0.00000	0.52089	-0.07924
9	C1	PY	-0.02225	0.06288	0.00000	0.03885	-0.00664
10	C1	PZ	0.00000	0.00000	-0.05861	0.00000	0.00000
11	C1	S	-0.27150	0.54082	0.00000	-1.66412	-0.59511
12	C1	PX	0.95466	0.35591	0.00000	-1.66545	0.64059
13	C1	PY	-0.09910	-0.26463	0.00000	0.22595	0.29425
14	C1	PZ	0.00000	0.00000	0.23216	0.00000	0.00000
15	C1	DXX	0.04140	-0.04731	0.00000	-0.03676	0.02138
16	C1	DYY	-0.06643	-0.01103	0.00000	0.08879	-0.00015
17	C1	DZZ	-0.00940	0.00429	0.00000	0.05198	-0.01072
18	C1	DXY	-0.00658	0.01855	0.00000	-0.02110	0.03078
19	C1	DXZ	0.00000	0.00000	-0.01507	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.01475	0.00000	0.00000
21	C2	S	0.01744	-0.00974	0.00000	-0.00053	0.01863
22	C2	S	-0.19955	0.37680	0.00000	-0.50007	0.28768
23	C2	PX	0.61669	-0.41299	0.00000	0.29509	-0.11117
24	C2	PY	0.03052	-0.09357	0.00000	-0.08586	-0.35667
25	C2	PZ	0.00000	0.00000	-0.07457	0.00000	0.00000
26	C2	S	-0.24573	-0.80353	0.00000	1.44286	-0.40700
27	C2	PX	-2.62724	1.28102	0.00000	-1.01842	0.54528
28	C2	PY	0.26037	0.30025	0.00000	-0.36456	2.15583
29	C2	PZ	0.00000	0.00000	-0.11507	0.00000	0.00000
30	C2	DXX	0.04660	-0.09229	0.00000	-0.00239	0.04515
31	C2	DYY	-0.05839	0.07137	0.00000	-0.03967	0.02490
32	C2	DZZ	-0.02718	0.05375	0.00000	-0.03092	-0.00417
33	C2	DXY	0.00263	0.01523	0.00000	-0.02829	0.05090
34	C2	DXZ	0.00000	0.00000	0.02125	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.02027	0.00000	0.00000
36	C3	S	-0.01159	0.01287	0.00000	-0.00169	0.00883
37	C3	S	-0.13696	-0.24890	0.00000	0.12116	0.49063
38	C3	PX	-0.09697	-0.04589	0.00000	-0.08666	0.05638
39	C3	PY	-0.05431	0.19556	0.00000	-0.08325	-0.21550
40	C3	PZ	0.00000	0.00000	0.17743	0.00000	0.00000
41	C3	S	-0.85795	1.38983	0.00000	-1.16502	-0.68981
42	C3	PX	0.60926	0.09813	0.00000	0.84679	-0.57817
43	C3	PY	0.80799	-1.12068	0.00000	0.64242	1.16653
44	C3	PZ	0.00000	0.00000	-0.50215	0.00000	0.00000
45	C3	DXX	-0.03794	-0.00208	0.00000	-0.01382	0.03525
46	C3	DYY	-0.03821	0.03121	0.00000	-0.00701	0.01420
47	C3	DZZ	0.01945	-0.02614	0.00000	0.01010	0.00326
48	C3	DXY	-0.00990	-0.07622	0.00000	0.03715	0.05070
49	C3	DXZ	0.00000	0.00000	-0.03186	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.01463	0.00000	0.00000
51	C4	S	-0.00956	-0.01251	0.00000	0.00004	0.00111
52	C4	S	0.07598	0.40280	0.00000	0.21763	0.12736
53	C4	PX	0.12961	0.25064	0.00000	-0.19605	0.03407
54	C4	PY	0.07370	0.40080	0.00000	-0.02031	0.28412

55	C4	PZ	0.00000	0.00000	0.05565	0.00000	0.00000
56	C4	S	-0.25789	-0.52527	0.00000	-1.40315	-0.67559
57	C4	PX	0.15831	-0.73135	0.00000	0.92884	-0.07601
58	C4	PY	-0.43667	-1.07665	0.00000	0.85378	-0.83388
59	C4	PZ	0.00000	0.00000	-0.14579	0.00000	0.00000
60	C4	DXX	-0.02195	0.06281	0.00000	-0.01076	-0.02057
61	C4	DYY	0.00202	-0.07214	0.00000	-0.01269	0.01305
62	C4	DZZ	0.02112	0.05569	0.00000	0.01629	0.01415
63	C4	DXY	-0.04709	-0.09860	0.00000	-0.04468	-0.01680
64	C4	DXZ	0.00000	0.00000	-0.00406	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	-0.01977	0.00000	0.00000
66	C5	S	-0.00416	-0.01300	0.00000	-0.01236	-0.00470
67	C5	S	0.16433	0.61231	0.00000	0.21094	0.13825
68	C5	PX	-0.13295	-0.21572	0.00000	-0.45296	-0.24431
69	C5	PY	0.21547	0.31920	0.00000	0.41744	-0.01744
70	C5	PZ	0.00000	0.00000	0.05784	0.00000	0.00000
71	C5	S	0.43439	-1.96403	0.00000	0.25378	-1.52653
72	C5	PX	0.98076	0.14931	0.00000	1.44675	1.12850
73	C5	PY	-0.94135	-0.38798	0.00000	-1.51772	0.54397
74	C5	PZ	0.00000	0.00000	-0.03199	0.00000	0.00000
75	C5	DXX	-0.02186	0.04033	0.00000	0.04771	-0.00633
76	C5	DYY	0.04931	-0.07688	0.00000	-0.06809	-0.01810
77	C5	DZZ	0.00758	0.07605	0.00000	0.04842	0.01176
78	C5	DXY	0.05699	0.10955	0.00000	0.06139	-0.04465
79	C5	DXZ	0.00000	0.00000	0.01574	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	-0.02391	0.00000	0.00000
81	C6	S	-0.00697	0.00329	0.00000	0.01269	-0.00080
82	C6	S	-0.10397	-0.13040	0.00000	-0.01895	-0.41561
83	C6	PX	-0.10133	0.13253	0.00000	-0.20139	0.12261
84	C6	PY	-0.15027	-0.02744	0.00000	-0.02467	-0.04514
85	C6	PZ	0.00000	0.00000	-0.31306	0.00000	0.00000
86	C6	S	1.30742	0.11707	0.00000	1.22989	2.34602
87	C6	PX	0.49481	-0.77553	0.00000	1.08428	-1.61357
88	C6	PY	1.18253	-0.28445	0.00000	-1.30990	-0.51188
89	C6	PZ	0.00000	0.00000	0.96836	0.00000	0.00000
90	C6	DXX	-0.00501	0.00055	0.00000	0.01156	-0.01197
91	C6	DYY	0.01980	-0.01976	0.00000	0.04950	0.00856
92	C6	DZZ	-0.00707	-0.00085	0.00000	-0.01783	-0.02507
93	C6	DXY	-0.04410	0.03585	0.00000	0.03060	-0.03464
94	C6	DXZ	0.00000	0.00000	0.01148	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	-0.07510	0.00000	0.00000
96	C7	S	-0.00777	-0.00621	0.00000	0.01015	0.02339
97	C7	S	0.16953	0.20728	0.00000	-0.21837	0.76796
98	C7	PX	0.52263	0.12899	0.00000	-0.18729	-0.02504
99	C7	PY	-0.03350	0.26366	0.00000	-0.01214	-0.53624
100	C7	PZ	0.00000	0.00000	0.04454	0.00000	0.00000
101	C7	S	1.12712	-0.91158	0.00000	0.64794	-2.21606
102	C7	PX	-2.45689	-0.40255	0.00000	0.45995	0.86971
103	C7	PY	0.27356	-1.12461	0.00000	0.26469	2.17836
104	C7	PZ	0.00000	0.00000	-0.10557	0.00000	0.00000
105	C7	DXX	0.00214	0.03500	0.00000	0.03295	-0.03810
106	C7	DYY	0.05993	-0.04556	0.00000	-0.02340	0.14226
107	C7	DZZ	-0.00084	0.02233	0.00000	-0.03005	0.01067
108	C7	DXY	0.06603	0.05030	0.00000	-0.05488	-0.04904

109	C7	DXZ	0.00000	0.00000	-0.03184	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	-0.03660	0.00000	0.00000
111	H3	S	-0.09521	-0.30212	0.00000	-0.04840	-0.04673
112	H3	S	0.34364	1.28929	0.00000	-0.35559	0.57514
113	H3	PX	0.00035	-0.02612	0.00000	-0.01033	-0.02775
114	H3	PY	-0.02993	-0.08537	0.00000	0.00767	-0.03135
115	H3	PZ	0.00000	0.00000	-0.00950	0.00000	0.00000
116	H4	S	-0.12130	-0.31945	0.00000	-0.27894	0.06184
117	H4	S	0.78610	1.06050	0.00000	1.53118	0.17635
118	H4	PX	0.02252	0.03778	0.00000	0.02882	-0.00348
119	H4	PY	-0.03700	-0.07828	0.00000	-0.09209	-0.02060
120	H4	PZ	0.00000	0.00000	-0.00880	0.00000	0.00000
121	N1	S	0.00606	-0.00277	0.00000	0.01710	0.00780
122	N1	S	-0.02725	0.06148	0.00000	0.07680	-0.13461
123	N1	PX	0.05354	-0.21793	0.00000	-0.03580	0.01674
124	N1	PY	-0.12702	0.09998	0.00000	0.10893	0.05458
125	N1	PZ	0.00000	0.00000	0.94786	0.00000	0.00000
126	N1	S	0.27273	-0.22168	0.00000	-0.65558	-0.69961
127	N1	PX	-0.07039	0.49795	0.00000	-0.25869	-0.12042
128	N1	PY	0.32673	-0.36452	0.00000	-0.69708	-0.92731
129	N1	PZ	0.00000	0.00000	-1.51403	0.00000	0.00000
130	N1	DXX	0.02060	0.03103	0.00000	0.02813	-0.04825
131	N1	DYY	-0.00718	-0.00603	0.00000	0.03648	-0.06161
132	N1	DZZ	-0.01784	0.02609	0.00000	-0.00904	0.02173
133	N1	DXY	0.02780	0.00702	0.00000	-0.03907	-0.04660
134	N1	DXZ	0.00000	0.00000	0.04814	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.01921	0.00000	0.00000
136	H6	S	0.14534	-0.23023	0.00000	0.17851	0.13615
137	H6	S	-1.69128	1.23714	0.00000	-0.95466	0.37991
138	H6	PX	-0.08929	0.07584	0.00000	-0.06576	0.01048
139	H6	PY	-0.00209	-0.02689	0.00000	-0.01525	0.00183
140	H6	PZ	0.00000	0.00000	-0.01159	0.00000	0.00000
141	C8	S	0.00664	0.00054	0.00000	0.00278	-0.01994
142	C8	S	0.20223	0.17648	0.00000	0.14697	-0.27329
143	C8	PX	0.24871	0.09104	0.00000	-0.15870	-0.46762
144	C8	PY	0.11548	0.06466	0.00000	0.06945	-0.15561
145	C8	PZ	0.00000	0.00000	-0.17311	0.00000	0.00000
146	C8	S	-1.14689	-0.82305	0.00000	-0.13973	1.20743
147	C8	PX	-1.51533	-0.25296	0.00000	0.61968	2.24809
148	C8	PY	-0.87249	-0.61949	0.00000	-0.21094	1.39999
149	C8	PZ	0.00000	0.00000	0.65172	0.00000	0.00000
150	C8	DXX	0.00693	-0.04576	0.00000	0.00092	0.06237
151	C8	DYY	0.01364	0.02035	0.00000	0.02505	-0.08530
152	C8	DZZ	0.00576	0.01873	0.00000	0.00000	-0.00939
153	C8	DXY	-0.01691	0.02242	0.00000	0.01910	0.04331
154	C8	DXZ	0.00000	0.00000	0.02388	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.04817	0.00000	0.00000
156	H8	S	-0.07820	-0.02704	0.00000	0.10042	-0.12421
157	H8	S	1.41266	0.19734	0.00000	-0.55942	0.54773
158	H8	PX	-0.05885	-0.01592	0.00000	0.03632	-0.04408
159	H8	PY	0.03062	-0.00421	0.00000	-0.00304	0.02535
160	H8	PZ	0.00000	0.00000	-0.00961	0.00000	0.00000
161	C10	S	-0.01086	0.00475	0.00000	0.00313	-0.01620
162	C10	S	0.15292	0.11517	0.00000	-0.06240	-0.07303

163	C10	PX	-0.53911	0.12922	0.00000	0.00792	-0.10317
164	C10	PY	0.02316	0.01869	0.00000	0.00615	-0.22663
165	C10	PZ	0.00000	0.00000	-0.05425	0.00000	0.00000
166	C10	S	-0.61062	-0.41966	0.00000	0.06110	0.72734
167	C10	PX	1.76168	-0.30700	0.00000	-0.15516	-0.01185
168	C10	PY	-0.20853	-0.25237	0.00000	-0.08945	0.91707
169	C10	PZ	0.00000	0.00000	-0.08302	0.00000	0.00000
170	C10	DXX	-0.02818	0.01462	0.00000	0.01487	-0.08763
171	C10	DYY	0.00385	0.01055	0.00000	-0.00947	0.01405
172	C10	DZZ	0.02680	-0.00346	0.00000	-0.01576	0.04924
173	C10	DXY	-0.07116	0.00044	0.00000	0.01269	0.00423
174	C10	DXZ	0.00000	0.00000	0.04584	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	-0.01389	0.00000	0.00000
176	H16	S	0.06006	0.01312	0.00000	-0.03790	-0.28706
177	H16	S	-0.90755	0.07101	0.00000	0.03554	0.44720
178	H16	PX	0.03399	-0.01343	0.00000	0.00581	-0.00686
179	H16	PY	-0.03953	0.00762	0.00000	0.00704	0.02563
180	H16	PZ	0.00000	0.00000	0.00919	0.00000	0.00000
181	H18	S	-0.20992	-0.02972	0.00000	0.07859	-0.02687
182	H18	S	1.13908	-0.17302	0.00000	-0.20210	0.35309
183	H18	PX	0.06440	-0.01160	0.00000	-0.00488	0.04027
184	H18	PY	0.04515	-0.00043	0.00000	-0.01018	-0.02164
185	H18	PZ	0.00000	0.00000	-0.01369	0.00000	0.00000

MO:	86	87	88	89	90
Eigenvalues:	1.17402	1.20020	1.20276	1.21434	1.26398
(ev):	31.94659	32.65918	32.72891	33.04385	34.39462

		A	A	A	A	A	
1	H1	S	0.02982	0.15425	-0.02512	-0.00349	0.17840
2	H1	S	-0.01642	-0.18456	-0.13090	-0.06578	0.63368
3	H1	PX	-0.00079	0.01526	0.00471	-0.00137	-0.02843
4	H1	PY	-0.00075	0.01216	-0.00375	-0.00353	0.02074
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00043	-0.00549	-0.00708	-0.00081	-0.00759
7	C1	S	-0.06755	0.34765	-0.27529	0.12050	0.00406
8	C1	PX	0.04921	-0.18605	-0.02605	-0.08978	0.30258
9	C1	PY	-0.02900	-0.11016	0.23567	0.66862	0.25385
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.05709	-1.55995	0.23819	-1.29299	-0.83817
12	C1	PX	0.03460	0.23998	0.03533	0.40369	-0.76290
13	C1	PY	0.13812	0.23158	-0.96220	-3.81727	-2.51393
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.01506	0.09285	-0.00417	0.02323	-0.01546
16	C1	DYY	0.00244	-0.05461	-0.05176	-0.03558	-0.03666
17	C1	DZZ	0.00448	-0.00586	-0.00328	0.01214	0.04332
18	C1	DXY	-0.00012	-0.00791	0.02814	0.13399	0.07887
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00378	0.00391	0.00514	-0.00095	0.00602
22	C2	S	0.22732	-0.36090	-0.14346	-0.01731	0.15227
23	C2	PX	-0.01359	-0.14057	0.23699	-0.00288	0.22004
24	C2	PY	0.02847	-0.17489	-0.44312	0.12019	-0.18691
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

26	C2	S	-0.62406	1.88838	0.72687	0.35458	0.57820
27	C2	PX	-0.08463	0.34407	-0.24005	-0.05462	-0.79441
28	C2	PY	0.21044	1.32691	2.62770	-1.22201	3.18247
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01515	-0.07404	0.04534	-0.03311	0.00484
31	C2	DYY	0.01010	0.04205	-0.02651	0.02238	0.06641
32	C2	DZZ	0.00189	-0.00075	-0.02789	0.01855	-0.03776
33	C2	DXY	-0.01155	0.02994	0.10390	-0.03178	0.03956
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00064	-0.01691	0.01196	0.01546	-0.00012
37	C3	S	0.09304	-0.25381	0.17235	0.39603	0.12115
38	C3	PX	0.07569	-0.16453	-0.15801	0.28299	0.39109
39	C3	PY	-0.09202	-0.22271	0.22287	0.27148	-0.01952
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.41952	1.51557	0.24854	-3.02710	0.41529
42	C3	PX	-0.22632	0.57515	0.01236	-1.22808	-2.81676
43	C3	PY	0.40820	-0.02519	-0.48145	-0.92170	-1.37299
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.01984	-0.00689	0.02157	-0.02161	0.10048
46	C3	DYY	-0.02341	-0.01259	0.05255	0.03138	-0.04985
47	C3	DZZ	0.00830	-0.00794	-0.02493	0.01637	-0.00246
48	C3	DXY	0.01598	0.00546	-0.09004	-0.09059	-0.00497
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00389	0.03589	-0.00719	0.00592	-0.00346
52	C4	S	-0.06130	0.95229	-0.29495	-0.29042	-0.43402
53	C4	PX	0.15713	-0.24603	-0.21065	-0.53497	-0.02683
54	C4	PY	0.10127	0.38069	-0.18968	0.17592	0.37645
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.09990	-3.68930	0.69608	2.17466	0.62021
57	C4	PX	-0.47829	1.91673	0.96408	3.17756	1.96570
58	C4	PY	-0.19932	-1.62233	0.09430	-1.30887	-1.90869
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00332	-0.02465	-0.03117	-0.02011	-0.04903
61	C4	DYY	-0.03247	0.15276	0.02758	0.03902	-0.01408
62	C4	DZZ	0.01167	0.01379	-0.02476	-0.02185	0.00498
63	C4	DXY	-0.00875	0.01329	0.02124	-0.13067	-0.01064
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00506	-0.03562	0.00534	-0.02091	0.01112
67	C5	S	0.12064	-0.71041	0.37952	-0.64821	0.28367
68	C5	PX	0.04192	-0.34590	-0.19971	-0.08425	-0.15529
69	C5	PY	0.13953	-0.40662	-0.21747	-0.10079	-0.01835
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.56635	2.04909	-1.85001	3.38599	-1.49108
72	C5	PX	-0.13249	2.54989	1.52706	0.57690	2.54843
73	C5	PY	-0.26009	2.02415	0.81927	0.46335	1.50861
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.01340	0.01516	0.01666	0.00844	-0.00670
76	C5	DYY	0.02403	-0.13713	0.02368	-0.09960	0.02490
77	C5	DZZ	0.00180	-0.00064	0.00325	0.00221	0.00326
78	C5	DXY	0.01664	-0.02790	-0.09909	0.08860	-0.01449
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00362	0.01127	-0.01671	-0.00441	0.00683
82	C6	S	0.22548	0.00731	-0.71668	0.21291	0.47793
83	C6	PX	0.01189	0.00726	0.28164	-0.22466	0.45889
84	C6	PY	-0.12125	0.13837	-0.03506	-0.00409	-0.07566
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.05713	0.38652	3.58425	-1.43611	-1.33693
87	C6	PX	-0.31697	-0.33185	-1.75955	1.19538	-3.22320
88	C6	PY	0.17908	-0.09473	-0.31675	-0.05305	1.58787
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01593	0.02789	-0.01338	-0.02724	0.04086
91	C6	DYY	0.03097	0.01510	0.02129	0.00037	0.03170
92	C6	DZZ	-0.00401	-0.01444	-0.03711	0.02904	-0.00852
93	C6	DXY	-0.03440	-0.00245	0.03290	0.01251	-0.10589
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00345	0.00828	-0.01009	-0.00074	-0.01602
97	C7	S	0.08350	-0.27386	0.27957	0.43891	-0.57739
98	C7	PX	0.11993	0.13093	-0.04332	0.18815	-0.08773
99	C7	PY	-0.15456	-0.06913	0.38695	0.09112	-0.01390
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.15908	-0.01967	-0.24102	-0.49171	0.91196
102	C7	PX	-0.47843	-0.15750	0.06766	-0.50881	1.00507
103	C7	PY	0.72599	-0.58314	-1.04769	0.25107	0.03226
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.04215	-0.04086	0.03900	0.00997	-0.07766
106	C7	DYY	0.04307	0.00038	-0.01082	0.03111	0.00811
107	C7	DZZ	0.00897	-0.00496	-0.00030	0.01406	-0.01006
108	C7	DXY	-0.00554	0.03024	0.05358	-0.01270	0.01595
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.04781	0.15901	0.13852	-0.06487	0.12199
112	H3	S	0.28303	0.81409	-0.63899	-0.21501	0.35505
113	H3	PX	-0.00370	-0.02095	0.00474	0.00375	0.00010
114	H3	PY	-0.01988	-0.04504	0.04639	0.02075	-0.01778
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00839	-0.07042	0.17849	-0.22074	0.01434
117	H4	S	0.19953	-0.62980	0.05735	-0.24348	0.18890
118	H4	PX	0.01387	-0.01809	-0.01617	-0.01871	0.02825
119	H4	PY	-0.00895	0.03032	-0.00574	0.00930	-0.00002
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.01386	-0.00735	-0.00269	0.00488	0.00297
122	N1	S	-0.05895	0.04656	-0.22175	-0.04685	-0.07672
123	N1	PX	0.13272	0.06901	-0.11266	-0.08660	-0.01055
124	N1	PY	-0.08366	0.13138	0.25103	-0.03497	-0.31504
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.01992	-0.04897	-0.38978	0.36216	0.16757
127	N1	PX	-0.31967	-0.02024	0.52236	-0.16813	0.34862
128	N1	PY	-0.05802	-0.16423	-1.28405	0.29980	0.67328
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00473	0.03278	-0.02793	-0.01518	0.02806
131	N1	DYY	0.00108	-0.03702	-0.13240	0.01536	-0.02815
132	N1	DZZ	-0.03357	-0.00731	0.01309	-0.00058	-0.01728
133	N1	DXY	0.01098	-0.01298	-0.04327	0.03308	0.04829

134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.02761	-0.07790	0.20001	-0.00233	-0.20073
137	H6	S	0.06008	0.14334	-0.41071	0.03213	-0.41419
138	H6	PX	0.00982	0.00600	-0.04339	-0.00182	-0.01086
139	H6	PY	0.01174	-0.00761	-0.01114	-0.01366	0.01810
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00514	0.00803	0.01300	-0.01142	-0.00522
142	C8	S	-0.27157	0.21871	0.36240	-0.35597	-0.20155
143	C8	PX	-0.09786	0.10837	-0.03349	-0.08860	0.11672
144	C8	PY	0.08733	0.15060	0.18001	-0.08374	0.02727
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.72681	-0.59598	-1.40413	1.01669	0.88660
147	C8	PX	0.28867	-0.14063	0.35052	-0.11025	-0.25600
148	C8	PY	0.00175	-0.15192	-0.55630	-0.45321	0.43465
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.01477	-0.00023	-0.03786	-0.06146	-0.00267
151	C8	DYY	-0.00163	0.04755	0.06814	-0.02468	0.00842
152	C8	DZZ	-0.01630	-0.00853	-0.00500	0.01393	-0.00880
153	C8	DXY	-0.01850	-0.01860	0.03514	0.00282	-0.02917
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.03794	-0.18092	-0.18951	0.10342	-0.06811
157	H8	S	0.61753	0.08502	-0.08783	0.43705	-0.65646
158	H8	PX	-0.01725	-0.01819	-0.00725	-0.03463	0.01572
159	H8	PY	0.01462	0.00080	-0.01749	-0.01368	-0.02375
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.01956	-0.00068	0.00709	0.01095	-0.00503
162	C10	S	-1.08540	-0.04953	-0.10628	0.08333	0.31377
163	C10	PX	-0.03293	0.02342	0.19243	-0.01595	0.09102
164	C10	PY	0.52524	0.18242	0.24474	-0.00558	0.01001
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	2.26069	0.35197	0.49022	-0.83420	-0.55050
167	C10	PX	0.07093	-0.26290	-0.52147	0.21881	-0.35028
168	C10	PY	-0.89295	-0.28458	-0.57391	-0.32526	0.15355
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.15461	0.03697	0.07684	0.02278	-0.01016
171	C10	DYY	-0.11933	-0.01599	-0.01465	0.00019	-0.00017
172	C10	DZZ	-0.13357	-0.02425	-0.05887	-0.00187	0.04114
173	C10	DXY	-0.02055	-0.04529	0.00171	0.02498	-0.02062
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.50713	0.19854	0.05267	-0.01495	0.04475
177	H16	S	-1.33270	-0.25463	-0.22129	-0.05092	0.39493
178	H16	PX	0.11384	0.01373	0.01124	0.00628	-0.02611
179	H16	PY	-0.02789	-0.02136	0.00888	0.01244	-0.00809
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.55364	-0.07371	0.15066	0.17433	-0.16281
182	H18	S	-1.22153	-0.27387	-0.75350	0.03319	0.15690
183	H18	PX	-0.09914	-0.01813	-0.04504	-0.00080	0.00088
184	H18	PY	-0.01555	0.01729	-0.01413	-0.01162	0.01957
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

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Eigenvalues:	1.28550	1.29727	1.37046	1.40396	1.42126
(ev):	34.98037	35.30045	37.29226	38.20382	38.67438

		A	A	A	A	A	
1	H1	S	0.08176	0.32724	0.15722	-0.30634	-0.03606
2	H1	S	-0.02695	0.38163	0.42653	-0.30806	-0.04483
3	H1	PX	0.01234	0.00127	-0.02084	-0.01848	-0.00855
4	H1	PY	0.01871	-0.01196	0.01444	-0.00484	-0.02472
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00066	0.01213	0.01388	0.02867	0.01285
7	C1	S	0.29001	0.69833	-0.10942	0.49163	0.16520
8	C1	PX	-0.14965	-0.02991	0.29158	-0.12523	0.03211
9	C1	PY	-0.02896	-0.04825	-0.03227	0.13323	-0.11749
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.12888	-2.00109	-1.35539	-2.39296	-1.03875
12	C1	PX	-0.11789	-0.19617	-0.65799	1.55221	0.31980
13	C1	PY	1.04893	-1.92623	1.63202	0.46968	0.29624
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.05804	0.08845	0.02382	0.00571	0.03950
16	C1	DYY	-0.00334	-0.00541	-0.07681	0.02875	-0.00672
17	C1	DZZ	-0.00271	0.02603	0.01414	-0.01331	-0.03332
18	C1	DXY	0.04332	0.04223	-0.04458	-0.01454	-0.06889
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.00488	0.02849	0.00422	0.01894	0.01561
22	C2	S	0.10943	0.71394	0.68584	0.38720	0.43304
23	C2	PX	-0.09137	0.04622	0.32807	-0.12236	0.03778
24	C2	PY	0.25441	0.03002	0.10944	-0.11050	-0.17597
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.85015	-2.66294	-1.04144	-2.34365	-1.60061
27	C2	PX	0.52175	0.02981	-0.17769	0.23828	-0.35260
28	C2	PY	-1.59912	-0.34802	-1.28915	1.04880	-0.08324
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.02458	0.10596	0.09063	0.08192	0.04987
31	C2	DYY	-0.04705	-0.01826	0.02015	-0.01507	0.01613
32	C2	DZZ	0.03518	0.00385	0.00305	-0.01658	-0.02109
33	C2	DXY	-0.06637	-0.00258	-0.06779	0.02503	0.06818
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.01468	-0.02188	-0.02150	-0.00165	-0.00108
37	C3	S	0.75768	-0.34630	-0.59223	-0.20060	-0.16853
38	C3	PX	-0.34584	0.24689	-0.22166	-0.21903	0.03637
39	C3	PY	-0.06371	-0.14317	0.04520	0.06427	-0.40622
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.92276	0.44397	2.72739	2.56475	-0.24545
42	C3	PX	2.14701	-2.05724	1.80153	1.20666	0.16241
43	C3	PY	-0.36205	-0.70337	0.79418	0.58811	1.61450
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.06279	-0.08470	-0.00898	0.01259	-0.03283
46	C3	DYY	0.09910	-0.02870	-0.02030	0.04790	-0.00016
47	C3	DZZ	-0.02325	0.04019	-0.01903	-0.04811	-0.01672
48	C3	DXY	0.00575	0.00763	-0.01232	0.02368	-0.00616
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

51	C4	S	-0.01411	-0.02515	0.00801	-0.00098	0.00729
52	C4	S	-0.48466	-0.56098	0.22895	-0.00156	0.34241
53	C4	PX	0.06291	-0.11912	0.09107	-0.10442	-0.07766
54	C4	PY	0.18599	0.05491	0.03764	-0.08651	-0.22133
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.88028	3.08138	-1.51700	0.91761	-0.00728
57	C4	PX	-1.31833	1.37951	-0.50643	-0.04630	0.43602
58	C4	PY	0.19437	-0.47262	-0.48189	-0.24234	0.64138
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.06072	-0.01445	-0.01793	-0.01309	0.06553
61	C4	DYY	-0.03733	-0.07835	0.03797	0.08045	0.02918
62	C4	DZZ	0.01574	0.01011	0.01225	-0.05523	-0.05023
63	C4	DXY	-0.04375	-0.09783	0.04114	-0.04163	-0.00685
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00082	-0.01153	-0.02313	-0.00057	-0.00013
67	C5	S	-0.32325	-0.09708	-0.70142	-0.30423	0.05905
68	C5	PX	0.08772	0.25010	0.14531	-0.17029	0.08149
69	C5	PY	0.39333	-0.07417	0.17228	0.15922	-0.13632
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.30782	1.53529	2.47264	-0.01419	0.96419
72	C5	PX	-1.28314	-1.02690	-0.74840	0.11005	-0.63324
73	C5	PY	-1.69900	0.00968	-0.15886	-0.30626	0.40362
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.08350	-0.01309	-0.07596	-0.03750	0.04544
76	C5	DYY	0.02216	0.01425	-0.03177	-0.01234	0.00866
77	C5	DZZ	0.01574	-0.00742	0.00444	-0.00675	-0.05144
78	C5	DXY	0.03588	0.08726	0.09820	-0.01128	0.02265
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.01131	-0.01195	0.00271	-0.01395	-0.02923
82	C6	S	-0.11480	-0.59621	0.20704	-0.18734	-0.34913
83	C6	PX	-0.26191	0.08022	0.12299	0.05287	-0.03888
84	C6	PY	0.14445	0.08223	0.11042	-0.34829	-0.52072
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.90232	0.77606	-0.29715	0.06570	0.49993
87	C6	PX	1.66999	-1.34615	0.42272	-0.51427	0.91178
88	C6	PY	-1.19651	-0.26400	-1.37201	2.21260	1.51123
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.08865	-0.12690	0.01935	0.01684	-0.03221
91	C6	DYY	-0.05800	0.03266	0.02509	-0.10169	-0.06317
92	C6	DZZ	-0.00934	0.00975	-0.00121	0.01960	0.01284
93	C6	DXY	0.01740	0.01748	0.00033	-0.10850	-0.05043
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01781	0.01049	0.00780	-0.01511	0.00797
97	C7	S	-0.16064	-0.21952	0.46560	0.00645	0.09638
98	C7	PX	0.13173	0.01317	-0.23737	0.06710	-0.11892
99	C7	PY	-0.10337	-0.08076	0.00901	0.22930	0.11754
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.29567	0.04003	-0.20298	-0.07480	1.04069
102	C7	PX	0.24149	0.87128	-0.21329	-0.44117	0.11201
103	C7	PY	-0.90890	0.54323	-1.16364	-1.70549	0.21837
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

105	C7	DXX	-0.04811	-0.04501	0.10678	-0.00598	-0.02124
106	C7	DYY	0.00944	0.04401	-0.00731	-0.02627	0.05857
107	C7	DZZ	-0.01769	-0.01898	-0.00852	0.01823	-0.01690
108	C7	DXY	0.03029	0.03877	0.06300	0.02121	-0.03033
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.02153	-0.35358	0.35934	0.03713	-0.19324
112	H3	S	0.14151	-0.24210	0.38368	-0.12784	-0.35953
113	H3	PX	-0.01774	0.02202	0.02805	-0.00887	0.01961
114	H3	PY	-0.00126	-0.01223	-0.00942	0.02440	-0.00494
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.18353	-0.19809	-0.33728	-0.03815	-0.30464
117	H4	S	0.40461	-0.34485	-0.30493	0.14481	-0.41194
118	H4	PX	0.00331	-0.02407	0.02287	-0.00591	-0.01451
119	H4	PY	-0.01175	0.00270	0.00630	-0.02448	-0.01057
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.00220	-0.00896	-0.00331	0.01448	0.01691
122	N1	S	-0.21259	0.09644	-0.32931	0.02551	-0.05693
123	N1	PX	-0.15482	-0.04556	-0.19598	0.14738	0.06348
124	N1	PY	-0.07960	0.21213	-0.04439	-0.56504	-0.20312
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.18370	0.43118	-0.37392	-0.36359	0.02813
127	N1	PX	0.02983	0.65977	0.29038	-0.60997	-0.49118
128	N1	PY	0.16782	-1.14489	0.24206	1.80582	1.35697
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.06661	0.06116	-0.12914	0.00278	-0.02666
131	N1	DYY	-0.05870	-0.01632	-0.05546	0.08035	0.03666
132	N1	DZZ	0.01829	0.00402	0.01874	-0.01576	-0.00077
133	N1	DXY	-0.02600	-0.06159	-0.01238	0.02902	0.06025
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.20989	0.15595	0.15235	0.33899	0.09566
137	H6	S	0.32292	0.30529	-0.03528	0.32257	0.02483
138	H6	PX	0.00097	0.00663	-0.02504	0.00758	0.00531
139	H6	PY	0.02640	-0.01923	-0.00505	0.03134	-0.01595
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00231	0.01392	0.01506	0.02035	-0.03931
142	C8	S	-0.18717	0.61489	0.23334	0.50812	-0.93291
143	C8	PX	0.12829	-0.01745	0.13013	0.13961	0.01819
144	C8	PY	0.26971	0.10939	-0.00452	-0.35960	0.44445
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	1.08124	-1.70960	-0.97578	-2.61031	5.01961
147	C8	PX	-0.38628	1.58371	-1.64355	-1.67094	-1.11321
148	C8	PY	-0.82178	-0.76463	-0.34514	3.58371	-1.67611
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.04540	0.06596	0.04613	0.09253	-0.03749
151	C8	DYY	0.04923	0.00335	-0.00123	-0.03046	0.03081
152	C8	DZZ	-0.03020	-0.00166	-0.01707	0.01237	-0.02865
153	C8	DXY	-0.00019	0.02652	0.06281	-0.09352	-0.02367
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.45381	-0.16295	-0.02720	0.00512	-0.04302
157	H8	S	-0.05111	-0.28127	-0.05851	-0.06090	-0.13454
158	H8	PX	-0.04372	-0.00453	0.01627	-0.00897	0.01128

159	H8	PY	-0.00411	0.01594	0.00625	-0.02494	-0.01819
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00400	-0.00729	0.00009	-0.02719	0.02444
162	C10	S	0.60982	-0.38589	-0.09142	-0.59623	0.96214
163	C10	PX	0.11875	-0.01897	0.04527	0.12245	0.06046
164	C10	PY	0.26909	-0.10203	-0.02381	-0.04487	0.18165
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-1.77339	0.75961	0.12338	4.24857	-4.34075
167	C10	PX	-0.39742	-0.78787	1.04415	0.02630	0.18280
168	C10	PY	-0.85700	0.21952	-0.13781	1.76899	-1.60957
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.08486	-0.02775	0.01331	-0.13557	0.13646
171	C10	DYY	-0.02228	0.00075	-0.00499	0.06026	-0.10051
172	C10	DZZ	0.01225	-0.02774	-0.02066	0.01375	0.05349
173	C10	DXY	-0.03093	-0.07979	0.09428	0.01271	0.00941
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.12906	0.16168	-0.32658	-0.00299	0.05007
177	H16	S	0.10385	0.02986	-0.31721	0.00135	0.19028
178	H16	PX	-0.01155	0.00665	-0.00145	-0.02060	-0.01462
179	H16	PY	0.00178	-0.02161	0.04309	-0.03947	0.02355
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.04625	-0.24915	0.30252	-0.18571	0.17691
182	H18	S	-0.10693	-0.30206	0.14054	-0.06206	0.27466
183	H18	PX	-0.01338	0.00056	-0.01028	-0.02758	-0.00115
184	H18	PY	0.02227	0.02082	-0.03963	-0.00168	0.01812
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	96	97	98	99	100
Eigenvalues:	1.46880	1.47855	1.48237	1.57062	1.58697
(ev):	39.96810	40.23338	40.33727	42.73883	43.18366

		A	A	A	A	A	
1	H1	S	0.35209	0.00000	0.23318	0.00000	0.00000
2	H1	S	0.35735	0.00000	0.30278	0.00000	0.00000
3	H1	PX	0.02038	0.00000	-0.00957	0.00000	0.00000
4	H1	PY	-0.00626	0.00000	-0.00076	0.00000	0.00000
5	H1	PZ	0.00000	0.04687	0.00000	0.08627	0.13416
6	C1	S	0.02858	0.00000	0.02352	0.00000	0.00000
7	C1	S	0.83761	0.00000	0.11966	0.00000	0.00000
8	C1	PX	-0.20786	0.00000	0.15425	0.00000	0.00000
9	C1	PY	0.11396	0.00000	-0.03319	0.00000	0.00000
10	C1	PZ	0.00000	-0.00086	0.00000	0.05904	0.10554
11	C1	S	-2.56910	0.00000	-2.10165	0.00000	0.00000
12	C1	PX	-0.33384	0.00000	-0.54411	0.00000	0.00000
13	C1	PY	0.02333	0.00000	1.67934	0.00000	0.00000
14	C1	PZ	0.00000	0.02684	0.00000	-0.04023	-0.07801
15	C1	DXX	0.13022	0.00000	0.10175	0.00000	0.00000
16	C1	DYY	-0.01550	0.00000	-0.06327	0.00000	0.00000
17	C1	DZZ	-0.02005	0.00000	-0.03850	0.00000	0.00000
18	C1	DXY	-0.00044	0.00000	-0.00892	0.00000	0.00000
19	C1	DXZ	0.00000	0.10179	0.00000	0.20242	0.31469
20	C1	DYZ	0.00000	0.28078	0.00000	-0.16259	0.12329
21	C2	S	-0.00312	0.00000	-0.01794	0.00000	0.00000

22	C2	S	-0.26941	0.00000	-0.27514	0.00000	0.00000
23	C2	PX	-0.17505	0.00000	0.13011	0.00000	0.00000
24	C2	PY	-0.11624	0.00000	0.04906	0.00000	0.00000
25	C2	PZ	0.00000	-0.01510	0.00000	0.08056	-0.02043
26	C2	S	-0.50902	0.00000	2.14573	0.00000	0.00000
27	C2	PX	-0.77960	0.00000	-1.28472	0.00000	0.00000
28	C2	PY	0.82483	0.00000	-1.95828	0.00000	0.00000
29	C2	PZ	0.00000	0.04217	0.00000	-0.02004	-0.04447
30	C2	DXX	-0.05654	0.00000	-0.13208	0.00000	0.00000
31	C2	DYY	-0.00653	0.00000	0.09923	0.00000	0.00000
32	C2	DZZ	0.01135	0.00000	-0.01296	0.00000	0.00000
33	C2	DXY	0.03686	0.00000	0.01120	0.00000	0.00000
34	C2	DXZ	0.00000	-0.10342	0.00000	-0.25299	0.04389
35	C2	DYZ	0.00000	0.25735	0.00000	-0.13521	-0.13824
36	C3	S	-0.02373	0.00000	0.01995	0.00000	0.00000
37	C3	S	-0.70914	0.00000	0.00682	0.00000	0.00000
38	C3	PX	-0.24486	0.00000	-0.14085	0.00000	0.00000
39	C3	PY	-0.06796	0.00000	-0.31938	0.00000	0.00000
40	C3	PZ	0.00000	-0.02475	0.00000	-0.04917	-0.05419
41	C3	S	2.74285	0.00000	0.27212	0.00000	0.00000
42	C3	PX	1.81043	0.00000	3.79255	0.00000	0.00000
43	C3	PY	-0.90454	0.00000	1.09394	0.00000	0.00000
44	C3	PZ	0.00000	-0.02445	0.00000	0.12206	0.00673
45	C3	DXX	-0.01649	0.00000	-0.04923	0.00000	0.00000
46	C3	DYY	-0.01161	0.00000	0.09565	0.00000	0.00000
47	C3	DZZ	-0.01584	0.00000	-0.06522	0.00000	0.00000
48	C3	DXY	0.00806	0.00000	-0.04340	0.00000	0.00000
49	C3	DXZ	0.00000	-0.24107	0.00000	0.17967	0.13608
50	C3	DYZ	0.00000	-0.25201	0.00000	-0.09060	-0.32590
51	C4	S	-0.01305	0.00000	-0.00744	0.00000	0.00000
52	C4	S	-0.48679	0.00000	-0.22960	0.00000	0.00000
53	C4	PX	-0.10235	0.00000	0.07744	0.00000	0.00000
54	C4	PY	0.09991	0.00000	-0.01972	0.00000	0.00000
55	C4	PZ	0.00000	-0.02140	0.00000	0.04130	0.02045
56	C4	S	1.15906	0.00000	0.34801	0.00000	0.00000
57	C4	PX	0.91413	0.00000	-0.64028	0.00000	0.00000
58	C4	PY	0.56774	0.00000	0.03957	0.00000	0.00000
59	C4	PZ	0.00000	0.01092	0.00000	-0.00419	-0.02130
60	C4	DXX	-0.04617	0.00000	0.03550	0.00000	0.00000
61	C4	DYY	-0.01891	0.00000	-0.00475	0.00000	0.00000
62	C4	DZZ	-0.01320	0.00000	-0.04808	0.00000	0.00000
63	C4	DXY	-0.08643	0.00000	0.03964	0.00000	0.00000
64	C4	DXZ	0.00000	0.26205	0.00000	-0.11781	0.08316
65	C4	DYZ	0.00000	-0.02566	0.00000	0.23723	0.16087
66	C5	S	0.00752	0.00000	0.01711	0.00000	0.00000
67	C5	S	0.26518	0.00000	0.50402	0.00000	0.00000
68	C5	PX	-0.08230	0.00000	0.08124	0.00000	0.00000
69	C5	PY	-0.03450	0.00000	-0.21202	0.00000	0.00000
70	C5	PZ	0.00000	-0.01841	0.00000	0.03776	0.02920
71	C5	S	-0.51248	0.00000	-0.16967	0.00000	0.00000
72	C5	PX	0.90215	0.00000	-0.82078	0.00000	0.00000
73	C5	PY	-0.80435	0.00000	0.36843	0.00000	0.00000
74	C5	PZ	0.00000	0.00622	0.00000	-0.01744	0.02584
75	C5	DXX	0.00715	0.00000	0.04775	0.00000	0.00000

76	C5	DYY	0.05002	0.00000	0.03697	0.00000	0.00000
77	C5	DZZ	-0.01279	0.00000	-0.03464	0.00000	0.00000
78	C5	DXY	-0.05132	0.00000	0.02029	0.00000	0.00000
79	C5	DXZ	0.00000	-0.25596	0.00000	0.08227	-0.01447
80	C5	DYZ	0.00000	-0.04628	0.00000	0.25346	0.12361
81	C6	S	0.00336	0.00000	-0.00846	0.00000	0.00000
82	C6	S	0.25616	0.00000	0.00842	0.00000	0.00000
83	C6	PX	0.10424	0.00000	-0.46359	0.00000	0.00000
84	C6	PY	-0.06757	0.00000	-0.02901	0.00000	0.00000
85	C6	PZ	0.00000	-0.00656	0.00000	-0.02943	-0.04813
86	C6	S	-0.42322	0.00000	0.24520	0.00000	0.00000
87	C6	PX	0.15126	0.00000	4.68138	0.00000	0.00000
88	C6	PY	2.23739	0.00000	0.36925	0.00000	0.00000
89	C6	PZ	0.00000	-0.02832	0.00000	-0.01305	0.22659
90	C6	DXX	0.05100	0.00000	0.02919	0.00000	0.00000
91	C6	DYY	-0.02527	0.00000	-0.08077	0.00000	0.00000
92	C6	DZZ	-0.01269	0.00000	0.01819	0.00000	0.00000
93	C6	DXY	-0.00342	0.00000	-0.06839	0.00000	0.00000
94	C6	DXZ	0.00000	0.26754	0.00000	-0.21345	-0.09119
95	C6	DYZ	0.00000	-0.20465	0.00000	-0.16717	0.08240
96	C7	S	-0.00372	0.00000	0.03741	0.00000	0.00000
97	C7	S	0.03504	0.00000	0.61443	0.00000	0.00000
98	C7	PX	-0.02993	0.00000	-0.08502	0.00000	0.00000
99	C7	PY	-0.18598	0.00000	0.08666	0.00000	0.00000
100	C7	PZ	0.00000	-0.09141	0.00000	-0.05841	-0.04640
101	C7	S	0.00293	0.00000	-2.79485	0.00000	0.00000
102	C7	PX	-1.20302	0.00000	1.74568	0.00000	0.00000
103	C7	PY	-1.77834	0.00000	-2.05526	0.00000	0.00000
104	C7	PZ	0.00000	0.11677	0.00000	-0.07420	-0.00298
105	C7	DXX	0.06880	0.00000	-0.03590	0.00000	0.00000
106	C7	DYY	-0.05533	0.00000	0.10270	0.00000	0.00000
107	C7	DZZ	0.00568	0.00000	-0.04428	0.00000	0.00000
108	C7	DXY	0.03810	0.00000	0.01162	0.00000	0.00000
109	C7	DXZ	0.00000	-0.20173	0.00000	-0.28350	0.12062
110	C7	DYZ	0.00000	0.07140	0.00000	0.03346	0.36828
111	H3	S	-0.42691	0.00000	-0.01238	0.00000	0.00000
112	H3	S	-0.49435	0.00000	-0.06675	0.00000	0.00000
113	H3	PX	-0.01519	0.00000	0.01670	0.00000	0.00000
114	H3	PY	-0.01343	0.00000	-0.00601	0.00000	0.00000
115	H3	PZ	0.00000	0.02945	0.00000	0.07090	0.06825
116	H4	S	0.39287	0.00000	-0.09257	0.00000	0.00000
117	H4	S	0.46767	0.00000	-0.24050	0.00000	0.00000
118	H4	PX	-0.02004	0.00000	0.00794	0.00000	0.00000
119	H4	PY	0.00576	0.00000	0.01490	0.00000	0.00000
120	H4	PZ	0.00000	0.02986	0.00000	0.07325	0.06004
121	N1	S	-0.00358	0.00000	-0.00023	0.00000	0.00000
122	N1	S	-0.14004	0.00000	0.02303	0.00000	0.00000
123	N1	PX	0.07524	0.00000	-0.15027	0.00000	0.00000
124	N1	PY	0.03745	0.00000	-0.13100	0.00000	0.00000
125	N1	PZ	0.00000	-0.08370	0.00000	-0.03790	0.11746
126	N1	S	0.19625	0.00000	-0.30537	0.00000	0.00000
127	N1	PX	-0.20929	0.00000	-1.16943	0.00000	0.00000
128	N1	PY	1.40402	0.00000	1.39159	0.00000	0.00000
129	N1	PZ	0.00000	0.08964	0.00000	-0.03504	-0.28934

130	N1	DXX	-0.08345	0.00000	-0.00689	0.00000	0.00000
131	N1	DYY	0.00184	0.00000	0.02265	0.00000	0.00000
132	N1	DZZ	-0.00168	0.00000	0.01057	0.00000	0.00000
133	N1	DXY	0.04268	0.00000	0.06570	0.00000	0.00000
134	N1	DXZ	0.00000	0.14574	0.00000	0.01123	0.04183
135	N1	DYZ	0.00000	0.00931	0.00000	0.20030	-0.10882
136	H6	S	-0.23095	0.00000	-0.44504	0.00000	0.00000
137	H6	S	-0.17698	0.00000	-0.70455	0.00000	0.00000
138	H6	PX	0.02866	0.00000	0.00152	0.00000	0.00000
139	H6	PY	0.01429	0.00000	-0.01798	0.00000	0.00000
140	H6	PZ	0.00000	0.03852	0.00000	0.11335	-0.02391
141	C8	S	0.00335	0.00000	0.00297	0.00000	0.00000
142	C8	S	0.02437	0.00000	0.15914	0.00000	0.00000
143	C8	PX	0.33581	0.00000	-0.06204	0.00000	0.00000
144	C8	PY	-0.00788	0.00000	-0.40484	0.00000	0.00000
145	C8	PZ	0.00000	0.09873	0.00000	0.01253	-0.02662
146	C8	S	-0.30531	0.00000	-0.68199	0.00000	0.00000
147	C8	PX	-3.57722	0.00000	-0.48597	0.00000	0.00000
148	C8	PY	0.21873	0.00000	5.04708	0.00000	0.00000
149	C8	PZ	0.00000	-0.24358	0.00000	0.05252	0.10779
150	C8	DXX	0.00931	0.00000	0.00429	0.00000	0.00000
151	C8	DYY	0.01051	0.00000	-0.00100	0.00000	0.00000
152	C8	DZZ	-0.00341	0.00000	0.01512	0.00000	0.00000
153	C8	DXY	-0.00802	0.00000	-0.00142	0.00000	0.00000
154	C8	DXZ	0.00000	0.00858	0.00000	0.23838	-0.31908
155	C8	DYZ	0.00000	0.20601	0.00000	0.15923	-0.15634
156	H8	S	0.14954	0.00000	-0.43854	0.00000	0.00000
157	H8	S	0.19932	0.00000	-0.59414	0.00000	0.00000
158	H8	PX	-0.00306	0.00000	-0.05076	0.00000	0.00000
159	H8	PY	-0.02030	0.00000	-0.02237	0.00000	0.00000
160	H8	PZ	0.00000	-0.06973	0.00000	-0.14697	-0.01716
161	C10	S	0.00261	0.00000	-0.02273	0.00000	0.00000
162	C10	S	0.06467	0.00000	-0.36424	0.00000	0.00000
163	C10	PX	-0.02956	0.00000	0.16886	0.00000	0.00000
164	C10	PY	0.04756	0.00000	0.09353	0.00000	0.00000
165	C10	PZ	0.00000	0.04396	0.00000	0.03654	-0.07658
166	C10	S	-0.03913	0.00000	4.51643	0.00000	0.00000
167	C10	PX	2.03054	0.00000	-0.29469	0.00000	0.00000
168	C10	PY	-0.24883	0.00000	1.74596	0.00000	0.00000
169	C10	PZ	0.00000	0.07836	0.00000	-0.01761	0.02753
170	C10	DXX	0.02321	0.00000	-0.12451	0.00000	0.00000
171	C10	DYY	-0.01209	0.00000	0.08516	0.00000	0.00000
172	C10	DZZ	-0.00545	0.00000	0.00617	0.00000	0.00000
173	C10	DXY	0.14377	0.00000	-0.01235	0.00000	0.00000
174	C10	DXZ	0.00000	-0.00871	0.00000	0.13069	-0.16458
175	C10	DYZ	0.00000	-0.15089	0.00000	-0.12950	0.17589
176	H16	S	-0.39299	0.00000	0.00913	0.00000	0.00000
177	H16	S	-0.62793	0.00000	0.08507	0.00000	0.00000
178	H16	PX	0.00307	0.00000	-0.02055	0.00000	0.00000
179	H16	PY	0.04130	0.00000	-0.03147	0.00000	0.00000
180	H16	PZ	0.00000	0.04569	0.00000	0.08034	-0.10348
181	H18	S	0.41741	0.00000	-0.09664	0.00000	0.00000
182	H18	S	0.51922	0.00000	-0.24699	0.00000	0.00000
183	H18	PX	-0.00320	0.00000	-0.02819	0.00000	0.00000

184	H18	PY	-0.04204	0.00000	-0.02539	0.00000	0.00000
185	H18	PZ	0.00000	0.04294	0.00000	-0.01564	0.01945

MO:		101	102	103	104	105
Eigenvalues:		1.60573	1.61528	1.62909	1.64045	1.67320
(ev):		43.69417	43.95390	44.32986	44.63889	45.53021

		A	A	A	A	A	
1	H1	S	0.23470	0.00000	0.05320	0.00000	0.64365
2	H1	S	0.43635	0.00000	-0.06868	0.00000	1.09696
3	H1	PX	0.01240	0.00000	-0.02394	0.00000	0.03991
4	H1	PY	0.01161	0.00000	0.03883	0.00000	-0.00900
5	H1	PZ	0.00000	0.06181	0.00000	-0.02292	0.00000
6	C1	S	-0.00321	0.00000	0.04221	0.00000	-0.02074
7	C1	S	-0.06720	0.00000	0.56814	0.00000	-0.60185
8	C1	PX	0.02954	0.00000	-0.01459	0.00000	0.26696
9	C1	PY	0.00961	0.00000	0.09405	0.00000	0.12267
10	C1	PZ	0.00000	0.03294	0.00000	0.00550	0.00000
11	C1	S	1.30979	0.00000	-4.60293	0.00000	1.50755
12	C1	PX	-1.47670	0.00000	1.06435	0.00000	-3.36563
13	C1	PY	0.37033	0.00000	2.44930	0.00000	0.39395
14	C1	PZ	0.00000	0.07764	0.00000	-0.04001	0.00000
15	C1	DXX	0.03508	0.00000	0.09068	0.00000	0.06796
16	C1	DYY	-0.02836	0.00000	-0.01168	0.00000	-0.10330
17	C1	DZZ	0.01968	0.00000	-0.06557	0.00000	0.02037
18	C1	DXY	0.03328	0.00000	-0.02864	0.00000	-0.03828
19	C1	DXZ	0.00000	0.08318	0.00000	-0.04438	0.00000
20	C1	DYZ	0.00000	-0.05265	0.00000	0.15297	0.00000
21	C2	S	-0.03955	0.00000	0.03774	0.00000	-0.02240
22	C2	S	-0.39828	0.00000	0.68530	0.00000	-0.58081
23	C2	PX	0.02904	0.00000	0.15409	0.00000	-0.22243
24	C2	PY	-0.25256	0.00000	0.11771	0.00000	0.03574
25	C2	PZ	0.00000	-0.03971	0.00000	-0.06354	0.00000
26	C2	S	3.96853	0.00000	-3.59111	0.00000	1.89652
27	C2	PX	1.13775	0.00000	-2.34958	0.00000	3.08026
28	C2	PY	-1.09815	0.00000	0.29035	0.00000	0.09477
29	C2	PZ	0.00000	0.13075	0.00000	0.07116	0.00000
30	C2	DXX	-0.05529	0.00000	-0.00505	0.00000	0.04023
31	C2	DYY	0.01490	0.00000	0.02005	0.00000	-0.09318
32	C2	DZZ	0.06170	0.00000	-0.02452	0.00000	0.03575
33	C2	DXY	-0.07482	0.00000	0.02012	0.00000	0.01844
34	C2	DXZ	0.00000	0.11161	0.00000	0.22930	0.00000
35	C2	DYZ	0.00000	-0.15221	0.00000	0.01240	0.00000
36	C3	S	-0.02363	0.00000	0.00302	0.00000	0.01699
37	C3	S	-0.66667	0.00000	-0.35574	0.00000	0.22284
38	C3	PX	-0.10405	0.00000	-0.43006	0.00000	-0.40360
39	C3	PY	0.34631	0.00000	-0.06764	0.00000	-0.14553
40	C3	PZ	0.00000	0.06151	0.00000	-0.00847	0.00000
41	C3	S	1.20682	0.00000	1.25758	0.00000	-1.32959
42	C3	PX	1.00935	0.00000	4.09456	0.00000	1.70346
43	C3	PY	-1.99571	0.00000	3.27783	0.00000	0.54717
44	C3	PZ	0.00000	-0.20145	0.00000	0.04106	0.00000
45	C3	DXX	-0.12205	0.00000	0.03196	0.00000	0.07715
46	C3	DYY	0.01818	0.00000	0.03822	0.00000	-0.05557

47	C3	DZZ	0.03394	0.00000	-0.09836	0.00000	0.00415
48	C3	DXY	-0.03233	0.00000	-0.01399	0.00000	-0.03982
49	C3	DXZ	0.00000	-0.06615	0.00000	0.14317	0.00000
50	C3	DYZ	0.00000	-0.02239	0.00000	-0.28288	0.00000
51	C4	S	-0.00132	0.00000	-0.00856	0.00000	0.01375
52	C4	S	0.06266	0.00000	-0.41206	0.00000	0.35643
53	C4	PX	-0.04035	0.00000	0.17537	0.00000	-0.24352
54	C4	PY	0.00240	0.00000	0.13305	0.00000	-0.05123
55	C4	PZ	0.00000	-0.01856	0.00000	-0.08921	0.00000
56	C4	S	-1.06085	0.00000	0.21046	0.00000	-1.81053
57	C4	PX	-0.03521	0.00000	-0.89652	0.00000	0.81995
58	C4	PY	0.95012	0.00000	-0.75453	0.00000	1.99137
59	C4	PZ	0.00000	-0.02418	0.00000	0.06265	0.00000
60	C4	DXX	-0.00841	0.00000	-0.08338	0.00000	0.07306
61	C4	DYY	-0.05312	0.00000	0.05946	0.00000	-0.07764
62	C4	DZZ	0.06484	0.00000	-0.03161	0.00000	0.02548
63	C4	DXY	0.00738	0.00000	-0.01505	0.00000	0.00204
64	C4	DXZ	0.00000	-0.26325	0.00000	-0.10994	0.00000
65	C4	DYZ	0.00000	-0.04471	0.00000	-0.30412	0.00000
66	C5	S	-0.00129	0.00000	-0.01284	0.00000	0.00479
67	C5	S	0.07479	0.00000	-0.29164	0.00000	0.23483
68	C5	PX	0.01428	0.00000	-0.09271	0.00000	0.28473
69	C5	PY	0.09426	0.00000	0.01119	0.00000	0.01024
70	C5	PZ	0.00000	-0.01748	0.00000	-0.08131	0.00000
71	C5	S	-0.66601	0.00000	1.37744	0.00000	-0.98912
72	C5	PX	0.20175	0.00000	0.26432	0.00000	-0.78882
73	C5	PY	-0.49973	0.00000	-1.20466	0.00000	0.99533
74	C5	PZ	0.00000	-0.02070	0.00000	0.05941	0.00000
75	C5	DXX	-0.01134	0.00000	-0.07592	0.00000	0.07414
76	C5	DYY	-0.05646	0.00000	0.08550	0.00000	-0.07159
77	C5	DZZ	0.08503	0.00000	-0.04297	0.00000	0.02465
78	C5	DXY	-0.04963	0.00000	0.03577	0.00000	0.00121
79	C5	DXZ	0.00000	0.30798	0.00000	0.18005	0.00000
80	C5	DYZ	0.00000	-0.06338	0.00000	-0.30973	0.00000
81	C6	S	-0.01564	0.00000	-0.02094	0.00000	0.02038
82	C6	S	0.16709	0.00000	-0.36215	0.00000	0.41215
83	C6	PX	-0.19417	0.00000	0.14815	0.00000	0.28917
84	C6	PY	0.39410	0.00000	-0.06301	0.00000	-0.04230
85	C6	PZ	0.00000	0.07717	0.00000	0.04945	0.00000
86	C6	S	-1.80798	0.00000	5.99370	0.00000	-0.13841
87	C6	PX	2.92039	0.00000	-0.16674	0.00000	-1.09720
88	C6	PY	-3.31005	0.00000	0.33309	0.00000	-1.67574
89	C6	PZ	0.00000	-0.12498	0.00000	-0.18171	0.00000
90	C6	DXX	-0.05657	0.00000	0.06072	0.00000	0.08067
91	C6	DYY	-0.04720	0.00000	0.07254	0.00000	-0.00808
92	C6	DZZ	0.09747	0.00000	-0.08619	0.00000	-0.00100
93	C6	DXY	-0.06010	0.00000	0.01974	0.00000	0.04359
94	C6	DXZ	0.00000	0.10668	0.00000	-0.18580	0.00000
95	C6	DYZ	0.00000	0.16496	0.00000	-0.03529	0.00000
96	C7	S	0.04381	0.00000	0.01866	0.00000	-0.00284
97	C7	S	0.83474	0.00000	0.11226	0.00000	-0.19352
98	C7	PX	-0.21692	0.00000	0.12044	0.00000	0.06689
99	C7	PY	0.15999	0.00000	0.20574	0.00000	-0.00639
100	C7	PZ	0.00000	-0.06268	0.00000	-0.12865	0.00000

101	C7	S	-3.45760	0.00000	-1.37941	0.00000	-0.48163
102	C7	PX	0.83051	0.00000	-2.18185	0.00000	-0.86266
103	C7	PY	-0.70204	0.00000	0.69440	0.00000	0.47067
104	C7	PZ	0.00000	0.15542	0.00000	0.07644	0.00000
105	C7	DXX	0.09430	0.00000	0.09873	0.00000	0.00439
106	C7	DYY	0.01718	0.00000	-0.03440	0.00000	-0.01474
107	C7	DZZ	-0.03555	0.00000	-0.04725	0.00000	0.02414
108	C7	DXY	0.05791	0.00000	-0.10896	0.00000	-0.05843
109	C7	DXZ	0.00000	-0.09901	0.00000	-0.21162	0.00000
110	C7	DYZ	0.00000	0.01264	0.00000	0.23441	0.00000
111	H3	S	-0.12234	0.00000	0.18169	0.00000	-0.35215
112	H3	S	-0.19015	0.00000	0.30020	0.00000	-0.64776
113	H3	PX	-0.01628	0.00000	-0.00251	0.00000	0.01010
114	H3	PY	-0.00625	0.00000	0.00095	0.00000	-0.03423
115	H3	PZ	0.00000	-0.07731	0.00000	-0.15162	0.00000
116	H4	S	0.22069	0.00000	0.16750	0.00000	-0.19237
117	H4	S	0.37220	0.00000	0.23115	0.00000	-0.39060
118	H4	PX	-0.00019	0.00000	0.00030	0.00000	-0.01944
119	H4	PY	0.00706	0.00000	0.01587	0.00000	-0.02379
120	H4	PZ	0.00000	-0.09620	0.00000	-0.15832	0.00000
121	N1	S	0.00471	0.00000	-0.00225	0.00000	0.00044
122	N1	S	0.09928	0.00000	0.18761	0.00000	-0.08806
123	N1	PX	0.15628	0.00000	-0.01977	0.00000	-0.03524
124	N1	PY	-0.33350	0.00000	0.15179	0.00000	-0.06519
125	N1	PZ	0.00000	-0.01191	0.00000	-0.02854	0.00000
126	N1	S	-0.15982	0.00000	-0.14620	0.00000	-0.42149
127	N1	PX	-0.75668	0.00000	0.35364	0.00000	0.23253
128	N1	PY	1.41658	0.00000	-1.99517	0.00000	-1.08595
129	N1	PZ	0.00000	0.01214	0.00000	0.09910	0.00000
130	N1	DXX	0.06359	0.00000	0.04519	0.00000	-0.01318
131	N1	DYY	-0.00175	0.00000	0.00075	0.00000	-0.03579
132	N1	DZZ	0.00113	0.00000	-0.00001	0.00000	0.02305
133	N1	DXY	-0.05802	0.00000	-0.01337	0.00000	0.00304
134	N1	DXZ	0.00000	0.20278	0.00000	-0.10764	0.00000
135	N1	DYZ	0.00000	-0.23406	0.00000	0.13400	0.00000
136	H6	S	-0.00172	0.00000	-0.25534	0.00000	0.56581
137	H6	S	0.08559	0.00000	-0.52950	0.00000	0.97426
138	H6	PX	-0.01493	0.00000	0.02173	0.00000	-0.04102
139	H6	PY	0.02641	0.00000	0.00877	0.00000	-0.01611
140	H6	PZ	0.00000	-0.01781	0.00000	-0.10407	0.00000
141	C8	S	-0.00205	0.00000	-0.01933	0.00000	0.00202
142	C8	S	-0.34885	0.00000	-0.47075	0.00000	-0.00898
143	C8	PX	-0.20779	0.00000	-0.44455	0.00000	-0.21274
144	C8	PY	0.33708	0.00000	-0.08884	0.00000	-0.20834
145	C8	PZ	0.00000	-0.00388	0.00000	0.01628	0.00000
146	C8	S	4.36494	0.00000	-0.45535	0.00000	-1.78246
147	C8	PX	0.58506	0.00000	3.08165	0.00000	1.64697
148	C8	PY	-4.19067	0.00000	0.40119	0.00000	1.44049
149	C8	PZ	0.00000	0.01917	0.00000	-0.03718	0.00000
150	C8	DXX	0.11733	0.00000	-0.10037	0.00000	-0.07435
151	C8	DYY	0.02887	0.00000	-0.00886	0.00000	-0.03904
152	C8	DZZ	-0.07850	0.00000	0.01934	0.00000	0.06899
153	C8	DXY	-0.01820	0.00000	0.02019	0.00000	0.00163
154	C8	DXZ	0.00000	-0.18752	0.00000	0.14082	0.00000

155	C8	DYZ	0.00000	0.37288	0.00000	-0.05044	0.00000
156	H8	S	0.12507	0.00000	0.67939	0.00000	0.26270
157	H8	S	-0.07844	0.00000	0.95111	0.00000	0.39436
158	H8	PX	0.02544	0.00000	0.03823	0.00000	0.02108
159	H8	PY	0.01667	0.00000	-0.03878	0.00000	-0.01580
160	H8	PZ	0.00000	-0.01468	0.00000	-0.14691	0.00000
161	C10	S	0.03075	0.00000	0.00390	0.00000	-0.01121
162	C10	S	0.20284	0.00000	0.16609	0.00000	-0.12054
163	C10	PX	0.09807	0.00000	0.00150	0.00000	0.00136
164	C10	PY	-0.29059	0.00000	0.11132	0.00000	0.07779
165	C10	PZ	0.00000	0.13965	0.00000	-0.02475	0.00000
166	C10	S	-4.78029	0.00000	0.23405	0.00000	1.83212
167	C10	PX	-1.26447	0.00000	-1.56879	0.00000	-0.74253
168	C10	PY	-1.68857	0.00000	0.09094	0.00000	0.81819
169	C10	PZ	0.00000	-0.10333	0.00000	0.02708	0.00000
170	C10	DXX	0.08434	0.00000	0.01743	0.00000	-0.06108
171	C10	DYY	-0.10277	0.00000	0.03004	0.00000	0.05091
172	C10	DZZ	-0.00200	0.00000	-0.01360	0.00000	0.02693
173	C10	DXY	-0.09188	0.00000	-0.09460	0.00000	-0.03470
174	C10	DXZ	0.00000	-0.17938	0.00000	0.16650	0.00000
175	C10	DYZ	0.00000	-0.32017	0.00000	0.04691	0.00000
176	H16	S	0.33587	0.00000	0.25345	0.00000	0.09543
177	H16	S	0.43461	0.00000	0.45279	0.00000	0.24638
178	H16	PX	-0.02746	0.00000	0.00459	0.00000	0.00900
179	H16	PY	-0.00259	0.00000	-0.02302	0.00000	-0.01947
180	H16	PZ	0.00000	0.02362	0.00000	0.05373	0.00000
181	H18	S	-0.10308	0.00000	-0.27759	0.00000	-0.16883
182	H18	S	-0.28653	0.00000	-0.47463	0.00000	-0.22871
183	H18	PX	-0.00794	0.00000	0.01184	0.00000	-0.00055
184	H18	PY	0.04578	0.00000	0.02161	0.00000	0.00430
185	H18	PZ	0.00000	0.13878	0.00000	-0.07727	0.00000

MO:	106	107	108	109	110
Eigenvalues:	1.67544	1.69183	1.70830	1.71739	1.75678
(ev):	45.59108	46.03698	46.48529	46.73262	47.80450

		A	A	A	A	A	
1	H1	S	0.00000	0.00000	0.00000	0.18877	0.00000
2	H1	S	0.00000	0.00000	0.00000	0.39725	0.00000
3	H1	PX	0.00000	0.00000	0.00000	0.01369	0.00000
4	H1	PY	0.00000	0.00000	0.00000	0.02313	0.00000
5	H1	PZ	-0.11533	-0.08923	-0.13202	0.00000	-0.05594
6	C1	S	0.00000	0.00000	0.00000	-0.00257	0.00000
7	C1	S	0.00000	0.00000	0.00000	0.06141	0.00000
8	C1	PX	0.00000	0.00000	0.00000	-0.01189	0.00000
9	C1	PY	0.00000	0.00000	0.00000	-0.27039	0.00000
10	C1	PZ	-0.08720	-0.05664	-0.08988	0.00000	-0.04050
11	C1	S	0.00000	0.00000	0.00000	-0.16957	0.00000
12	C1	PX	0.00000	0.00000	0.00000	-0.95131	0.00000
13	C1	PY	0.00000	0.00000	0.00000	0.46300	0.00000
14	C1	PZ	0.12742	-0.00768	0.06374	0.00000	0.07131
15	C1	DXX	0.00000	0.00000	0.00000	0.03049	0.00000
16	C1	DYY	0.00000	0.00000	0.00000	-0.02803	0.00000
17	C1	DZZ	0.00000	0.00000	0.00000	0.04741	0.00000

18	C1	DXY	0.00000	0.00000	0.00000	0.08502	0.00000
19	C1	DXZ	-0.27503	-0.15978	-0.20844	0.00000	-0.09342
20	C1	DYZ	0.15515	0.20716	-0.08253	0.00000	-0.07058
21	C2	S	0.00000	0.00000	0.00000	-0.01510	0.00000
22	C2	S	0.00000	0.00000	0.00000	-0.26223	0.00000
23	C2	PX	0.00000	0.00000	0.00000	-0.09078	0.00000
24	C2	PY	0.00000	0.00000	0.00000	0.17020	0.00000
25	C2	PZ	0.13779	-0.02831	-0.07732	0.00000	-0.00489
26	C2	S	0.00000	0.00000	0.00000	1.96870	0.00000
27	C2	PX	0.00000	0.00000	0.00000	1.18305	0.00000
28	C2	PY	0.00000	0.00000	0.00000	-0.09343	0.00000
29	C2	PZ	-0.15731	0.08355	-0.01151	0.00000	-0.05747
30	C2	DXX	0.00000	0.00000	0.00000	-0.02408	0.00000
31	C2	DYY	0.00000	0.00000	0.00000	-0.01570	0.00000
32	C2	DZZ	0.00000	0.00000	0.00000	0.02371	0.00000
33	C2	DXY	0.00000	0.00000	0.00000	0.09297	0.00000
34	C2	DXZ	-0.37765	0.06346	0.17859	0.00000	-0.01868
35	C2	DYZ	-0.12088	-0.31640	0.02135	0.00000	0.04371
36	C3	S	0.00000	0.00000	0.00000	0.01646	0.00000
37	C3	S	0.00000	0.00000	0.00000	0.28890	0.00000
38	C3	PX	0.00000	0.00000	0.00000	-0.24303	0.00000
39	C3	PY	0.00000	0.00000	0.00000	0.43542	0.00000
40	C3	PZ	0.02903	-0.02479	0.05502	0.00000	0.02598
41	C3	S	0.00000	0.00000	0.00000	-0.36275	0.00000
42	C3	PX	0.00000	0.00000	0.00000	3.64418	0.00000
43	C3	PY	0.00000	0.00000	0.00000	-4.71179	0.00000
44	C3	PZ	-0.15028	0.14342	-0.10873	0.00000	-0.14665
45	C3	DXX	0.00000	0.00000	0.00000	0.01213	0.00000
46	C3	DYY	0.00000	0.00000	0.00000	0.05542	0.00000
47	C3	DZZ	0.00000	0.00000	0.00000	-0.01514	0.00000
48	C3	DXY	0.00000	0.00000	0.00000	-0.01658	0.00000
49	C3	DXZ	-0.01274	-0.06082	0.34403	0.00000	0.22271
50	C3	DYZ	-0.06707	-0.02286	0.09469	0.00000	0.03032
51	C4	S	0.00000	0.00000	0.00000	-0.03518	0.00000
52	C4	S	0.00000	0.00000	0.00000	-0.66185	0.00000
53	C4	PX	0.00000	0.00000	0.00000	-0.10352	0.00000
54	C4	PY	0.00000	0.00000	0.00000	0.28739	0.00000
55	C4	PZ	-0.12278	-0.04437	0.02767	0.00000	0.00589
56	C4	S	0.00000	0.00000	0.00000	2.05968	0.00000
57	C4	PX	0.00000	0.00000	0.00000	-1.28250	0.00000
58	C4	PY	0.00000	0.00000	0.00000	-2.78021	0.00000
59	C4	PZ	0.05443	0.02186	-0.01387	0.00000	-0.00793
60	C4	DXX	0.00000	0.00000	0.00000	-0.03755	0.00000
61	C4	DYY	0.00000	0.00000	0.00000	-0.01356	0.00000
62	C4	DZZ	0.00000	0.00000	0.00000	0.05610	0.00000
63	C4	DXY	0.00000	0.00000	0.00000	0.06489	0.00000
64	C4	DXZ	-0.12380	0.22358	0.24843	0.00000	0.03639
65	C4	DYZ	-0.36740	-0.12138	0.00313	0.00000	-0.01615
66	C5	S	0.00000	0.00000	0.00000	0.03517	0.00000
67	C5	S	0.00000	0.00000	0.00000	0.74956	0.00000
68	C5	PX	0.00000	0.00000	0.00000	0.03968	0.00000
69	C5	PY	0.00000	0.00000	0.00000	-0.22056	0.00000
70	C5	PZ	0.06371	0.12183	0.00690	0.00000	-0.00069
71	C5	S	0.00000	0.00000	0.00000	-3.32226	0.00000

72	C5	PX	0.00000	0.00000	0.00000	-1.59912	0.00000
73	C5	PY	0.00000	0.00000	0.00000	3.19302	0.00000
74	C5	PZ	-0.01307	-0.08621	0.01572	0.00000	0.01088
75	C5	DXX	0.00000	0.00000	0.00000	-0.01023	0.00000
76	C5	DYY	0.00000	0.00000	0.00000	-0.03074	0.00000
77	C5	DZZ	0.00000	0.00000	0.00000	0.04315	0.00000
78	C5	DXY	0.00000	0.00000	0.00000	0.05761	0.00000
79	C5	DXZ	0.11412	-0.14703	-0.26506	0.00000	-0.06402
80	C5	DYZ	0.23229	0.29717	-0.06080	0.00000	-0.01869
81	C6	S	0.00000	0.00000	0.00000	-0.03676	0.00000
82	C6	S	0.00000	0.00000	0.00000	-0.65305	0.00000
83	C6	PX	0.00000	0.00000	0.00000	-0.03058	0.00000
84	C6	PY	0.00000	0.00000	0.00000	-0.20266	0.00000
85	C6	PZ	-0.05427	0.07636	-0.00733	0.00000	-0.01603
86	C6	S	0.00000	0.00000	0.00000	1.94103	0.00000
87	C6	PX	0.00000	0.00000	0.00000	2.91116	0.00000
88	C6	PY	0.00000	0.00000	0.00000	2.38710	0.00000
89	C6	PZ	0.19009	-0.23437	0.11718	0.00000	0.20531
90	C6	DXX	0.00000	0.00000	0.00000	-0.02017	0.00000
91	C6	DYY	0.00000	0.00000	0.00000	-0.11488	0.00000
92	C6	DZZ	0.00000	0.00000	0.00000	0.05800	0.00000
93	C6	DXY	0.00000	0.00000	0.00000	0.02438	0.00000
94	C6	DXZ	-0.04750	-0.08304	-0.33565	0.00000	-0.06527
95	C6	DYZ	-0.20113	0.38902	-0.04034	0.00000	-0.12448
96	C7	S	0.00000	0.00000	0.00000	0.01508	0.00000
97	C7	S	0.00000	0.00000	0.00000	0.12410	0.00000
98	C7	PX	0.00000	0.00000	0.00000	-0.01986	0.00000
99	C7	PY	0.00000	0.00000	0.00000	-0.20481	0.00000
100	C7	PZ	-0.00385	-0.04932	-0.03279	0.00000	0.06456
101	C7	S	0.00000	0.00000	0.00000	-3.26782	0.00000
102	C7	PX	0.00000	0.00000	0.00000	-0.30467	0.00000
103	C7	PY	0.00000	0.00000	0.00000	-2.43614	0.00000
104	C7	PZ	0.04210	0.02234	0.00253	0.00000	-0.10467
105	C7	DXX	0.00000	0.00000	0.00000	0.03273	0.00000
106	C7	DYY	0.00000	0.00000	0.00000	-0.05899	0.00000
107	C7	DZZ	0.00000	0.00000	0.00000	0.00418	0.00000
108	C7	DXY	0.00000	0.00000	0.00000	0.05152	0.00000
109	C7	DXZ	0.07121	-0.14705	-0.05723	0.00000	0.28102
110	C7	DYZ	0.09275	0.00454	0.04467	0.00000	0.17154
111	H3	S	0.00000	0.00000	0.00000	0.52633	0.00000
112	H3	S	0.00000	0.00000	0.00000	0.93395	0.00000
113	H3	PX	0.00000	0.00000	0.00000	0.02609	0.00000
114	H3	PY	0.00000	0.00000	0.00000	0.02738	0.00000
115	H3	PZ	-0.20349	-0.02175	0.07109	0.00000	0.00757
116	H4	S	0.00000	0.00000	0.00000	-0.52319	0.00000
117	H4	S	0.00000	0.00000	0.00000	-0.97332	0.00000
118	H4	PX	0.00000	0.00000	0.00000	0.03694	0.00000
119	H4	PY	0.00000	0.00000	0.00000	-0.02806	0.00000
120	H4	PZ	0.08027	0.18870	0.05172	0.00000	0.00870
121	N1	S	0.00000	0.00000	0.00000	0.02570	0.00000
122	N1	S	0.00000	0.00000	0.00000	0.53496	0.00000
123	N1	PX	0.00000	0.00000	0.00000	0.24219	0.00000
124	N1	PY	0.00000	0.00000	0.00000	-0.03141	0.00000
125	N1	PZ	-0.02838	0.09573	-0.02963	0.00000	-0.09685

126	N1	S	0.00000	0.00000	0.00000	-1.03275	0.00000
127	N1	PX	0.00000	0.00000	0.00000	-1.36071	0.00000
128	N1	PY	0.00000	0.00000	0.00000	1.87505	0.00000
129	N1	PZ	-0.13507	0.09192	-0.17085	0.00000	-0.14473
130	N1	DXX	0.00000	0.00000	0.00000	0.11647	0.00000
131	N1	DYY	0.00000	0.00000	0.00000	0.10846	0.00000
132	N1	DZZ	0.00000	0.00000	0.00000	0.00202	0.00000
133	N1	DXY	0.00000	0.00000	0.00000	0.00885	0.00000
134	N1	DXZ	0.11699	-0.16583	0.11267	0.00000	0.34653
135	N1	DYZ	0.08287	-0.21007	0.12886	0.00000	-0.05238
136	H6	S	0.00000	0.00000	0.00000	0.16673	0.00000
137	H6	S	0.00000	0.00000	0.00000	0.28139	0.00000
138	H6	PX	0.00000	0.00000	0.00000	-0.01158	0.00000
139	H6	PY	0.00000	0.00000	0.00000	0.00123	0.00000
140	H6	PZ	0.17994	-0.02468	-0.12280	0.00000	-0.00432
141	C8	S	0.00000	0.00000	0.00000	-0.00204	0.00000
142	C8	S	0.00000	0.00000	0.00000	-0.17247	0.00000
143	C8	PX	0.00000	0.00000	0.00000	0.13001	0.00000
144	C8	PY	0.00000	0.00000	0.00000	0.05338	0.00000
145	C8	PZ	0.00559	-0.01512	-0.01864	0.00000	-0.02693
146	C8	S	0.00000	0.00000	0.00000	2.13005	0.00000
147	C8	PX	0.00000	0.00000	0.00000	-2.81803	0.00000
148	C8	PY	0.00000	0.00000	0.00000	-0.12328	0.00000
149	C8	PZ	0.01338	0.01420	0.18985	0.00000	0.18452
150	C8	DXX	0.00000	0.00000	0.00000	0.03195	0.00000
151	C8	DYY	0.00000	0.00000	0.00000	0.01777	0.00000
152	C8	DZZ	0.00000	0.00000	0.00000	-0.01522	0.00000
153	C8	DXY	0.00000	0.00000	0.00000	-0.06177	0.00000
154	C8	DXZ	-0.12675	0.07347	-0.04130	0.00000	-0.28764
155	C8	DYZ	-0.02792	0.07264	0.19323	0.00000	0.12181
156	H8	S	0.00000	0.00000	0.00000	0.17034	0.00000
157	H8	S	0.00000	0.00000	0.00000	0.03792	0.00000
158	H8	PX	0.00000	0.00000	0.00000	-0.01419	0.00000
159	H8	PY	0.00000	0.00000	0.00000	-0.03700	0.00000
160	H8	PZ	0.02629	-0.07149	-0.04780	0.00000	0.09909
161	C10	S	0.00000	0.00000	0.00000	0.01201	0.00000
162	C10	S	0.00000	0.00000	0.00000	0.08936	0.00000
163	C10	PX	0.00000	0.00000	0.00000	0.01742	0.00000
164	C10	PY	0.00000	0.00000	0.00000	-0.06026	0.00000
165	C10	PZ	-0.02580	0.04612	0.05719	0.00000	0.02630
166	C10	S	0.00000	0.00000	0.00000	-1.07349	0.00000
167	C10	PX	0.00000	0.00000	0.00000	1.00817	0.00000
168	C10	PY	0.00000	0.00000	0.00000	-0.51510	0.00000
169	C10	PZ	0.02478	-0.05342	-0.09662	0.00000	-0.07295
170	C10	DXX	0.00000	0.00000	0.00000	0.00928	0.00000
171	C10	DYY	0.00000	0.00000	0.00000	-0.03298	0.00000
172	C10	DZZ	0.00000	0.00000	0.00000	0.01390	0.00000
173	C10	DXY	0.00000	0.00000	0.00000	0.05278	0.00000
174	C10	DXZ	-0.19235	0.20254	-0.33956	0.00000	0.45400
175	C10	DYZ	0.06200	-0.10906	-0.14789	0.00000	-0.12588
176	H16	S	0.00000	0.00000	0.00000	-0.07752	0.00000
177	H16	S	0.00000	0.00000	0.00000	-0.33391	0.00000
178	H16	PX	0.00000	0.00000	0.00000	-0.01413	0.00000
179	H16	PY	0.00000	0.00000	0.00000	0.00651	0.00000

180	H16	PZ	-0.09591	0.11699	-0.11468	0.00000	0.27146
181	H18	S	0.00000	0.00000	0.00000	0.20173	0.00000
182	H18	S	0.00000	0.00000	0.00000	0.30292	0.00000
183	H18	PX	0.00000	0.00000	0.00000	-0.00734	0.00000
184	H18	PY	0.00000	0.00000	0.00000	-0.00620	0.00000
185	H18	PZ	0.07312	-0.07348	0.19352	0.00000	-0.22480

MO:		111	112	113	114	115
Eigenvalues:		1.90008	1.98176	2.03536	2.08417	2.11203
(ev):		51.70382	53.92646	55.38507	56.71307	57.47129

		A	A	A	A	A	
1	H1	S	0.02940	0.17515	0.09118	-0.11837	0.00000
2	H1	S	0.14438	0.08649	0.17843	-0.63434	0.00000
3	H1	PX	-0.00262	0.03372	0.03374	-0.00606	0.00000
4	H1	PY	-0.06170	0.05499	-0.04336	-0.01170	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.20587
6	C1	S	-0.00964	-0.00174	-0.01986	0.03230	0.00000
7	C1	S	-0.00433	-0.11068	-0.27589	0.56810	0.00000
8	C1	PX	-0.01352	0.02930	0.03824	-0.09780	0.00000
9	C1	PY	-0.07302	0.14042	-0.00328	-0.17965	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.00250
11	C1	S	0.05080	0.14900	1.08214	-1.85854	0.00000
12	C1	PX	-0.37038	-0.33056	-0.81329	2.24590	0.00000
13	C1	PY	0.53350	-0.14059	-0.23857	-0.87888	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.48008
15	C1	DXX	0.01871	-0.09201	-0.00736	-0.14035	0.00000
16	C1	DYY	-0.12964	0.07321	0.10109	-0.04864	0.00000
17	C1	DZZ	0.15966	-0.00226	-0.12691	0.12514	0.00000
18	C1	DXY	-0.17550	0.05258	-0.09140	-0.09792	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.34103
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.42207
21	C2	S	0.00104	0.00416	-0.02034	-0.01253	0.00000
22	C2	S	0.31604	-0.05888	-0.19422	-0.52261	0.00000
23	C2	PX	0.14188	-0.04077	-0.03856	-0.20266	0.00000
24	C2	PY	-0.26215	0.04597	-0.05319	0.08971	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.01522
26	C2	S	-0.09818	0.18751	1.08387	1.07143	0.00000
27	C2	PX	-0.31860	1.26788	-0.08509	2.22179	0.00000
28	C2	PY	0.18056	1.21552	-0.93133	1.90685	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.14380
30	C2	DXX	-0.00630	0.04090	-0.00894	0.12069	0.00000
31	C2	DYY	-0.10289	0.06570	0.06111	-0.04176	0.00000
32	C2	DZZ	0.15039	-0.13318	-0.09575	-0.06630	0.00000
33	C2	DXY	0.11501	-0.15403	0.09875	0.12149	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.05656
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.20281
36	C3	S	0.02047	-0.01786	0.01937	-0.07343	0.00000
37	C3	S	0.29296	-0.28471	0.04949	-0.91219	0.00000
38	C3	PX	0.11855	0.03057	0.17901	0.21764	0.00000
39	C3	PY	-0.05758	-0.12683	0.06107	0.12365	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.04555
41	C3	S	-0.86425	3.39861	-3.17790	9.96294	0.00000
42	C3	PX	0.54557	-1.04434	0.70849	-4.36380	0.00000

43	C3	PY	1.26861	-0.06530	-0.25172	-3.25528	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.86932
45	C3	DXX	0.11577	0.04921	0.31377	0.03545	0.00000
46	C3	DYY	-0.15884	0.02215	-0.08473	-0.03810	0.00000
47	C3	DZZ	0.06128	-0.12858	-0.27590	0.15337	0.00000
48	C3	DXY	-0.29012	0.10117	0.05356	0.06636	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.01080
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01178
51	C4	S	0.00941	0.00724	-0.00239	-0.02620	0.00000
52	C4	S	0.24552	0.04898	-0.08888	-0.18904	0.00000
53	C4	PX	-0.07291	0.04056	-0.11248	-0.12492	0.00000
54	C4	PY	0.00246	-0.04635	0.08956	-0.00635	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.04257
56	C4	S	-1.32853	-0.57112	-0.11868	3.30968	0.00000
57	C4	PX	0.30213	0.27659	0.26037	-0.28252	0.00000
58	C4	PY	0.69161	0.46734	0.23824	-2.29405	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.13753
60	C4	DXX	-0.18743	0.10703	0.06213	-0.17453	0.00000
61	C4	DYY	0.04078	-0.09526	0.05877	0.06554	0.00000
62	C4	DZZ	0.15828	-0.03441	-0.18690	0.17716	0.00000
63	C4	DXY	-0.07492	0.00646	-0.03837	-0.13603	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.18362
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.11799
66	C5	S	-0.01443	-0.00687	-0.00064	0.02126	0.00000
67	C5	S	-0.08980	-0.22524	0.02461	0.40460	0.00000
68	C5	PX	0.09038	-0.03561	0.04777	0.08157	0.00000
69	C5	PY	0.08041	0.06799	-0.00656	-0.00174	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.04190
71	C5	S	0.74432	-0.54873	0.48183	-3.72751	0.00000
72	C5	PX	0.50777	0.72587	-0.45026	-0.55515	0.00000
73	C5	PY	-1.01402	-0.07987	0.31318	2.07201	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00538
75	C5	DXX	-0.19453	0.11786	0.05570	-0.19663	0.00000
76	C5	DYY	0.05276	-0.10846	0.09304	0.09085	0.00000
77	C5	DZZ	0.17750	-0.01503	-0.20972	0.07726	0.00000
78	C5	DXY	0.03836	-0.02432	0.02769	0.06622	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.11156
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.03737
81	C6	S	0.00641	0.01221	-0.00494	0.05276	0.00000
82	C6	S	0.16451	-0.05527	-0.35242	0.66161	0.00000
83	C6	PX	-0.12965	0.20537	-0.26857	0.09216	0.00000
84	C6	PY	0.08365	-0.01071	0.10788	-0.10468	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.01124
86	C6	S	2.85051	2.12872	-0.86057	-5.96872	0.00000
87	C6	PX	0.25890	-3.05906	2.60886	-5.17520	0.00000
88	C6	PY	-2.70575	-2.76494	0.66650	1.85488	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.49251
90	C6	DXX	0.05860	0.07198	0.28074	0.04098	0.00000
91	C6	DYY	-0.05791	0.18555	-0.13358	0.02239	0.00000
92	C6	DZZ	0.01835	-0.35302	-0.18986	-0.13657	0.00000
93	C6	DXY	0.30495	-0.04547	0.01114	0.03369	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.27417
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.05174
96	C7	S	0.01005	0.01926	-0.01921	0.05703	0.00000

97	C7	S	0.01090	0.47443	-0.49006	0.75172	0.00000
98	C7	PX	-0.03988	-0.01071	0.19701	0.00807	0.00000
99	C7	PY	0.08518	0.13521	0.04986	0.09658	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.02343
101	C7	S	0.12954	-2.28228	1.77772	-8.02278	0.00000
102	C7	PX	0.67999	2.26795	-1.63238	4.65758	0.00000
103	C7	PY	-0.39104	-1.10446	0.28462	-1.00422	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.61969
105	C7	DXX	-0.20204	0.06739	0.17453	0.13254	0.00000
106	C7	DYY	0.12064	0.01751	0.01897	-0.07171	0.00000
107	C7	DZZ	0.06219	-0.16725	-0.18614	-0.14434	0.00000
108	C7	DXY	0.17287	0.05864	0.18950	0.15017	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	-0.38225
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.30305
111	H3	S	-0.04368	-0.00948	-0.07350	0.24794	0.00000
112	H3	S	-0.12650	-0.19476	-0.13505	0.50404	0.00000
113	H3	PX	-0.04106	0.02859	-0.01167	-0.03247	0.00000
114	H3	PY	0.00068	-0.00418	-0.00478	0.07307	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.04617
116	H4	S	0.19260	0.16807	-0.17943	-0.11687	0.00000
117	H4	S	0.38859	0.16689	-0.23586	-0.42992	0.00000
118	H4	PX	0.02671	-0.02945	0.01889	0.09042	0.00000
119	H4	PY	0.03072	0.01270	-0.01598	0.02221	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.05559
121	N1	S	0.08565	0.08910	-0.04621	-0.04225	0.00000
122	N1	S	0.98045	1.33558	-0.55708	-0.43248	0.00000
123	N1	PX	0.03760	-0.07378	0.06332	0.03438	0.00000
124	N1	PY	-0.04858	0.09316	-0.02610	0.06970	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.03591
126	N1	S	-5.81602	-7.33317	2.92395	2.48490	0.00000
127	N1	PX	-1.75552	-1.30076	0.23340	1.17707	0.00000
128	N1	PY	-0.87967	-1.51130	1.08315	-1.01133	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.05002
130	N1	DXX	-0.04603	0.30220	-0.21267	-0.12999	0.00000
131	N1	DYY	0.29136	0.29127	0.05850	-0.02646	0.00000
132	N1	DZZ	0.08141	-0.22812	-0.05749	0.03002	0.00000
133	N1	DXY	-0.14204	-0.00832	-0.18790	0.11850	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.03257
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.25047
136	H6	S	-0.04391	0.28008	-0.09966	0.20662	0.00000
137	H6	S	-0.09299	0.40225	-0.10725	0.70521	0.00000
138	H6	PX	0.01467	-0.03041	-0.00295	0.01343	0.00000
139	H6	PY	-0.04319	0.09854	-0.04830	0.02880	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.01216
141	C8	S	0.01535	-0.02285	0.01501	-0.02609	0.00000
142	C8	S	0.10185	-0.45272	-0.08201	-0.66084	0.00000
143	C8	PX	-0.06922	0.09851	-0.07294	-0.11374	0.00000
144	C8	PY	-0.11535	-0.08615	-0.15752	-0.19249	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.02083
146	C8	S	0.10001	2.77681	-1.03706	2.03453	0.00000
147	C8	PX	-0.94532	-0.92407	-0.19404	4.09555	0.00000
148	C8	PY	3.32076	2.86887	-1.47792	3.46765	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.42237
150	C8	DXX	0.16161	0.06673	0.29160	-0.10719	0.00000

151	C8	DYY	-0.20008	0.08788	-0.03692	0.03962	0.00000
152	C8	DZZ	0.01833	-0.18769	-0.34929	0.06499	0.00000
153	C8	DXY	-0.04592	0.00779	0.06997	0.27434	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.14863
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.05066
156	H8	S	0.09455	-0.36557	0.13298	-0.28014	0.00000
157	H8	S	-0.40104	-0.70190	0.47527	-1.06420	0.00000
158	H8	PX	0.04276	-0.03650	0.07849	-0.02903	0.00000
159	H8	PY	-0.01062	0.06425	0.11473	0.13709	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	-0.27918
161	C10	S	-0.01241	-0.00095	-0.01290	-0.00471	0.00000
162	C10	S	0.07102	0.10602	-0.11128	0.06733	0.00000
163	C10	PX	0.01299	-0.00068	0.02936	0.08789	0.00000
164	C10	PY	0.25246	0.05011	-0.06122	0.11549	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.00791
166	C10	S	2.37426	1.10527	-0.50446	2.08001	0.00000
167	C10	PX	0.65192	0.70007	-0.12220	-1.78037	0.00000
168	C10	PY	0.83228	0.24483	-0.38357	0.96561	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.18896
170	C10	DXX	-0.03570	-0.01033	0.19438	-0.12890	0.00000
171	C10	DYY	-0.01321	0.03734	-0.00492	0.10434	0.00000
172	C10	DZZ	0.10981	-0.08323	-0.23412	0.02024	0.00000
173	C10	DXY	0.02910	0.02025	-0.07416	-0.15968	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00696
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.23782
176	H16	S	-0.13800	-0.11387	-0.16503	0.19646	0.00000
177	H16	S	-0.15476	-0.25671	0.01037	0.61402	0.00000
178	H16	PX	0.01717	-0.03017	-0.02351	-0.02358	0.00000
179	H16	PY	0.00567	-0.01681	0.06458	-0.01869	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.05896
181	H18	S	0.07762	0.12394	-0.11414	-0.12835	0.00000
182	H18	S	0.15755	0.15685	-0.09919	-0.60281	0.00000
183	H18	PX	-0.02789	0.00455	-0.01022	-0.00583	0.00000
184	H18	PY	0.01250	-0.02413	0.05826	-0.09602	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	-0.07617

MO:	116	117	118	119	120
Eigenvalues:	2.12691	2.14240	2.15746	2.17372	2.19360
(ev):	57.87625	58.29774	58.70737	59.15008	59.69093

		A	A	A	A	A	
1	H1	S	0.01742	0.37347	-0.09247	0.29242	0.00000
2	H1	S	0.18940	-0.07792	-0.20469	0.31275	0.00000
3	H1	PX	-0.03467	0.13368	-0.03003	0.04406	0.00000
4	H1	PY	0.00609	0.06497	0.10831	0.10359	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.09428
6	C1	S	-0.00392	0.01150	0.00565	0.00135	0.00000
7	C1	S	-0.34964	-0.01618	0.20186	-0.25968	0.00000
8	C1	PX	0.19154	-0.01397	-0.05269	0.09260	0.00000
9	C1	PY	0.01746	-0.00701	0.02009	0.25208	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.02419
11	C1	S	0.53132	-0.60716	-0.31334	-0.22156	0.00000
12	C1	PX	-0.68750	-0.01928	0.73971	-1.04841	0.00000
13	C1	PY	0.24403	0.23005	-0.82891	0.16925	0.00000

14	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.08162
15	C1	DXX	0.06965	-0.35439	0.00966	-0.12429	0.00000
16	C1	DYY	-0.01586	0.31288	0.00692	0.11781	0.00000
17	C1	DZZ	-0.13378	0.07588	-0.03529	0.02712	0.00000
18	C1	DXY	-0.14694	0.01810	0.24457	0.06518	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.11538
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.11178
21	C2	S	0.00809	0.00334	-0.02382	0.00701	0.00000
22	C2	S	0.00262	0.11543	-0.16572	0.28736	0.00000
23	C2	PX	-0.09164	0.09868	-0.00023	0.05482	0.00000
24	C2	PY	-0.07320	-0.15851	0.01481	-0.07285	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.03733
26	C2	S	-0.61206	0.05872	1.50775	-0.44557	0.00000
27	C2	PX	-0.19343	-0.36001	1.35445	-1.35181	0.00000
28	C2	PY	-0.01794	0.21352	0.68190	-0.64507	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.41519
30	C2	DXX	-0.03482	-0.19342	0.20738	0.29325	0.00000
31	C2	DYY	0.00613	0.11341	-0.17369	-0.28698	0.00000
32	C2	DZZ	-0.06660	0.12154	0.00876	-0.05484	0.00000
33	C2	DXY	0.21095	0.10497	0.08876	0.05256	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.35859
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.33951
36	C3	S	0.00549	0.01924	-0.02721	0.02585	0.00000
37	C3	S	0.03617	-0.23226	-0.72101	0.52035	0.00000
38	C3	PX	0.13170	0.05421	0.10131	-0.12823	0.00000
39	C3	PY	0.05849	-0.19197	0.13671	-0.27018	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00471
41	C3	S	-1.70075	0.22412	4.65998	-3.85308	0.00000
42	C3	PX	0.33738	0.32058	-1.99998	2.21387	0.00000
43	C3	PY	0.87950	0.50120	-2.12411	1.95329	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.17669
45	C3	DXX	0.07780	0.09961	-0.12605	-0.07378	0.00000
46	C3	DYY	0.01852	-0.09379	0.14237	0.00388	0.00000
47	C3	DZZ	-0.14383	0.00554	-0.07304	0.05103	0.00000
48	C3	DXY	0.10554	0.22235	-0.01445	0.31070	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.32473
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01075
51	C4	S	-0.00215	0.00942	-0.01884	0.00609	0.00000
52	C4	S	0.26979	-0.13377	-0.07337	0.24136	0.00000
53	C4	PX	-0.19624	0.00820	-0.01559	-0.17416	0.00000
54	C4	PY	-0.01472	0.03865	-0.05672	0.01216	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.04163
56	C4	S	-0.88120	-0.14615	1.70744	-1.39878	0.00000
57	C4	PX	0.52862	-0.18729	-0.29038	0.71316	0.00000
58	C4	PY	0.66899	-0.34480	-0.99117	0.70104	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.12790
60	C4	DXX	-0.24795	0.21109	0.08239	-0.05258	0.00000
61	C4	DYY	0.20173	-0.27708	-0.04925	-0.00101	0.00000
62	C4	DZZ	0.02491	0.10343	0.02468	0.05312	0.00000
63	C4	DXY	-0.17754	-0.22174	0.16447	0.03740	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.06279
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	-0.14790
66	C5	S	-0.01365	0.01465	0.01280	-0.01362	0.00000
67	C5	S	0.00029	-0.14755	0.15365	-0.09149	0.00000

68	C5	PX	0.21848	-0.12767	-0.06284	-0.09110	0.00000
69	C5	PY	0.08497	0.02004	-0.00301	-0.05660	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.02301
71	C5	S	0.83877	-0.09947	-2.02405	1.93913	0.00000
72	C5	PX	-0.20808	0.33478	-0.34585	0.39091	0.00000
73	C5	PY	-0.67340	-0.08526	1.38500	-0.64102	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.09400
75	C5	DXX	-0.30394	0.09110	-0.02763	-0.15004	0.00000
76	C5	DYY	0.23227	-0.13397	0.06291	0.21799	0.00000
77	C5	DZZ	0.06641	0.04671	-0.11173	-0.04758	0.00000
78	C5	DXY	0.15316	0.21340	-0.18267	-0.18986	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.21854
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	-0.15366
81	C6	S	-0.02569	0.01226	0.01697	-0.02591	0.00000
82	C6	S	-0.22715	-0.00046	0.58067	-0.08186	0.00000
83	C6	PX	-0.07954	-0.06033	0.09739	-0.06689	0.00000
84	C6	PY	0.13930	-0.05374	0.00043	0.15677	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.10351
86	C6	S	1.46429	0.41810	-3.13650	2.99920	0.00000
87	C6	PX	0.51505	0.55360	-2.09176	2.20825	0.00000
88	C6	PY	-0.66660	0.00133	0.02878	-0.92970	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.57872
90	C6	DXX	0.20101	0.15533	0.06372	-0.17317	0.00000
91	C6	DYY	-0.04649	-0.18000	-0.00689	0.05773	0.00000
92	C6	DZZ	-0.08499	0.07934	-0.10524	0.16222	0.00000
93	C6	DXY	-0.08923	0.05645	0.23303	0.12527	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	-0.04558
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.21656
96	C7	S	-0.02361	0.00750	0.02363	-0.00900	0.00000
97	C7	S	0.10695	0.24025	0.45916	-0.21567	0.00000
98	C7	PX	-0.18484	-0.09256	-0.00107	0.12410	0.00000
99	C7	PY	-0.08839	0.12970	-0.02281	0.17401	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.01998
101	C7	S	1.97028	-0.50443	-4.71436	2.72149	0.00000
102	C7	PX	-0.73801	0.40136	2.69082	-1.57631	0.00000
103	C7	PY	0.56671	-0.16564	-0.49673	-0.00121	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.12679
105	C7	DXX	0.08599	0.03052	-0.12921	0.28603	0.00000
106	C7	DYY	-0.08552	-0.12816	0.12686	-0.26589	0.00000
107	C7	DZZ	0.03514	0.18140	-0.09698	-0.00351	0.00000
108	C7	DXY	-0.22330	-0.06705	-0.13979	-0.13720	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.18491
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.16215
111	H3	S	-0.09472	0.38468	0.02067	-0.07433	0.00000
112	H3	S	-0.21243	0.05024	0.25429	-0.21186	0.00000
113	H3	PX	-0.13832	0.09029	0.04982	-0.02045	0.00000
114	H3	PY	0.05205	0.11025	-0.02312	-0.00323	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	-0.13255
116	H4	S	0.04142	0.24406	-0.28383	-0.24050	0.00000
117	H4	S	0.10287	0.02521	-0.28650	0.21856	0.00000
118	H4	PX	0.12114	-0.06326	0.04123	0.07270	0.00000
119	H4	PY	0.07923	0.06054	-0.09531	-0.06614	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.05147
121	N1	S	0.00474	-0.00093	0.00161	0.01045	0.00000

122	N1	S	0.07112	0.01978	-0.30916	0.40169	0.00000
123	N1	PX	-0.05743	0.11547	-0.15979	0.15101	0.00000
124	N1	PY	0.04102	0.06542	0.08349	-0.15864	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.15189
126	N1	S	-0.45473	0.15445	0.48504	-1.52365	0.00000
127	N1	PX	0.13288	-0.22824	0.29990	-0.80015	0.00000
128	N1	PY	0.01921	-0.12321	-0.66607	0.28769	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.44759
130	N1	DXX	0.28086	-0.17430	-0.23286	-0.15730	0.00000
131	N1	DYY	-0.09721	0.03841	0.17851	0.14846	0.00000
132	N1	DZZ	-0.16499	0.16304	-0.08410	0.05459	0.00000
133	N1	DXY	-0.02420	-0.15196	-0.20310	-0.05340	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.43058
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.22091
136	H6	S	0.00199	0.10496	-0.04035	-0.47999	0.00000
137	H6	S	-0.00285	-0.18365	0.42424	-0.33064	0.00000
138	H6	PX	0.01860	-0.06978	0.04534	0.14305	0.00000
139	H6	PY	-0.03033	-0.06997	-0.03733	-0.04902	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.24823
141	C8	S	-0.00714	0.01099	-0.01823	0.00744	0.00000
142	C8	S	-0.06164	0.13374	-0.20046	0.19464	0.00000
143	C8	PX	0.12178	-0.00514	0.05004	0.01403	0.00000
144	C8	PY	0.13915	0.03853	-0.12630	0.11751	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.07447
146	C8	S	0.29629	-0.11715	1.06627	-0.59982	0.00000
147	C8	PX	-0.85610	0.45738	2.01684	-1.19381	0.00000
148	C8	PY	-2.12853	0.47560	2.47951	-0.63981	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.40387
150	C8	DXX	-0.23275	-0.07741	0.12867	-0.04417	0.00000
151	C8	DYY	0.27722	-0.07699	-0.08607	0.03066	0.00000
152	C8	DZZ	-0.09188	0.18503	-0.04986	-0.00091	0.00000
153	C8	DXY	-0.24071	-0.09728	-0.24121	0.12990	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.05491
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.03811
156	H8	S	-0.14094	-0.08344	-0.14053	-0.20652	0.00000
157	H8	S	0.24746	-0.08957	-0.57794	0.43288	0.00000
158	H8	PX	-0.04384	0.00679	-0.08487	-0.04970	0.00000
159	H8	PY	-0.04813	0.03092	-0.09448	0.13107	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.04619
161	C10	S	0.00366	0.00628	-0.00850	0.00049	0.00000
162	C10	S	-0.14074	0.08254	0.07620	-0.00922	0.00000
163	C10	PX	-0.07439	-0.00217	-0.00904	0.00850	0.00000
164	C10	PY	-0.23805	0.09220	0.16679	-0.01835	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.01075
166	C10	S	-1.57266	0.27345	1.63386	-0.34240	0.00000
167	C10	PX	0.25312	-0.37596	-1.12029	0.50723	0.00000
168	C10	PY	-0.46002	0.16464	0.54687	-0.14582	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.23190
170	C10	DXX	-0.05174	-0.06585	0.10315	-0.05855	0.00000
171	C10	DYY	0.08432	-0.03125	-0.06578	0.05044	0.00000
172	C10	DZZ	-0.11644	0.15902	-0.01586	-0.01150	0.00000
173	C10	DXY	0.22905	0.10977	0.24681	-0.08766	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	-0.03228
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	-0.32286

176	H16	S	0.19392	0.20750	0.31019	-0.10703	0.00000
177	H16	S	-0.16299	0.08095	0.25155	-0.16122	0.00000
178	H16	PX	0.02709	0.05969	0.15239	-0.08540	0.00000
179	H16	PY	-0.07881	-0.02510	0.04458	-0.04363	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.09074
181	H18	S	-0.05963	-0.08658	-0.45216	0.17999	0.00000
182	H18	S	0.16481	-0.09134	-0.28434	0.09645	0.00000
183	H18	PX	0.10118	0.03001	0.12667	-0.05950	0.00000
184	H18	PY	-0.04532	-0.01909	-0.00296	0.00718	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.13287

MO:	121	122	123	124	125
Eigenvalues:	2.24660	2.27302	2.27957	2.28758	2.30563
(ev):	61.13308	61.85196	62.03024	62.24833	62.73932

		A	A	A	A	A	
1	H1	S	-0.04482	0.00000	0.00000	-0.31917	-0.17840
2	H1	S	0.05061	0.00000	0.00000	-0.04154	0.00015
3	H1	PX	0.00427	0.00000	0.00000	-0.11732	-0.10293
4	H1	PY	-0.08468	0.00000	0.00000	0.17058	-0.03839
5	H1	PZ	0.00000	0.14686	-0.28243	0.00000	0.00000
6	C1	S	-0.01796	0.00000	0.00000	-0.01003	-0.00436
7	C1	S	0.05068	0.00000	0.00000	-0.19661	-0.09140
8	C1	PX	-0.07968	0.00000	0.00000	0.04517	0.07037
9	C1	PY	0.00017	0.00000	0.00000	0.03658	0.11544
10	C1	PZ	0.00000	0.02669	0.05752	0.00000	0.00000
11	C1	S	0.90026	0.00000	0.00000	0.88039	-0.64083
12	C1	PX	-0.23012	0.00000	0.00000	0.25347	0.36290
13	C1	PY	-0.26285	0.00000	0.00000	-0.82668	-0.23861
14	C1	PZ	0.00000	-0.36469	0.41287	0.00000	0.00000
15	C1	DXX	0.06010	0.00000	0.00000	0.23997	0.20338
16	C1	DYY	-0.02342	0.00000	0.00000	-0.04159	-0.02086
17	C1	DZZ	-0.02159	0.00000	0.00000	-0.24311	-0.29187
18	C1	DXY	-0.07037	0.00000	0.00000	0.32532	-0.09623
19	C1	DXZ	0.00000	0.17301	-0.30008	0.00000	0.00000
20	C1	DYZ	0.00000	-0.18267	-0.01078	0.00000	0.00000
21	C2	S	-0.01548	0.00000	0.00000	0.01677	0.01005
22	C2	S	0.10322	0.00000	0.00000	0.17969	0.11105
23	C2	PX	0.09901	0.00000	0.00000	0.03273	0.05506
24	C2	PY	0.00002	0.00000	0.00000	-0.05623	0.12098
25	C2	PZ	0.00000	0.01243	0.04865	0.00000	0.00000
26	C2	S	0.68377	0.00000	0.00000	-0.88507	0.22192
27	C2	PX	0.37682	0.00000	0.00000	0.08817	0.48929
28	C2	PY	-0.10111	0.00000	0.00000	0.71356	-0.08458
29	C2	PZ	0.00000	0.56589	0.10975	0.00000	0.00000
30	C2	DXX	-0.01186	0.00000	0.00000	-0.26523	-0.21651
31	C2	DYY	0.03079	0.00000	0.00000	0.02430	0.06114
32	C2	DZZ	0.00794	0.00000	0.00000	0.30692	0.24943
33	C2	DXY	0.03736	0.00000	0.00000	0.17144	-0.09673
34	C2	DXZ	0.00000	0.33145	0.12661	0.00000	0.00000
35	C2	DYZ	0.00000	0.17821	-0.03643	0.00000	0.00000
36	C3	S	-0.00381	0.00000	0.00000	-0.00888	-0.00588
37	C3	S	-0.07604	0.00000	0.00000	-0.31704	-0.04207
38	C3	PX	0.14157	0.00000	0.00000	0.17059	0.16417

39	C3	PY	0.14222	0.00000	0.00000	-0.11090	-0.05280
40	C3	PZ	0.00000	-0.04563	-0.05181	0.00000	0.00000
41	C3	S	-0.01404	0.00000	0.00000	-0.26916	2.39976
42	C3	PX	-0.66751	0.00000	0.00000	-1.24083	-0.36528
43	C3	PY	-0.96341	0.00000	0.00000	-0.21593	-0.83834
44	C3	PZ	0.00000	0.27051	-0.18900	0.00000	0.00000
45	C3	DXX	0.15854	0.00000	0.00000	-0.09624	-0.00391
46	C3	DYY	-0.13510	0.00000	0.00000	0.25313	-0.04569
47	C3	DZZ	-0.02006	0.00000	0.00000	-0.25164	0.13701
48	C3	DXY	-0.08131	0.00000	0.00000	-0.05309	0.27162
49	C3	DXZ	0.00000	0.01266	-0.18146	0.00000	0.00000
50	C3	DYZ	0.00000	-0.05159	-0.24541	0.00000	0.00000
51	C4	S	-0.00759	0.00000	0.00000	-0.00284	-0.02078
52	C4	S	-0.26125	0.00000	0.00000	0.17553	-0.41889
53	C4	PX	0.06120	0.00000	0.00000	0.06775	0.00376
54	C4	PY	0.11096	0.00000	0.00000	-0.16573	0.15473
55	C4	PZ	0.00000	0.03011	-0.03222	0.00000	0.00000
56	C4	S	0.09369	0.00000	0.00000	0.56127	1.47117
57	C4	PX	-0.09082	0.00000	0.00000	-0.18365	-0.07630
58	C4	PY	0.09321	0.00000	0.00000	0.14237	-0.87487
59	C4	PZ	0.00000	0.58793	-0.32698	0.00000	0.00000
60	C4	DXX	0.12253	0.00000	0.00000	0.02527	-0.16250
61	C4	DYY	0.08054	0.00000	0.00000	-0.03955	0.34097
62	C4	DZZ	-0.29662	0.00000	0.00000	0.10764	-0.24973
63	C4	DXY	0.20023	0.00000	0.00000	0.07111	0.14771
64	C4	DXZ	0.00000	-0.37428	-0.07389	0.00000	0.00000
65	C4	DYZ	0.00000	-0.22440	0.27931	0.00000	0.00000
66	C5	S	-0.00820	0.00000	0.00000	0.01920	0.00811
67	C5	S	-0.26065	0.00000	0.00000	0.17659	0.27164
68	C5	PX	-0.03398	0.00000	0.00000	0.08177	0.13530
69	C5	PY	0.11784	0.00000	0.00000	0.01648	-0.04336
70	C5	PZ	0.00000	-0.04997	-0.01728	0.00000	0.00000
71	C5	S	0.06010	0.00000	0.00000	-0.82551	-0.85701
72	C5	PX	0.13812	0.00000	0.00000	-0.27631	-0.49249
73	C5	PY	-0.00601	0.00000	0.00000	0.05575	0.72496
74	C5	PZ	0.00000	-0.69317	0.04488	0.00000	0.00000
75	C5	DXX	0.17306	0.00000	0.00000	-0.12494	0.02069
76	C5	DYY	0.00230	0.00000	0.00000	-0.10360	-0.07550
77	C5	DZZ	-0.25072	0.00000	0.00000	0.23844	0.07806
78	C5	DXY	-0.17109	0.00000	0.00000	0.16101	-0.07419
79	C5	DXZ	0.00000	-0.29365	0.20294	0.00000	0.00000
80	C5	DYZ	0.00000	0.34193	0.11716	0.00000	0.00000
81	C6	S	0.00049	0.00000	0.00000	0.00237	0.02402
82	C6	S	-0.06211	0.00000	0.00000	0.12422	0.20333
83	C6	PX	-0.06709	0.00000	0.00000	0.15000	0.12658
84	C6	PY	0.13244	0.00000	0.00000	0.07795	-0.01097
85	C6	PZ	0.00000	0.00732	-0.03614	0.00000	0.00000
86	C6	S	-0.13055	0.00000	0.00000	-0.63945	-0.70144
87	C6	PX	0.02455	0.00000	0.00000	-1.02720	-0.54390
88	C6	PY	-1.18013	0.00000	0.00000	0.86839	0.04457
89	C6	PZ	0.00000	-0.36112	-0.03163	0.00000	0.00000
90	C6	DXX	0.14104	0.00000	0.00000	0.10591	0.02827
91	C6	DYY	-0.13433	0.00000	0.00000	-0.10971	-0.19631
92	C6	DZZ	-0.02972	0.00000	0.00000	0.03519	0.12999

93	C6	DXY	0.09592	0.00000	0.00000	0.04780	-0.15114
94	C6	DXZ	0.00000	0.15467	0.20742	0.00000	0.00000
95	C6	DYZ	0.00000	-0.08030	-0.08903	0.00000	0.00000
96	C7	S	0.00370	0.00000	0.00000	-0.02091	0.02802
97	C7	S	0.07099	0.00000	0.00000	-0.46971	0.43324
98	C7	PX	-0.07777	0.00000	0.00000	0.22588	-0.03712
99	C7	PY	-0.04251	0.00000	0.00000	-0.14950	0.22072
100	C7	PZ	0.00000	-0.01659	-0.02955	0.00000	0.00000
101	C7	S	-0.35665	0.00000	0.00000	1.06709	-2.77856
102	C7	PX	0.15076	0.00000	0.00000	-0.58804	1.70973
103	C7	PY	0.09820	0.00000	0.00000	0.72667	-1.22577
104	C7	PZ	0.00000	-0.13610	-0.18055	0.00000	0.00000
105	C7	DXX	0.06858	0.00000	0.00000	0.08549	0.12275
106	C7	DYY	-0.01716	0.00000	0.00000	0.01643	-0.26680
107	C7	DZZ	-0.00336	0.00000	0.00000	-0.23913	0.13885
108	C7	DXY	0.07780	0.00000	0.00000	-0.14441	0.01774
109	C7	DXZ	0.00000	0.09768	0.28454	0.00000	0.00000
110	C7	DYZ	0.00000	0.01494	0.35362	0.00000	0.00000
111	H3	S	-0.20543	0.00000	0.00000	-0.04845	-0.24530
112	H3	S	0.03969	0.00000	0.00000	-0.01489	0.31529
113	H3	PX	0.04110	0.00000	0.00000	0.01280	-0.16811
114	H3	PY	-0.12610	0.00000	0.00000	0.01576	-0.07321
115	H3	PZ	0.00000	-0.31817	0.21713	0.00000	0.00000
116	H4	S	-0.13578	0.00000	0.00000	0.20091	-0.08643
117	H4	S	0.06720	0.00000	0.00000	-0.11430	-0.23073
118	H4	PX	-0.05360	0.00000	0.00000	0.00990	-0.05639
119	H4	PY	-0.11202	0.00000	0.00000	0.08244	-0.03054
120	H4	PZ	0.00000	0.40042	0.01069	0.00000	0.00000
121	N1	S	-0.00136	0.00000	0.00000	-0.01325	0.00678
122	N1	S	0.07285	0.00000	0.00000	-0.03042	0.44267
123	N1	PX	0.10031	0.00000	0.00000	0.16047	0.15563
124	N1	PY	0.00017	0.00000	0.00000	0.03366	0.20498
125	N1	PZ	0.00000	-0.01118	0.05343	0.00000	0.00000
126	N1	S	-0.03064	0.00000	0.00000	0.79096	-1.11553
127	N1	PX	0.11571	0.00000	0.00000	0.19695	-0.50608
128	N1	PY	-0.40695	0.00000	0.00000	-0.02978	-0.31452
129	N1	PZ	0.00000	0.10204	-0.15163	0.00000	0.00000
130	N1	DXX	-0.04190	0.00000	0.00000	-0.12990	-0.14772
131	N1	DYY	0.05590	0.00000	0.00000	0.11412	0.14137
132	N1	DZZ	0.03872	0.00000	0.00000	0.02410	0.11977
133	N1	DXY	-0.05298	0.00000	0.00000	-0.07752	-0.10783
134	N1	DXZ	0.00000	0.01547	-0.27047	0.00000	0.00000
135	N1	DYZ	0.00000	0.12359	0.22284	0.00000	0.00000
136	H6	S	0.04701	0.00000	0.00000	0.29325	0.26285
137	H6	S	0.08944	0.00000	0.00000	0.01359	0.05487
138	H6	PX	-0.02698	0.00000	0.00000	-0.09563	-0.10442
139	H6	PY	-0.05944	0.00000	0.00000	-0.04563	0.07799
140	H6	PZ	0.00000	-0.30051	-0.10156	0.00000	0.00000
141	C8	S	0.01993	0.00000	0.00000	-0.00226	0.00262
142	C8	S	-0.13174	0.00000	0.00000	-0.04224	0.03940
143	C8	PX	-0.03462	0.00000	0.00000	0.11543	0.00608
144	C8	PY	0.30904	0.00000	0.00000	0.06866	-0.15362
145	C8	PZ	0.00000	0.01170	0.09928	0.00000	0.00000
146	C8	S	-0.05569	0.00000	0.00000	-0.43860	0.94869

147	C8	PX	0.50405	0.00000	0.00000	0.04533	0.53344
148	C8	PY	-1.64793	0.00000	0.00000	-0.41818	2.07394
149	C8	PZ	0.00000	0.09768	0.48173	0.00000	0.00000
150	C8	DXX	-0.19448	0.00000	0.00000	0.01370	0.01477
151	C8	DYY	0.09712	0.00000	0.00000	0.02139	-0.14185
152	C8	DZZ	0.04365	0.00000	0.00000	-0.07637	0.19988
153	C8	DXY	0.04008	0.00000	0.00000	0.14712	0.05275
154	C8	DXZ	0.00000	0.10355	0.13947	0.00000	0.00000
155	C8	DYZ	0.00000	-0.00723	-0.08979	0.00000	0.00000
156	H8	S	0.01592	0.00000	0.00000	-0.07377	-0.20786
157	H8	S	-0.02668	0.00000	0.00000	0.29858	-0.50466
158	H8	PX	0.00318	0.00000	0.00000	-0.10963	-0.02524
159	H8	PY	-0.02693	0.00000	0.00000	-0.03831	0.12481
160	H8	PZ	0.00000	0.06640	0.17044	0.00000	0.00000
161	C10	S	0.01585	0.00000	0.00000	-0.00163	0.00407
162	C10	S	0.06933	0.00000	0.00000	-0.00954	0.13109
163	C10	PX	0.00707	0.00000	0.00000	-0.05732	0.06234
164	C10	PY	-0.04666	0.00000	0.00000	-0.00288	0.14745
165	C10	PZ	0.00000	-0.00347	-0.03266	0.00000	0.00000
166	C10	S	-1.39816	0.00000	0.00000	-0.15692	1.12298
167	C10	PX	-0.28673	0.00000	0.00000	0.42683	-0.53078
168	C10	PY	0.09852	0.00000	0.00000	0.08794	0.12259
169	C10	PZ	0.00000	-0.05135	-0.29087	0.00000	0.00000
170	C10	DXX	-0.48807	0.00000	0.00000	-0.13303	0.14170
171	C10	DYY	0.24839	0.00000	0.00000	0.09752	-0.15573
172	C10	DZZ	0.33398	0.00000	0.00000	0.04809	0.02706
173	C10	DXY	0.07743	0.00000	0.00000	-0.19936	0.06428
174	C10	DXZ	0.00000	0.00024	-0.02430	0.00000	0.00000
175	C10	DYZ	0.00000	-0.05959	-0.36960	0.00000	0.00000
176	H16	S	0.39242	0.00000	0.00000	-0.14073	0.06803
177	H16	S	0.13277	0.00000	0.00000	-0.07143	0.09161
178	H16	PX	-0.02258	0.00000	0.00000	-0.16301	0.12777
179	H16	PY	-0.27421	0.00000	0.00000	-0.14095	0.18607
180	H16	PZ	0.00000	0.00826	0.12752	0.00000	0.00000
181	H18	S	0.28862	0.00000	0.00000	0.26943	-0.21006
182	H18	S	-0.05124	0.00000	0.00000	0.11380	-0.22681
183	H18	PX	0.02691	0.00000	0.00000	-0.13227	0.06830
184	H18	PY	-0.30189	0.00000	0.00000	0.00567	0.01707
185	H18	PZ	0.00000	0.03918	0.18883	0.00000	0.00000

MO:	126	127	128	129	130
Eigenvalues:	2.31922	2.35383	2.39048	2.39593	2.43253
(ev):	63.10911	64.05112	65.04840	65.19658	66.19258

		A	A	A	A	A	
1	H1	S	0.02400	-0.05257	-0.06064	0.07386	-0.07682
2	H1	S	-0.04584	-0.31394	0.07346	-0.04732	-0.03608
3	H1	PX	0.00933	0.01852	-0.03702	0.01199	-0.05109
4	H1	PY	0.00777	0.09691	-0.20188	-0.19909	-0.06050
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01541	0.02509	-0.01714	-0.00773	0.00557
7	C1	S	0.14187	0.52236	-0.16112	-0.03293	-0.04459
8	C1	PX	-0.04063	-0.20445	0.07104	0.06300	0.04492
9	C1	PY	0.05785	0.11613	-0.26290	-0.15749	-0.02599

10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-1.08849	-1.31710	0.49038	-0.29791	-1.10412
12	C1	PX	0.29685	1.15189	-0.23893	0.06825	0.40258
13	C1	PY	0.56297	0.14357	0.65664	0.31447	0.35839
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00962	-0.04746	0.10253	-0.04166	0.05896
16	C1	DYY	-0.07044	-0.12826	-0.02700	0.06460	0.01252
17	C1	DZZ	0.14106	0.28220	-0.17228	-0.10957	-0.14487
18	C1	DXY	-0.09582	0.06214	-0.09287	-0.24729	0.06128
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.02783	0.01446	-0.01074	-0.00111	0.00956
22	C2	S	0.41721	0.28022	-0.10279	0.08687	-0.12014
23	C2	PX	0.14917	0.06111	-0.02587	0.09779	-0.10106
24	C2	PY	0.09296	0.07419	-0.30445	0.00122	-0.03221
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-1.21524	-1.37794	0.82655	0.83701	-0.62052
27	C2	PX	-1.49807	-0.24806	0.75570	0.40278	-0.14514
28	C2	PY	-0.65051	0.85151	1.30602	0.42939	0.36493
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.02978	-0.16804	-0.00017	0.09507	-0.03407
31	C2	DYY	-0.15868	0.03977	-0.05175	-0.15157	-0.03393
32	C2	DZZ	0.29599	0.19430	0.01608	0.13582	0.03926
33	C2	DXY	-0.23722	0.28047	0.16681	-0.11645	0.05017
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00913	0.01098	-0.01259	-0.01486	0.02077
37	C3	S	0.24403	0.01868	0.18534	-0.24254	0.30393
38	C3	PX	0.01265	0.11396	-0.10762	0.08807	-0.25064
39	C3	PY	-0.18585	-0.18140	0.02728	0.18544	-0.14087
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-1.89903	1.75029	1.60294	2.24348	0.83156
42	C3	PX	1.25809	-0.32136	0.06378	-0.81245	1.16067
43	C3	PY	1.64478	0.68957	-0.93609	-0.90895	0.40005
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.08783	0.01466	-0.19564	-0.00535	-0.33302
46	C3	DYY	0.00745	-0.12969	0.10616	-0.00638	0.04717
47	C3	DZZ	-0.02410	0.22636	0.11949	0.04114	0.35293
48	C3	DXY	-0.04897	-0.05979	-0.19475	-0.02991	0.13904
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.02085	0.00570	-0.01888	-0.01079	-0.01029
52	C4	S	0.09585	-0.02400	-0.31732	-0.34192	-0.14514
53	C4	PX	0.02415	0.09411	0.14552	0.00457	0.05234
54	C4	PY	-0.00834	-0.06861	0.09867	0.18359	0.02251
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.48859	0.70809	-0.17340	0.19611	0.62837
57	C4	PX	0.04976	-0.55949	-0.58027	0.04394	-0.29873
58	C4	PY	0.00883	-0.03066	-0.44495	-0.99697	-0.57597
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.10444	0.08206	0.22574	0.00835	0.03779
61	C4	DYY	-0.08095	-0.09310	0.00536	0.09050	0.04638
62	C4	DZZ	0.21997	0.07468	-0.29487	-0.18298	-0.04493
63	C4	DXY	0.00732	0.27027	-0.19972	-0.14265	-0.11300

64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02145	0.00693	-0.00677	0.00633	-0.00055
67	C5	S	0.39117	-0.26055	-0.15859	0.18875	0.04355
68	C5	PX	-0.05476	-0.01853	-0.14620	-0.07951	-0.05666
69	C5	PY	-0.25976	0.16931	0.06819	-0.12790	-0.03783
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.74738	-0.41822	-1.37862	-0.85248	-0.41350
72	C5	PX	0.18539	0.04232	0.48132	0.43036	-0.18110
73	C5	PY	0.10243	-0.29387	0.22279	1.03334	0.12138
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.04592	-0.01080	0.16479	0.15028	-0.01858
76	C5	DYY	-0.29155	0.03579	-0.01628	-0.16996	0.08793
77	C5	DZZ	0.42176	-0.09298	-0.22356	0.05355	-0.08788
78	C5	DXY	-0.07494	-0.11394	0.25368	-0.06913	0.14311
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00275	0.01497	0.00102	0.00392	0.02227
82	C6	S	-0.31696	0.23902	0.39062	0.26287	0.44458
83	C6	PX	-0.04718	-0.01933	0.19040	0.04526	0.22778
84	C6	PY	-0.19022	-0.03060	0.16287	-0.11937	-0.05308
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.30953	0.17929	0.09572	-0.80912	-0.17304
87	C6	PX	1.55183	-1.14658	-1.29488	-1.19125	-0.37864
88	C6	PY	2.01923	0.82293	-0.95835	-0.28778	1.31706
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.06883	0.19275	-0.25249	0.01317	-0.21232
91	C6	DYY	0.06383	-0.22362	0.09199	0.07471	-0.03687
92	C6	DZZ	0.07968	0.15253	0.13844	-0.12049	0.31688
93	C6	DXY	0.07126	0.01424	0.24987	0.25484	-0.17436
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.02066	0.01017	0.00725	0.01110	0.00887
97	C7	S	-0.41745	0.33353	-0.07702	0.40147	0.04599
98	C7	PX	0.10627	-0.11130	0.07795	-0.14995	0.11629
99	C7	PY	-0.04701	-0.01796	-0.12664	-0.10712	0.14140
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	2.29039	-0.92377	-1.61896	-2.32243	-0.70336
102	C7	PX	-1.60818	0.69152	0.78896	1.41184	-0.04463
103	C7	PY	0.31636	-0.31305	-0.34553	0.15615	-1.02757
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.21210	0.04282	0.10907	-0.01716	-0.08488
106	C7	DYY	-0.11453	-0.16292	-0.10606	-0.02805	0.06059
107	C7	DZZ	-0.09331	0.12066	-0.16117	-0.00315	0.06117
108	C7	DXY	0.02784	0.05380	-0.10418	-0.21424	0.20934
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.08320	-0.09223	0.17524	0.14219	0.09092
112	H3	S	-0.01458	0.08536	0.19694	0.26734	0.17310
113	H3	PX	-0.01473	0.20077	0.05305	-0.11494	0.00039
114	H3	PY	0.01876	-0.14206	0.01868	0.04450	0.04701
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.08638	-0.02484	0.20490	-0.03144	0.02168
117	H4	S	-0.10082	0.14372	0.03747	-0.18459	-0.06340

118	H4	PX	-0.18089	0.00818	-0.07559	-0.19787	0.02458
119	H4	PY	-0.01371	-0.08526	0.02024	-0.09209	0.03058
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.02206	0.00619	0.01170	0.00431	0.02078
122	N1	S	-0.47109	0.19503	0.31108	-0.19741	-0.06058
123	N1	PX	-0.05830	0.02661	0.06649	-0.12635	-0.21449
124	N1	PY	-0.14845	0.06885	-0.23384	-0.04801	0.27645
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	2.30604	-0.73146	-1.67926	-0.02480	-0.66271
127	N1	PX	0.32939	-0.07045	-0.40807	0.22311	-0.27427
128	N1	PY	1.10545	-0.19937	-0.07041	-0.69503	0.33324
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.08537	0.24012	-0.04279	-0.10770	0.03914
131	N1	DYY	0.02630	-0.16779	0.09447	0.01971	0.03974
132	N1	DZZ	-0.03706	-0.01450	-0.06559	-0.01765	-0.07079
133	N1	DXY	-0.05662	0.01838	0.10273	-0.08063	-0.12073
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.14285	0.18737	0.09316	-0.04003	0.02647
137	H6	S	-0.43687	-0.02819	0.20793	0.11789	-0.02266
138	H6	PX	-0.02008	-0.06582	0.01133	-0.00326	0.01162
139	H6	PY	0.20070	-0.11082	-0.21931	0.09720	-0.09248
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01204	-0.02153	-0.01785	-0.01207	-0.02407
142	C8	S	-0.28035	-0.27247	-0.04869	-0.05461	-0.46380
143	C8	PX	-0.05877	0.00896	-0.03473	0.05447	-0.00188
144	C8	PY	0.04043	-0.12702	0.04173	0.00996	-0.03020
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-1.12274	0.36080	0.86075	0.59126	-0.24972
147	C8	PX	-0.42600	-0.02173	0.35245	0.96761	-0.97526
148	C8	PY	-0.16512	1.83608	0.82854	0.78784	3.01895
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.01494	-0.22312	-0.07463	-0.12076	0.41130
151	C8	DYY	0.17087	0.19206	0.09888	0.08271	-0.14758
152	C8	DZZ	-0.31549	-0.07992	-0.06138	0.03569	-0.40430
153	C8	DXY	0.00468	-0.06574	0.18156	-0.22495	-0.25645
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.00683	-0.02211	-0.17593	-0.12102	0.12301
157	H8	S	0.48318	-0.20710	-0.11012	-0.21648	-0.11692
158	H8	PX	0.02559	0.04123	-0.12540	-0.07168	0.17889
159	H8	PY	0.12029	0.12606	0.01057	-0.01186	0.25853
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.02448	-0.03219	-0.01673	-0.00978	-0.01561
162	C10	S	-0.18592	-0.25379	-0.13278	-0.07382	0.12045
163	C10	PX	0.06649	-0.03584	0.08469	-0.14618	-0.01506
164	C10	PY	-0.07453	-0.04572	-0.05343	0.01048	0.24608
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.54539	1.77216	0.66947	0.64729	2.19298
167	C10	PX	-0.30641	0.24452	-0.54573	0.31784	0.64563
168	C10	PY	0.49994	0.51108	0.22594	0.16616	1.04027
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.07704	0.14169	0.08127	0.04032	-0.15750
171	C10	DYY	0.23769	0.16417	0.06866	0.04873	0.21358

172	C10	DZZ	-0.25143	-0.50481	-0.26853	-0.14861	0.01614
173	C10	DXY	0.22302	-0.03133	0.05028	-0.10974	0.10035
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.16515	-0.23791	0.01802	-0.15587	0.00165
177	H16	S	0.11264	-0.10088	0.20543	-0.16491	-0.21629
178	H16	PX	0.10756	-0.12417	0.12222	-0.31587	-0.10020
179	H16	PY	0.01440	0.02260	0.22389	-0.29841	-0.30303
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.19514	-0.14546	-0.19796	0.03833	0.06204
182	H18	S	-0.04439	0.05447	-0.21438	0.15366	0.26595
183	H18	PX	0.18927	-0.00521	0.16114	-0.22896	-0.05106
184	H18	PY	-0.22599	0.18817	-0.14073	0.40441	-0.02772
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	131	132	133	134	135
Eigenvalues:	2.43724	2.52134	2.52181	2.56069	2.61248
(ev):	66.32070	68.60917	68.62186	69.68007	71.08919

		A	A	A	A	A	
1	H1	S	0.00000	0.00000	0.00933	0.00000	0.00000
2	H1	S	0.00000	0.00000	-0.11783	0.00000	0.00000
3	H1	PX	0.00000	0.00000	0.05784	0.00000	0.00000
4	H1	PY	0.00000	0.00000	-0.07784	0.00000	0.00000
5	H1	PZ	-0.13363	0.21529	0.00000	-0.23467	0.18022
6	C1	S	0.00000	0.00000	-0.02962	0.00000	0.00000
7	C1	S	0.00000	0.00000	-0.15863	0.00000	0.00000
8	C1	PX	0.00000	0.00000	0.05661	0.00000	0.00000
9	C1	PY	0.00000	0.00000	-0.10649	0.00000	0.00000
10	C1	PZ	-0.01006	-0.10910	0.00000	0.04925	-0.04378
11	C1	S	0.00000	0.00000	0.09679	0.00000	0.00000
12	C1	PX	0.00000	0.00000	0.26863	0.00000	0.00000
13	C1	PY	0.00000	0.00000	-1.02837	0.00000	0.00000
14	C1	PZ	0.04275	-0.11954	0.00000	0.11144	-0.00725
15	C1	DXX	0.00000	0.00000	-0.11695	0.00000	0.00000
16	C1	DYY	0.00000	0.00000	0.43344	0.00000	0.00000
17	C1	DZZ	0.00000	0.00000	-0.38986	0.00000	0.00000
18	C1	DXY	0.00000	0.00000	0.13279	0.00000	0.00000
19	C1	DXZ	0.02801	0.07069	0.00000	0.00392	-0.08212
20	C1	DYZ	0.02026	-0.05215	0.00000	0.36538	0.38216
21	C2	S	0.00000	0.00000	0.03630	0.00000	0.00000
22	C2	S	0.00000	0.00000	0.30031	0.00000	0.00000
23	C2	PX	0.00000	0.00000	0.05897	0.00000	0.00000
24	C2	PY	0.00000	0.00000	0.19739	0.00000	0.00000
25	C2	PZ	0.02912	0.05822	0.00000	0.07453	0.07395
26	C2	S	0.00000	0.00000	-0.58775	0.00000	0.00000
27	C2	PX	0.00000	0.00000	0.13407	0.00000	0.00000
28	C2	PY	0.00000	0.00000	1.13109	0.00000	0.00000
29	C2	PZ	-0.02122	0.05864	0.00000	0.08922	0.08940
30	C2	DXX	0.00000	0.00000	0.01281	0.00000	0.00000
31	C2	DYY	0.00000	0.00000	-0.36109	0.00000	0.00000
32	C2	DZZ	0.00000	0.00000	0.44815	0.00000	0.00000
33	C2	DXY	0.00000	0.00000	0.22441	0.00000	0.00000
34	C2	DXZ	0.03496	0.07806	0.00000	-0.01410	0.01289

35	C2	DYZ	-0.02226	-0.16727	0.00000	0.37430	0.41282
36	C3	S	0.00000	0.00000	-0.01666	0.00000	0.00000
37	C3	S	0.00000	0.00000	-0.41525	0.00000	0.00000
38	C3	PX	0.00000	0.00000	-0.08909	0.00000	0.00000
39	C3	PY	0.00000	0.00000	-0.22276	0.00000	0.00000
40	C3	PZ	-0.00715	-0.04010	0.00000	0.11091	0.00534
41	C3	S	0.00000	0.00000	2.01275	0.00000	0.00000
42	C3	PX	0.00000	0.00000	-2.29225	0.00000	0.00000
43	C3	PY	0.00000	0.00000	-0.55732	0.00000	0.00000
44	C3	PZ	-0.00133	-0.12949	0.00000	0.01900	-0.07404
45	C3	DXX	0.00000	0.00000	0.06478	0.00000	0.00000
46	C3	DYY	0.00000	0.00000	-0.02038	0.00000	0.00000
47	C3	DZZ	0.00000	0.00000	-0.10395	0.00000	0.00000
48	C3	DXY	0.00000	0.00000	-0.06751	0.00000	0.00000
49	C3	DXZ	0.51114	0.25624	0.00000	0.32824	0.12430
50	C3	DYZ	-0.22581	0.37128	0.00000	-0.19019	0.41583
51	C4	S	0.00000	0.00000	-0.02281	0.00000	0.00000
52	C4	S	0.00000	0.00000	-0.11859	0.00000	0.00000
53	C4	PX	0.00000	0.00000	-0.20204	0.00000	0.00000
54	C4	PY	0.00000	0.00000	0.12735	0.00000	0.00000
55	C4	PZ	-0.01595	-0.00370	0.00000	-0.07936	-0.09674
56	C4	S	0.00000	0.00000	0.84840	0.00000	0.00000
57	C4	PX	0.00000	0.00000	0.48953	0.00000	0.00000
58	C4	PY	0.00000	0.00000	-0.96939	0.00000	0.00000
59	C4	PZ	-0.05145	0.05489	0.00000	-0.10446	-0.06898
60	C4	DXX	0.00000	0.00000	0.22082	0.00000	0.00000
61	C4	DYY	0.00000	0.00000	-0.05502	0.00000	0.00000
62	C4	DZZ	0.00000	0.00000	-0.16007	0.00000	0.00000
63	C4	DXY	0.00000	0.00000	-0.11156	0.00000	0.00000
64	C4	DXZ	0.12894	0.35364	0.00000	-0.15512	-0.03353
65	C4	DYZ	-0.02468	-0.17800	0.00000	0.15777	0.04919
66	C5	S	0.00000	0.00000	0.02173	0.00000	0.00000
67	C5	S	0.00000	0.00000	0.03183	0.00000	0.00000
68	C5	PX	0.00000	0.00000	-0.14612	0.00000	0.00000
69	C5	PY	0.00000	0.00000	-0.10354	0.00000	0.00000
70	C5	PZ	0.01065	0.04800	0.00000	-0.07214	-0.06524
71	C5	S	0.00000	0.00000	-0.69980	0.00000	0.00000
72	C5	PX	0.00000	0.00000	0.40099	0.00000	0.00000
73	C5	PY	0.00000	0.00000	0.92561	0.00000	0.00000
74	C5	PZ	0.03717	0.01911	0.00000	-0.08744	-0.07857
75	C5	DXX	0.00000	0.00000	-0.23655	0.00000	0.00000
76	C5	DYY	0.00000	0.00000	0.07217	0.00000	0.00000
77	C5	DZZ	0.00000	0.00000	0.14360	0.00000	0.00000
78	C5	DXY	0.00000	0.00000	-0.24149	0.00000	0.00000
79	C5	DXZ	0.14037	0.21016	0.00000	0.24557	0.34323
80	C5	DYZ	0.05148	0.06897	0.00000	0.21756	0.24888
81	C6	S	0.00000	0.00000	0.01033	0.00000	0.00000
82	C6	S	0.00000	0.00000	0.26784	0.00000	0.00000
83	C6	PX	0.00000	0.00000	-0.12286	0.00000	0.00000
84	C6	PY	0.00000	0.00000	0.30452	0.00000	0.00000
85	C6	PZ	0.03768	-0.02035	0.00000	0.12206	0.04422
86	C6	S	0.00000	0.00000	-1.18067	0.00000	0.00000
87	C6	PX	0.00000	0.00000	-2.56225	0.00000	0.00000
88	C6	PY	0.00000	0.00000	0.22096	0.00000	0.00000

89	C6	PZ	0.05501	-0.02163	0.00000	0.15057	0.06500
90	C6	DXX	0.00000	0.00000	0.03671	0.00000	0.00000
91	C6	DYY	0.00000	0.00000	-0.06247	0.00000	0.00000
92	C6	DZZ	0.00000	0.00000	0.05467	0.00000	0.00000
93	C6	DXY	0.00000	0.00000	-0.08074	0.00000	0.00000
94	C6	DXZ	0.40408	0.43683	0.00000	-0.12382	0.06066
95	C6	DYZ	0.05399	-0.09786	0.00000	-0.23301	0.05364
96	C7	S	0.00000	0.00000	0.00705	0.00000	0.00000
97	C7	S	0.00000	0.00000	0.06385	0.00000	0.00000
98	C7	PX	0.00000	0.00000	0.04754	0.00000	0.00000
99	C7	PY	0.00000	0.00000	-0.04688	0.00000	0.00000
100	C7	PZ	-0.11001	0.09305	0.00000	-0.01461	0.06087
101	C7	S	0.00000	0.00000	-0.71747	0.00000	0.00000
102	C7	PX	0.00000	0.00000	0.97659	0.00000	0.00000
103	C7	PY	0.00000	0.00000	0.29625	0.00000	0.00000
104	C7	PZ	-0.15505	0.19656	0.00000	-0.02536	0.09791
105	C7	DXX	0.00000	0.00000	-0.26008	0.00000	0.00000
106	C7	DYY	0.00000	0.00000	0.18029	0.00000	0.00000
107	C7	DZZ	0.00000	0.00000	0.09879	0.00000	0.00000
108	C7	DXY	0.00000	0.00000	0.13087	0.00000	0.00000
109	C7	DXZ	0.12403	0.09388	0.00000	-0.12163	0.13682
110	C7	DYZ	-0.03786	0.14339	0.00000	-0.51171	0.23884
111	H3	S	0.00000	0.00000	0.11999	0.00000	0.00000
112	H3	S	0.00000	0.00000	0.14065	0.00000	0.00000
113	H3	PX	0.00000	0.00000	-0.12308	0.00000	0.00000
114	H3	PY	0.00000	0.00000	0.14389	0.00000	0.00000
115	H3	PZ	0.02575	-0.03140	0.00000	0.09579	0.15598
116	H4	S	0.00000	0.00000	-0.18521	0.00000	0.00000
117	H4	S	0.00000	0.00000	-0.08750	0.00000	0.00000
118	H4	PX	0.00000	0.00000	-0.09312	0.00000	0.00000
119	H4	PY	0.00000	0.00000	-0.20514	0.00000	0.00000
120	H4	PZ	-0.00711	-0.03715	0.00000	0.08889	0.08523
121	N1	S	0.00000	0.00000	-0.00556	0.00000	0.00000
122	N1	S	0.00000	0.00000	-0.00709	0.00000	0.00000
123	N1	PX	0.00000	0.00000	0.00958	0.00000	0.00000
124	N1	PY	0.00000	0.00000	0.09159	0.00000	0.00000
125	N1	PZ	0.01438	-0.00252	0.00000	-0.00764	0.00987
126	N1	S	0.00000	0.00000	0.07861	0.00000	0.00000
127	N1	PX	0.00000	0.00000	0.64376	0.00000	0.00000
128	N1	PY	0.00000	0.00000	-0.60885	0.00000	0.00000
129	N1	PZ	0.17542	0.11209	0.00000	-0.15096	-0.09936
130	N1	DXX	0.00000	0.00000	0.36798	0.00000	0.00000
131	N1	DYY	0.00000	0.00000	-0.13095	0.00000	0.00000
132	N1	DZZ	0.00000	0.00000	-0.17542	0.00000	0.00000
133	N1	DXY	0.00000	0.00000	0.16551	0.00000	0.00000
134	N1	DXZ	0.28263	0.13766	0.00000	-0.04888	-0.25885
135	N1	DYZ	-0.22432	0.03636	0.00000	-0.40313	0.13451
136	H6	S	0.00000	0.00000	0.06500	0.00000	0.00000
137	H6	S	0.00000	0.00000	0.11852	0.00000	0.00000
138	H6	PX	0.00000	0.00000	0.00010	0.00000	0.00000
139	H6	PY	0.00000	0.00000	0.10492	0.00000	0.00000
140	H6	PZ	0.04653	-0.03751	0.00000	-0.23215	-0.13815
141	C8	S	0.00000	0.00000	-0.00528	0.00000	0.00000
142	C8	S	0.00000	0.00000	-0.15238	0.00000	0.00000

143	C8	PX	0.00000	0.00000	0.10895	0.00000	0.00000
144	C8	PY	0.00000	0.00000	-0.06039	0.00000	0.00000
145	C8	PZ	-0.05703	0.02684	0.00000	-0.03956	0.06299
146	C8	S	0.00000	0.00000	0.29128	0.00000	0.00000
147	C8	PX	0.00000	0.00000	0.68627	0.00000	0.00000
148	C8	PY	0.00000	0.00000	0.26474	0.00000	0.00000
149	C8	PZ	-0.16443	-0.00738	0.00000	0.02903	-0.02407
150	C8	DXX	0.00000	0.00000	-0.04054	0.00000	0.00000
151	C8	DYY	0.00000	0.00000	0.02543	0.00000	0.00000
152	C8	DZZ	0.00000	0.00000	0.03006	0.00000	0.00000
153	C8	DXY	0.00000	0.00000	0.12589	0.00000	0.00000
154	C8	DXZ	0.59030	0.08955	0.00000	-0.15231	-0.09181
155	C8	DYZ	0.18479	-0.36479	0.00000	-0.27673	0.33328
156	H8	S	0.00000	0.00000	0.10583	0.00000	0.00000
157	H8	S	0.00000	0.00000	-0.37145	0.00000	0.00000
158	H8	PX	0.00000	0.00000	0.12595	0.00000	0.00000
159	H8	PY	0.00000	0.00000	-0.02791	0.00000	0.00000
160	H8	PZ	0.26040	-0.46690	0.00000	-0.07397	-0.23795
161	C10	S	0.00000	0.00000	-0.00085	0.00000	0.00000
162	C10	S	0.00000	0.00000	-0.01124	0.00000	0.00000
163	C10	PX	0.00000	0.00000	-0.01380	0.00000	0.00000
164	C10	PY	0.00000	0.00000	-0.02174	0.00000	0.00000
165	C10	PZ	0.06351	-0.10196	0.00000	-0.07262	0.11280
166	C10	S	0.00000	0.00000	0.13789	0.00000	0.00000
167	C10	PX	0.00000	0.00000	-0.18622	0.00000	0.00000
168	C10	PY	0.00000	0.00000	0.09473	0.00000	0.00000
169	C10	PZ	0.17192	-0.16267	0.00000	-0.11133	0.15985
170	C10	DXX	0.00000	0.00000	-0.01454	0.00000	0.00000
171	C10	DYY	0.00000	0.00000	0.02121	0.00000	0.00000
172	C10	DZZ	0.00000	0.00000	-0.01975	0.00000	0.00000
173	C10	DXY	0.00000	0.00000	-0.14470	0.00000	0.00000
174	C10	DXZ	0.07782	0.00772	0.00000	-0.03973	-0.02351
175	C10	DYZ	0.18327	-0.11365	0.00000	-0.04373	-0.06072
176	H16	S	0.00000	0.00000	-0.07659	0.00000	0.00000
177	H16	S	0.00000	0.00000	0.16247	0.00000	0.00000
178	H16	PX	0.00000	0.00000	0.05113	0.00000	0.00000
179	H16	PY	0.00000	0.00000	0.15767	0.00000	0.00000
180	H16	PZ	-0.32011	0.24909	0.00000	0.25278	-0.33808
181	H18	S	0.00000	0.00000	0.04937	0.00000	0.00000
182	H18	S	0.00000	0.00000	-0.10386	0.00000	0.00000
183	H18	PX	0.00000	0.00000	0.02754	0.00000	0.00000
184	H18	PY	0.00000	0.00000	-0.14848	0.00000	0.00000
185	H18	PZ	-0.02902	0.31855	0.00000	0.15261	-0.38947

MO:	136	137	138	139	140
Eigenvalues:	2.61465	2.64801	2.68326	2.70446	2.71343
(ev):	71.14828	72.05602	73.01517	73.59204	73.83611

		A	A	A	A	A	
1	H1	S	-0.09206	-0.25088	0.00000	-0.08840	0.00000
2	H1	S	0.19493	0.28337	0.00000	0.06172	0.00000
3	H1	PX	-0.11708	-0.19510	0.00000	0.07800	0.00000
4	H1	PY	0.14465	0.06234	0.00000	-0.21260	0.00000
5	H1	PZ	0.00000	0.00000	-0.11704	0.00000	-0.41877

6	C1	S	-0.03692	-0.03252	0.00000	-0.02264	0.00000
7	C1	S	-0.17754	-0.19199	0.00000	-0.07861	0.00000
8	C1	PX	-0.08620	-0.12851	0.00000	-0.02648	0.00000
9	C1	PY	-0.10895	0.07528	0.00000	0.03435	0.00000
10	C1	PZ	0.00000	0.00000	-0.02317	0.00000	0.08906
11	C1	S	1.17478	1.47144	0.00000	1.37082	0.00000
12	C1	PX	-0.51479	-0.51233	0.00000	-0.27330	0.00000
13	C1	PY	-1.04810	0.33824	0.00000	0.01394	0.00000
14	C1	PZ	0.00000	0.00000	-0.04034	0.00000	0.10352
15	C1	DXX	0.14670	0.33758	0.00000	0.02122	0.00000
16	C1	DYY	0.16207	-0.11719	0.00000	0.19067	0.00000
17	C1	DZZ	-0.37733	-0.32251	0.00000	-0.16279	0.00000
18	C1	DXY	0.24754	-0.02500	0.00000	0.09412	0.00000
19	C1	DXZ	0.00000	0.00000	0.14002	0.00000	0.17718
20	C1	DYZ	0.00000	0.00000	-0.29975	0.00000	0.31707
21	C2	S	-0.03420	-0.00885	0.00000	0.00087	0.00000
22	C2	S	-0.38728	-0.23808	0.00000	0.02558	0.00000
23	C2	PX	-0.00835	-0.02266	0.00000	0.05246	0.00000
24	C2	PY	-0.13875	0.00515	0.00000	-0.02196	0.00000
25	C2	PZ	0.00000	0.00000	0.09680	0.00000	-0.01636
26	C2	S	2.46070	1.29304	0.00000	-0.82821	0.00000
27	C2	PX	1.45002	0.63600	0.00000	0.23888	0.00000
28	C2	PY	-0.76482	0.52839	0.00000	-0.39811	0.00000
29	C2	PZ	0.00000	0.00000	0.07559	0.00000	-0.01625
30	C2	DXX	0.12751	0.21129	0.00000	0.01648	0.00000
31	C2	DYY	0.09218	-0.25571	0.00000	0.01802	0.00000
32	C2	DZZ	-0.20539	-0.00833	0.00000	-0.05893	0.00000
33	C2	DXY	-0.23642	0.14156	0.00000	-0.08795	0.00000
34	C2	DXZ	0.00000	0.00000	-0.19892	0.00000	-0.05076
35	C2	DYZ	0.00000	0.00000	-0.17584	0.00000	0.14695
36	C3	S	0.01412	-0.01576	0.00000	-0.04053	0.00000
37	C3	S	-0.03108	0.03405	0.00000	-0.23874	0.00000
38	C3	PX	0.03949	0.06444	0.00000	-0.10646	0.00000
39	C3	PY	-0.28984	-0.21388	0.00000	-0.05873	0.00000
40	C3	PZ	0.00000	0.00000	-0.03095	0.00000	0.04004
41	C3	S	0.43175	0.95389	0.00000	1.39066	0.00000
42	C3	PX	-0.66388	0.56320	0.00000	-0.67912	0.00000
43	C3	PY	-1.73162	-1.25206	0.00000	-1.04298	0.00000
44	C3	PZ	0.00000	0.00000	-0.01475	0.00000	-0.04548
45	C3	DXX	0.05738	0.16001	0.00000	0.18318	0.00000
46	C3	DYY	-0.07293	0.05620	0.00000	0.06182	0.00000
47	C3	DZZ	0.06065	-0.11470	0.00000	-0.29726	0.00000
48	C3	DXY	-0.14085	-0.02089	0.00000	-0.17911	0.00000
49	C3	DXZ	0.00000	0.00000	0.06658	0.00000	-0.09623
50	C3	DYZ	0.00000	0.00000	-0.09551	0.00000	0.19569
51	C4	S	-0.00585	0.00533	0.00000	-0.02168	0.00000
52	C4	S	-0.08371	-0.03233	0.00000	-0.01223	0.00000
53	C4	PX	-0.00698	0.02249	0.00000	-0.19518	0.00000
54	C4	PY	0.05442	0.10026	0.00000	0.02679	0.00000
55	C4	PZ	0.00000	0.00000	0.07986	0.00000	0.03600
56	C4	S	0.78756	-0.48513	0.00000	0.52772	0.00000
57	C4	PX	0.18403	-0.89441	0.00000	-0.81419	0.00000
58	C4	PY	-0.29582	0.23931	0.00000	0.50646	0.00000
59	C4	PZ	0.00000	0.00000	0.07964	0.00000	0.01630

60	C4	DXX	0.00243	0.06691	0.00000	0.28686	0.00000
61	C4	DYY	-0.02774	-0.16205	0.00000	-0.16292	0.00000
62	C4	DZZ	0.06076	0.12809	0.00000	-0.15866	0.00000
63	C4	DXY	0.00653	0.01150	0.00000	0.15462	0.00000
64	C4	DXZ	0.00000	0.00000	0.37087	0.00000	-0.12311
65	C4	DYZ	0.00000	0.00000	-0.01564	0.00000	0.45216
66	C5	S	-0.00669	0.01643	0.00000	0.02150	0.00000
67	C5	S	0.18391	0.25496	0.00000	-0.05821	0.00000
68	C5	PX	0.06035	-0.07371	0.00000	-0.12538	0.00000
69	C5	PY	-0.03672	-0.02326	0.00000	0.02490	0.00000
70	C5	PZ	0.00000	0.00000	0.10815	0.00000	0.00558
71	C5	S	-0.69566	-1.73806	0.00000	-0.37698	0.00000
72	C5	PX	-0.59483	-0.02037	0.00000	-1.05266	0.00000
73	C5	PY	0.62978	0.59455	0.00000	-0.59731	0.00000
74	C5	PZ	0.00000	0.00000	0.05773	0.00000	0.03510
75	C5	DXX	0.08059	-0.01073	0.00000	-0.23735	0.00000
76	C5	DYY	-0.03768	-0.10552	0.00000	0.08194	0.00000
77	C5	DZZ	-0.08370	0.10205	0.00000	0.19398	0.00000
78	C5	DXY	0.05249	0.16438	0.00000	-0.02018	0.00000
79	C5	DXZ	0.00000	0.00000	-0.01984	0.00000	-0.18050
80	C5	DYZ	0.00000	0.00000	0.22190	0.00000	0.18965
81	C6	S	0.00150	-0.04089	0.00000	0.04185	0.00000
82	C6	S	0.08275	-0.25181	0.00000	0.26334	0.00000
83	C6	PX	-0.05032	-0.16567	0.00000	-0.05627	0.00000
84	C6	PY	-0.12817	0.18178	0.00000	-0.17544	0.00000
85	C6	PZ	0.00000	0.00000	0.04903	0.00000	-0.04708
86	C6	S	-1.12585	0.54185	0.00000	-1.11792	0.00000
87	C6	PX	0.50935	0.23886	0.00000	-0.87857	0.00000
88	C6	PY	-1.97624	-0.52710	0.00000	0.05899	0.00000
89	C6	PZ	0.00000	0.00000	0.06809	0.00000	-0.06340
90	C6	DXX	-0.00364	0.01886	0.00000	-0.21037	0.00000
91	C6	DYY	0.05376	0.20638	0.00000	-0.02565	0.00000
92	C6	DZZ	-0.19118	-0.27908	0.00000	0.26220	0.00000
93	C6	DXY	0.20349	0.05876	0.00000	-0.00424	0.00000
94	C6	DXZ	0.00000	0.00000	0.13624	0.00000	-0.08953
95	C6	DYZ	0.00000	0.00000	-0.33636	0.00000	0.31243
96	C7	S	0.06646	0.01851	0.00000	-0.05602	0.00000
97	C7	S	0.53837	0.15280	0.00000	-0.31054	0.00000
98	C7	PX	0.05854	-0.10026	0.00000	-0.08097	0.00000
99	C7	PY	-0.09486	-0.16758	0.00000	-0.29922	0.00000
100	C7	PZ	0.00000	0.00000	-0.01205	0.00000	0.04490
101	C7	S	-3.23497	-0.61543	0.00000	1.11071	0.00000
102	C7	PX	1.84783	-0.22212	0.00000	-0.66083	0.00000
103	C7	PY	-0.57815	-1.39467	0.00000	-0.91919	0.00000
104	C7	PZ	0.00000	0.00000	-0.03867	0.00000	0.08431
105	C7	DXX	-0.30280	0.19510	0.00000	0.24090	0.00000
106	C7	DYY	-0.16183	-0.34548	0.00000	0.09636	0.00000
107	C7	DZZ	0.57237	0.21706	0.00000	-0.44906	0.00000
108	C7	DXY	0.12771	0.24901	0.00000	0.37722	0.00000
109	C7	DXZ	0.00000	0.00000	-0.08143	0.00000	0.18946
110	C7	DYZ	0.00000	0.00000	-0.08347	0.00000	0.13420
111	H3	S	-0.00854	0.12381	0.00000	-0.07845	0.00000
112	H3	S	0.02774	0.04368	0.00000	-0.04898	0.00000
113	H3	PX	-0.11012	0.38307	0.00000	-0.03131	0.00000

114	H3	PY	0.11773	-0.09853	0.00000	0.00823	0.00000
115	H3	PZ	0.00000	0.00000	-0.34926	0.00000	-0.52580
116	H4	S	-0.06628	0.15601	0.00000	0.02656	0.00000
117	H4	S	-0.23820	-0.17784	0.00000	0.02732	0.00000
118	H4	PX	0.15511	-0.22871	0.00000	0.27370	0.00000
119	H4	PY	0.12606	-0.04689	0.00000	0.16225	0.00000
120	H4	PZ	0.00000	0.00000	-0.45584	0.00000	-0.36233
121	N1	S	0.01604	-0.01205	0.00000	0.03130	0.00000
122	N1	S	0.28868	-0.28323	0.00000	0.53464	0.00000
123	N1	PX	-0.00493	-0.03443	0.00000	0.03385	0.00000
124	N1	PY	-0.18940	-0.15470	0.00000	0.04155	0.00000
125	N1	PZ	0.00000	0.00000	0.00106	0.00000	0.00422
126	N1	S	-1.49822	0.45830	0.00000	-1.60388	0.00000
127	N1	PX	-0.64756	0.34532	0.00000	-0.44114	0.00000
128	N1	PY	-0.26016	0.17271	0.00000	0.13320	0.00000
129	N1	PZ	0.00000	0.00000	-0.20641	0.00000	0.17005
130	N1	DXX	-0.30268	0.18835	0.00000	-0.12110	0.00000
131	N1	DYY	0.04876	-0.03640	0.00000	-0.17841	0.00000
132	N1	DZZ	0.22093	-0.21662	0.00000	0.35398	0.00000
133	N1	DXY	-0.05321	0.05224	0.00000	0.14733	0.00000
134	N1	DXZ	0.00000	0.00000	-0.35963	0.00000	0.27251
135	N1	DYZ	0.00000	0.00000	-0.10636	0.00000	0.13749
136	H6	S	0.00894	-0.11712	0.00000	0.09631	0.00000
137	H6	S	0.35563	0.27300	0.00000	0.10484	0.00000
138	H6	PX	0.03440	0.12657	0.00000	0.06755	0.00000
139	H6	PY	0.02180	-0.09204	0.00000	0.09041	0.00000
140	H6	PZ	0.00000	0.00000	-0.46890	0.00000	-0.02809
141	C8	S	0.00379	0.02905	0.00000	0.03256	0.00000
142	C8	S	0.11219	0.17125	0.00000	0.21766	0.00000
143	C8	PX	-0.01278	-0.01867	0.00000	-0.35182	0.00000
144	C8	PY	0.48011	-0.19099	0.00000	0.02018	0.00000
145	C8	PZ	0.00000	0.00000	0.04253	0.00000	-0.00909
146	C8	S	0.21694	-0.01755	0.00000	-0.86443	0.00000
147	C8	PX	0.86154	-0.67616	0.00000	-1.70817	0.00000
148	C8	PY	1.17511	-1.91425	0.00000	-0.16588	0.00000
149	C8	PZ	0.00000	0.00000	0.07206	0.00000	-0.06726
150	C8	DXX	-0.08392	-0.17401	0.00000	-0.24546	0.00000
151	C8	DYY	-0.09239	0.06719	0.00000	0.00436	0.00000
152	C8	DZZ	0.08676	0.20041	0.00000	0.23982	0.00000
153	C8	DXY	0.06275	-0.06662	0.00000	-0.20400	0.00000
154	C8	DXZ	0.00000	0.00000	-0.20092	0.00000	0.17058
155	C8	DYZ	0.00000	0.00000	0.08220	0.00000	-0.01544
156	H8	S	0.15711	-0.00229	0.00000	-0.07922	0.00000
157	H8	S	-0.64405	-0.07421	0.00000	0.06641	0.00000
158	H8	PX	0.16779	0.14920	0.00000	0.04767	0.00000
159	H8	PY	-0.06119	0.27364	0.00000	0.19302	0.00000
160	H8	PZ	0.00000	0.00000	0.10368	0.00000	-0.26763
161	C10	S	-0.04215	0.03573	0.00000	-0.00380	0.00000
162	C10	S	-0.18499	0.13951	0.00000	-0.01127	0.00000
163	C10	PX	0.01598	0.02293	0.00000	0.11245	0.00000
164	C10	PY	0.15744	-0.11772	0.00000	0.04355	0.00000
165	C10	PZ	0.00000	0.00000	0.04001	0.00000	-0.00579
166	C10	S	1.50496	-1.90112	0.00000	0.11564	0.00000
167	C10	PX	-0.35932	0.03218	0.00000	0.73954	0.00000

168	C10	PY	0.86383	-1.01612	0.00000	-0.13294	0.00000
169	C10	PZ	0.00000	0.00000	0.04393	0.00000	-0.00095
170	C10	DXX	-0.05676	0.03225	0.00000	-0.00204	0.00000
171	C10	DYY	0.43259	-0.27831	0.00000	0.00307	0.00000
172	C10	DZZ	-0.48699	0.30718	0.00000	-0.05968	0.00000
173	C10	DXY	-0.00133	0.06890	0.00000	0.30814	0.00000
174	C10	DXZ	0.00000	0.00000	-0.09883	0.00000	0.10578
175	C10	DYZ	0.00000	0.00000	-0.12299	0.00000	0.03998
176	H16	S	-0.05945	0.14256	0.00000	0.04006	0.00000
177	H16	S	0.22526	-0.20011	0.00000	-0.45350	0.00000
178	H16	PX	-0.11975	0.04621	0.00000	-0.00107	0.00000
179	H16	PY	-0.03603	-0.01734	0.00000	-0.17392	0.00000
180	H16	PZ	0.00000	0.00000	-0.08143	0.00000	-0.06377
181	H18	S	-0.12373	0.04471	0.00000	-0.03018	0.00000
182	H18	S	-0.09542	-0.01667	0.00000	0.30977	0.00000
183	H18	PX	0.09912	-0.05610	0.00000	0.05884	0.00000
184	H18	PY	-0.08305	0.14605	0.00000	0.29543	0.00000
185	H18	PZ	0.00000	0.00000	-0.28515	0.00000	0.15609

MO:	141	142	143	144	145
Eigenvalues:	2.72800	2.73003	2.74124	2.80231	2.80292
(ev):	74.23264	74.28780	74.59310	76.25478	76.27139

		A	A	A	A	A	
1	H1	S	0.07951	0.00000	0.00941	0.00000	0.05690
2	H1	S	-0.22101	0.00000	-0.12936	0.00000	0.16581
3	H1	PX	0.14472	0.00000	0.12504	0.00000	-0.00788
4	H1	PY	0.05354	0.00000	0.22061	0.00000	-0.44815
5	H1	PZ	0.00000	0.44587	0.00000	0.15800	0.00000
6	C1	S	0.00012	0.00000	0.00666	0.00000	0.00846
7	C1	S	0.33103	0.00000	-0.08909	0.00000	0.02845
8	C1	PX	-0.05826	0.00000	0.20044	0.00000	-0.05718
9	C1	PY	0.03976	0.00000	-0.16372	0.00000	0.18510
10	C1	PZ	0.00000	-0.02550	0.00000	-0.03798	0.00000
11	C1	S	-0.87578	0.00000	0.41085	0.00000	-0.30726
12	C1	PX	0.54749	0.00000	0.23894	0.00000	-0.39225
13	C1	PY	-0.38709	0.00000	-0.89007	0.00000	1.03366
14	C1	PZ	0.00000	-0.06795	0.00000	-0.05023	0.00000
15	C1	DXX	-0.18810	0.00000	-0.12130	0.00000	0.06113
16	C1	DYY	0.27594	0.00000	0.00275	0.00000	0.00391
17	C1	DZZ	-0.03703	0.00000	0.15248	0.00000	0.00161
18	C1	DXY	0.01032	0.00000	0.11040	0.00000	-0.03098
19	C1	DXZ	0.00000	-0.30058	0.00000	-0.08709	0.00000
20	C1	DYZ	0.00000	0.06428	0.00000	0.03195	0.00000
21	C2	S	0.02492	0.00000	-0.00904	0.00000	-0.03735
22	C2	S	0.24398	0.00000	-0.15362	0.00000	0.04382
23	C2	PX	-0.00846	0.00000	0.09906	0.00000	0.27581
24	C2	PY	0.02129	0.00000	0.05206	0.00000	0.38836
25	C2	PZ	0.00000	0.03237	0.00000	0.02993	0.00000
26	C2	S	-1.12159	0.00000	0.24962	0.00000	1.46243
27	C2	PX	-0.26596	0.00000	0.41065	0.00000	0.29138
28	C2	PY	0.71335	0.00000	0.38125	0.00000	2.09176
29	C2	PZ	0.00000	0.07224	0.00000	0.03870	0.00000
30	C2	DXX	-0.14912	0.00000	0.18666	0.00000	0.17248

31	C2	DYY	0.04720	0.00000	-0.17479	0.00000	0.22050
32	C2	DZZ	0.21501	0.00000	-0.12150	0.00000	-0.41272
33	C2	DXY	0.00954	0.00000	0.11861	0.00000	0.31598
34	C2	DXZ	0.00000	-0.31434	0.00000	0.04431	0.00000
35	C2	DYZ	0.00000	0.02044	0.00000	0.29577	0.00000
36	C3	S	0.00109	0.00000	0.00444	0.00000	-0.00809
37	C3	S	0.02857	0.00000	-0.02435	0.00000	-0.13041
38	C3	PX	-0.11174	0.00000	-0.04534	0.00000	0.02669
39	C3	PY	-0.14863	0.00000	0.21546	0.00000	0.03722
40	C3	PZ	0.00000	-0.02964	0.00000	-0.05079	0.00000
41	C3	S	0.76155	0.00000	0.85078	0.00000	1.14407
42	C3	PX	-0.02944	0.00000	-1.28556	0.00000	1.07016
43	C3	PY	-0.61299	0.00000	-1.72428	0.00000	-0.03209
44	C3	PZ	0.00000	0.08268	0.00000	0.04556	0.00000
45	C3	DXX	0.06765	0.00000	0.07073	0.00000	-0.16960
46	C3	DYY	-0.06780	0.00000	-0.16050	0.00000	0.18259
47	C3	DZZ	0.06953	0.00000	0.07691	0.00000	-0.05076
48	C3	DXY	-0.05549	0.00000	0.17597	0.00000	0.12019
49	C3	DXZ	0.00000	-0.18436	0.00000	0.12202	0.00000
50	C3	DYZ	0.00000	0.06573	0.00000	0.10945	0.00000
51	C4	S	-0.02196	0.00000	-0.07218	0.00000	0.02873
52	C4	S	-0.41984	0.00000	-0.27853	0.00000	0.06612
53	C4	PX	-0.12417	0.00000	-0.14353	0.00000	-0.08635
54	C4	PY	0.04541	0.00000	-0.21440	0.00000	0.04641
55	C4	PZ	0.00000	-0.04182	0.00000	-0.01725	0.00000
56	C4	S	1.86832	0.00000	2.64223	0.00000	-1.64901
57	C4	PX	-0.29552	0.00000	-0.89041	0.00000	0.20561
58	C4	PY	-0.79401	0.00000	-0.73911	0.00000	-0.01802
59	C4	PZ	0.00000	-0.03483	0.00000	0.00979	0.00000
60	C4	DXX	0.01671	0.00000	0.26047	0.00000	0.00112
61	C4	DYY	0.06110	0.00000	0.25221	0.00000	-0.18875
62	C4	DZZ	-0.12672	0.00000	-0.63768	0.00000	0.20128
63	C4	DXY	0.32043	0.00000	0.06615	0.00000	0.22680
64	C4	DXZ	0.00000	-0.21925	0.00000	0.12739	0.00000
65	C4	DYZ	0.00000	-0.07930	0.00000	0.02453	0.00000
66	C5	S	0.02189	0.00000	0.05951	0.00000	0.04656
67	C5	S	0.20435	0.00000	0.35880	0.00000	-0.01495
68	C5	PX	0.01184	0.00000	-0.25360	0.00000	0.15239
69	C5	PY	-0.00841	0.00000	0.11036	0.00000	0.37138
70	C5	PZ	0.00000	0.03607	0.00000	-0.00937	0.00000
71	C5	S	-1.04886	0.00000	-2.48083	0.00000	-1.97098
72	C5	PX	-0.63280	0.00000	-0.98136	0.00000	1.40965
73	C5	PY	0.28970	0.00000	0.67426	0.00000	1.27365
74	C5	PZ	0.00000	0.03277	0.00000	-0.00767	0.00000
75	C5	DXX	0.01411	0.00000	-0.32674	0.00000	0.08944
76	C5	DYY	-0.15643	0.00000	-0.05302	0.00000	-0.50192
77	C5	DZZ	0.14861	0.00000	0.50463	0.00000	0.44801
78	C5	DXY	-0.02581	0.00000	0.28957	0.00000	-0.29711
79	C5	DXZ	0.00000	-0.21524	0.00000	0.15128	0.00000
80	C5	DYZ	0.00000	0.15367	0.00000	0.30911	0.00000
81	C6	S	-0.04122	0.00000	0.01665	0.00000	-0.01424
82	C6	S	-0.42051	0.00000	0.09400	0.00000	0.01889
83	C6	PX	-0.01723	0.00000	-0.08037	0.00000	0.04998
84	C6	PY	0.12241	0.00000	-0.08050	0.00000	-0.21090

85	C6	PZ	0.00000	0.05786	0.00000	-0.01567	0.00000
86	C6	S	0.30326	0.00000	-1.34429	0.00000	1.83171
87	C6	PX	-0.40726	0.00000	-0.90460	0.00000	-0.53427
88	C6	PY	1.28408	0.00000	1.12200	0.00000	0.56502
89	C6	PZ	0.00000	-0.06221	0.00000	-0.06710	0.00000
90	C6	DXX	-0.20477	0.00000	-0.03445	0.00000	0.21249
91	C6	DYY	0.31698	0.00000	0.01030	0.00000	-0.00910
92	C6	DZZ	-0.20970	0.00000	0.06222	0.00000	-0.11386
93	C6	DXY	0.24800	0.00000	-0.01061	0.00000	-0.06752
94	C6	DXZ	0.00000	-0.26106	0.00000	0.11639	0.00000
95	C6	DYZ	0.00000	-0.05345	0.00000	0.33632	0.00000
96	C7	S	0.02128	0.00000	0.01142	0.00000	-0.00207
97	C7	S	0.08842	0.00000	0.24917	0.00000	0.03229
98	C7	PX	0.00963	0.00000	0.01890	0.00000	-0.00579
99	C7	PY	-0.00921	0.00000	0.11859	0.00000	-0.04803
100	C7	PZ	0.00000	-0.00562	0.00000	-0.03790	0.00000
101	C7	S	-0.76733	0.00000	-2.18589	0.00000	-0.78496
102	C7	PX	0.11592	0.00000	1.39910	0.00000	-0.02549
103	C7	PY	-0.38857	0.00000	0.08232	0.00000	-0.42775
104	C7	PZ	0.00000	-0.03443	0.00000	-0.08312	0.00000
105	C7	DXX	0.03400	0.00000	-0.14991	0.00000	-0.03763
106	C7	DYY	-0.14668	0.00000	0.18501	0.00000	0.03251
107	C7	DZZ	0.17218	0.00000	0.00652	0.00000	-0.03458
108	C7	DXY	-0.01386	0.00000	-0.00258	0.00000	0.00126
109	C7	DXZ	0.00000	0.03838	0.00000	-0.31451	0.00000
110	C7	DYZ	0.00000	0.20142	0.00000	0.14139	0.00000
111	H3	S	-0.14745	0.00000	-0.19907	0.00000	0.12223
112	H3	S	0.31744	0.00000	0.38344	0.00000	0.03787
113	H3	PX	-0.27722	0.00000	0.14050	0.00000	-0.27173
114	H3	PY	-0.05995	0.00000	-0.33295	0.00000	0.05676
115	H3	PZ	0.00000	0.27787	0.00000	-0.07095	0.00000
116	H4	S	0.04625	0.00000	0.19999	0.00000	0.13884
117	H4	S	-0.21203	0.00000	-0.40450	0.00000	-0.12272
118	H4	PX	0.38887	0.00000	-0.20385	0.00000	-0.13430
119	H4	PY	0.27073	0.00000	0.20700	0.00000	0.03294
120	H4	PZ	0.00000	-0.36407	0.00000	-0.20669	0.00000
121	N1	S	-0.02263	0.00000	-0.00151	0.00000	0.00580
122	N1	S	-0.69843	0.00000	-0.07506	0.00000	0.11891
123	N1	PX	-0.12177	0.00000	-0.01195	0.00000	0.04825
124	N1	PY	-0.21566	0.00000	0.05864	0.00000	-0.01411
125	N1	PZ	0.00000	-0.01279	0.00000	0.03025	0.00000
126	N1	S	1.88877	0.00000	0.70473	0.00000	-0.56244
127	N1	PX	0.67318	0.00000	0.16033	0.00000	-0.15790
128	N1	PY	0.58448	0.00000	-0.12580	0.00000	-0.38995
129	N1	PZ	0.00000	0.04591	0.00000	0.04067	0.00000
130	N1	DXX	0.10140	0.00000	-0.00863	0.00000	0.10584
131	N1	DYY	0.11649	0.00000	-0.03566	0.00000	-0.15606
132	N1	DZZ	-0.32409	0.00000	0.06002	0.00000	0.05665
133	N1	DXY	0.19719	0.00000	-0.02942	0.00000	-0.24838
134	N1	DXZ	0.00000	0.17535	0.00000	-0.02629	0.00000
135	N1	DYZ	0.00000	-0.31348	0.00000	0.35095	0.00000
136	H6	S	0.14026	0.00000	-0.06776	0.00000	-0.13289
137	H6	S	-0.10674	0.00000	0.21389	0.00000	0.14746
138	H6	PX	-0.11151	0.00000	0.21451	0.00000	0.15853

139	H6	PY	-0.37149	0.00000	0.07541	0.00000	-0.45151
140	H6	PZ	0.00000	-0.48866	0.00000	0.01617	0.00000
141	C8	S	-0.01268	0.00000	-0.00858	0.00000	0.01215
142	C8	S	-0.05399	0.00000	-0.19782	0.00000	-0.06554
143	C8	PX	0.04069	0.00000	0.04504	0.00000	0.09581
144	C8	PY	-0.14114	0.00000	0.04351	0.00000	0.01744
145	C8	PZ	0.00000	-0.04123	0.00000	-0.09450	0.00000
146	C8	S	0.44980	0.00000	0.56885	0.00000	-0.50594
147	C8	PX	0.15356	0.00000	0.96643	0.00000	0.04683
148	C8	PY	-0.65859	0.00000	1.27436	0.00000	0.92799
149	C8	PZ	0.00000	-0.01438	0.00000	0.06524	0.00000
150	C8	DXX	0.04741	0.00000	0.06827	0.00000	-0.04711
151	C8	DYY	0.11554	0.00000	-0.05051	0.00000	-0.12566
152	C8	DZZ	-0.10744	0.00000	-0.00394	0.00000	0.14054
153	C8	DXY	0.00552	0.00000	0.00825	0.00000	-0.02988
154	C8	DXZ	0.00000	0.27627	0.00000	-0.09923	0.00000
155	C8	DYZ	0.00000	-0.03819	0.00000	0.28066	0.00000
156	H8	S	0.00539	0.00000	0.01868	0.00000	0.03790
157	H8	S	-0.02613	0.00000	-0.37774	0.00000	0.01150
158	H8	PX	0.05960	0.00000	0.00481	0.00000	0.03214
159	H8	PY	0.08063	0.00000	-0.17792	0.00000	0.08916
160	H8	PZ	0.00000	0.07380	0.00000	0.46125	0.00000
161	C10	S	0.01796	0.00000	-0.01448	0.00000	-0.01100
162	C10	S	0.04967	0.00000	-0.03399	0.00000	0.02105
163	C10	PX	-0.00148	0.00000	-0.02269	0.00000	-0.03337
164	C10	PY	-0.13088	0.00000	0.07883	0.00000	0.15357
165	C10	PZ	0.00000	-0.01671	0.00000	-0.01882	0.00000
166	C10	S	-0.86119	0.00000	0.98955	0.00000	0.91813
167	C10	PX	-0.18228	0.00000	-0.29683	0.00000	-0.07597
168	C10	PY	-0.39744	0.00000	0.51295	0.00000	0.37314
169	C10	PZ	0.00000	-0.02534	0.00000	-0.08583	0.00000
170	C10	DXX	0.03922	0.00000	-0.01108	0.00000	-0.05152
171	C10	DYY	-0.17959	0.00000	0.11550	0.00000	0.12765
172	C10	DZZ	0.18052	0.00000	-0.12758	0.00000	-0.09884
173	C10	DXY	0.01050	0.00000	-0.06741	0.00000	-0.10720
174	C10	DXZ	0.00000	0.18881	0.00000	-0.17661	0.00000
175	C10	DYZ	0.00000	0.06983	0.00000	0.49385	0.00000
176	H16	S	0.07833	0.00000	-0.03637	0.00000	-0.04618
177	H16	S	0.00689	0.00000	0.19381	0.00000	0.08794
178	H16	PX	0.03185	0.00000	-0.03923	0.00000	-0.02963
179	H16	PY	-0.02550	0.00000	0.01748	0.00000	0.10737
180	H16	PZ	0.00000	-0.09590	0.00000	0.54474	0.00000
181	H18	S	-0.01562	0.00000	-0.04678	0.00000	0.01610
182	H18	S	-0.02876	0.00000	-0.08595	0.00000	-0.10962
183	H18	PX	-0.06373	0.00000	0.01572	0.00000	0.03195
184	H18	PY	0.05579	0.00000	-0.07388	0.00000	-0.13180
185	H18	PZ	0.00000	0.28722	0.00000	0.15489	0.00000

MO:	146	147	148	149	150
Eigenvalues:	2.83549	2.86871	2.88238	2.92014	2.93390
(ev):	77.15767	78.06173	78.43366	79.46111	79.83563

	A	A	A	A	A	
1 H1	S	-0.11053	0.00000	0.02070	0.02042	0.00000

2	H1	S	-0.22806	0.00000	-0.18686	-0.10142	0.00000
3	H1	PX	0.02147	0.00000	0.03877	0.13183	0.00000
4	H1	PY	-0.33753	0.00000	0.26944	0.12702	0.00000
5	H1	PZ	0.00000	0.07024	0.00000	0.00000	0.46301
6	C1	S	-0.01175	0.00000	0.01300	0.03175	0.00000
7	C1	S	0.15017	0.00000	-0.04484	0.05942	0.00000
8	C1	PX	-0.12926	0.00000	0.14938	0.19820	0.00000
9	C1	PY	0.39424	0.00000	0.03088	0.07818	0.00000
10	C1	PZ	0.00000	0.02070	0.00000	0.00000	0.00216
11	C1	S	0.79627	0.00000	-0.80424	-1.09373	0.00000
12	C1	PX	0.36224	0.00000	0.57113	0.39278	0.00000
13	C1	PY	3.02780	0.00000	-2.22389	-0.12888	0.00000
14	C1	PZ	0.00000	0.05966	0.00000	0.00000	-0.07591
15	C1	DXX	0.04076	0.00000	-0.13468	-0.09068	0.00000
16	C1	DYY	0.10053	0.00000	-0.02451	-0.13470	0.00000
17	C1	DZZ	-0.16760	0.00000	0.10571	0.23832	0.00000
18	C1	DXY	-0.55572	0.00000	0.04204	-0.06454	0.00000
19	C1	DXZ	0.00000	-0.12268	0.00000	0.00000	-0.45311
20	C1	DYZ	0.00000	0.14675	0.00000	0.00000	0.00600
21	C2	S	0.03975	0.00000	0.02124	0.00849	0.00000
22	C2	S	-0.01429	0.00000	0.06993	0.01764	0.00000
23	C2	PX	-0.14907	0.00000	-0.06280	-0.09390	0.00000
24	C2	PY	0.02230	0.00000	0.18390	-0.17506	0.00000
25	C2	PZ	0.00000	-0.01910	0.00000	0.00000	0.01093
26	C2	S	-1.30912	0.00000	0.23453	-0.68295	0.00000
27	C2	PX	0.05757	0.00000	-0.10038	-0.30532	0.00000
28	C2	PY	-0.41774	0.00000	3.41226	-0.40653	0.00000
29	C2	PZ	0.00000	-0.06268	0.00000	0.00000	-0.04349
30	C2	DXX	-0.08004	0.00000	-0.06033	-0.03836	0.00000
31	C2	DYY	-0.16029	0.00000	-0.01476	-0.07945	0.00000
32	C2	DZZ	0.30841	0.00000	0.15271	0.10547	0.00000
33	C2	DXY	-0.08100	0.00000	0.31022	-0.16441	0.00000
34	C2	DXZ	0.00000	-0.02912	0.00000	0.00000	0.45540
35	C2	DYZ	0.00000	-0.18724	0.00000	0.00000	0.16740
36	C3	S	-0.03809	0.00000	-0.03552	-0.06482	0.00000
37	C3	S	-0.17460	0.00000	-0.10277	-0.26420	0.00000
38	C3	PX	-0.04702	0.00000	-0.05147	-0.02265	0.00000
39	C3	PY	0.16156	0.00000	0.08096	0.18314	0.00000
40	C3	PZ	0.00000	0.04301	0.00000	0.00000	-0.02375
41	C3	S	2.26004	0.00000	1.11753	2.22459	0.00000
42	C3	PX	0.41988	0.00000	-2.52314	0.55554	0.00000
43	C3	PY	1.73242	0.00000	-0.81150	-0.81585	0.00000
44	C3	PZ	0.00000	-0.02495	0.00000	0.00000	0.06028
45	C3	DXX	0.13474	0.00000	0.11895	-0.07838	0.00000
46	C3	DYY	0.07947	0.00000	0.03404	0.38624	0.00000
47	C3	DZZ	-0.22205	0.00000	-0.21965	-0.43971	0.00000
48	C3	DXY	0.29211	0.00000	0.19197	-0.02802	0.00000
49	C3	DXZ	0.00000	0.25789	0.00000	0.00000	0.02258
50	C3	DYZ	0.00000	-0.23038	0.00000	0.00000	-0.14255
51	C4	S	0.01772	0.00000	0.01922	-0.01063	0.00000
52	C4	S	-0.12424	0.00000	0.04796	-0.10927	0.00000
53	C4	PX	-0.23712	0.00000	0.13826	0.10063	0.00000
54	C4	PY	0.29705	0.00000	-0.10858	-0.12421	0.00000
55	C4	PZ	0.00000	-0.02071	0.00000	0.00000	-0.01648

56	C4	S	-0.75845	0.00000	-0.17209	0.66591	0.00000
57	C4	PX	-2.94965	0.00000	2.39084	0.16565	0.00000
58	C4	PY	1.25371	0.00000	-1.18627	-0.41084	0.00000
59	C4	PZ	0.00000	-0.08589	0.00000	0.00000	0.04178
60	C4	DXX	0.04560	0.00000	-0.41867	-0.19576	0.00000
61	C4	DYY	-0.29477	0.00000	0.30920	0.22646	0.00000
62	C4	DZZ	0.22479	0.00000	0.11471	-0.07542	0.00000
63	C4	DXY	0.26703	0.00000	-0.17396	-0.09937	0.00000
64	C4	DXZ	0.00000	-0.39796	0.00000	0.00000	0.10176
65	C4	DYZ	0.00000	-0.09778	0.00000	0.00000	0.30435
66	C5	S	0.02164	0.00000	-0.01320	-0.03081	0.00000
67	C5	S	0.20728	0.00000	0.01569	0.01334	0.00000
68	C5	PX	-0.05495	0.00000	0.21065	-0.02140	0.00000
69	C5	PY	-0.17561	0.00000	0.07441	-0.11709	0.00000
70	C5	PZ	0.00000	0.02285	0.00000	0.00000	-0.02360
71	C5	S	-1.47441	0.00000	-0.65738	0.85016	0.00000
72	C5	PX	-1.77527	0.00000	2.85683	-0.08818	0.00000
73	C5	PY	-0.89437	0.00000	1.49421	-0.40465	0.00000
74	C5	PZ	0.00000	0.10040	0.00000	0.00000	0.01477
75	C5	DXX	-0.22763	0.00000	0.21183	0.10569	0.00000
76	C5	DYY	0.15597	0.00000	-0.18226	0.12168	0.00000
77	C5	DZZ	0.08029	0.00000	-0.08020	-0.23909	0.00000
78	C5	DXY	0.03135	0.00000	-0.09978	0.14188	0.00000
79	C5	DXZ	0.00000	-0.42890	0.00000	0.00000	0.03720
80	C5	DYZ	0.00000	0.10321	0.00000	0.00000	0.33771
81	C6	S	-0.00675	0.00000	-0.01934	0.00402	0.00000
82	C6	S	0.08790	0.00000	0.05945	0.02751	0.00000
83	C6	PX	-0.07532	0.00000	-0.08007	-0.03542	0.00000
84	C6	PY	0.06368	0.00000	0.15713	-0.09036	0.00000
85	C6	PZ	0.00000	-0.08007	0.00000	0.00000	-0.00529
86	C6	S	0.14539	0.00000	0.30014	-0.35577	0.00000
87	C6	PX	-0.45831	0.00000	-2.98467	-0.02692	0.00000
88	C6	PY	-0.36683	0.00000	1.20472	0.25282	0.00000
89	C6	PZ	0.00000	-0.02934	0.00000	0.00000	0.01397
90	C6	DXX	-0.20936	0.00000	-0.27942	-0.09990	0.00000
91	C6	DYY	0.19861	0.00000	0.30605	0.12970	0.00000
92	C6	DZZ	-0.11158	0.00000	-0.17132	0.02989	0.00000
93	C6	DXY	-0.22459	0.00000	-0.19267	0.15269	0.00000
94	C6	DXZ	0.00000	0.31365	0.00000	0.00000	-0.07152
95	C6	DYZ	0.00000	0.27658	0.00000	0.00000	-0.09723
96	C7	S	0.01815	0.00000	-0.02372	-0.02231	0.00000
97	C7	S	0.16284	0.00000	-0.09242	-0.03607	0.00000
98	C7	PX	0.03417	0.00000	0.10048	-0.05720	0.00000
99	C7	PY	0.09896	0.00000	0.00054	-0.26904	0.00000
100	C7	PZ	0.00000	-0.02316	0.00000	0.00000	-0.01612
101	C7	S	-0.78373	0.00000	0.54758	-0.08009	0.00000
102	C7	PX	0.78379	0.00000	0.44401	-0.68984	0.00000
103	C7	PY	0.67382	0.00000	0.02291	-1.41074	0.00000
104	C7	PZ	0.00000	0.02843	0.00000	0.00000	-0.02201
105	C7	DXX	-0.16415	0.00000	-0.05682	-0.10968	0.00000
106	C7	DYY	0.07869	0.00000	0.20335	0.09539	0.00000
107	C7	DZZ	0.10763	0.00000	-0.14787	-0.09940	0.00000
108	C7	DXY	-0.22588	0.00000	0.18032	-0.02488	0.00000
109	C7	DXZ	0.00000	0.12589	0.00000	0.00000	-0.17231

110	C7	DYZ	0.00000	-0.29412	0.00000	0.00000	-0.10595
111	H3	S	0.08370	0.00000	0.02559	-0.03274	0.00000
112	H3	S	0.04401	0.00000	0.05662	0.13767	0.00000
113	H3	PX	0.50944	0.00000	-0.08037	0.01544	0.00000
114	H3	PY	-0.21713	0.00000	-0.04681	-0.12918	0.00000
115	H3	PZ	0.00000	0.31913	0.00000	0.00000	-0.30932
116	H4	S	0.10025	0.00000	0.05204	-0.02117	0.00000
117	H4	S	0.04565	0.00000	0.08183	0.07930	0.00000
118	H4	PX	0.25186	0.00000	-0.35066	0.01850	0.00000
119	H4	PY	0.02179	0.00000	-0.24867	0.01423	0.00000
120	H4	PZ	0.00000	-0.37763	0.00000	0.00000	-0.25126
121	N1	S	0.00587	0.00000	0.02123	-0.01235	0.00000
122	N1	S	0.12488	0.00000	0.29863	-0.17324	0.00000
123	N1	PX	-0.06037	0.00000	0.01053	-0.02260	0.00000
124	N1	PY	0.03294	0.00000	-0.07011	-0.11479	0.00000
125	N1	PZ	0.00000	0.03210	0.00000	0.00000	-0.01366
126	N1	S	-0.73325	0.00000	-1.38895	0.69912	0.00000
127	N1	PX	-0.22945	0.00000	-0.28613	0.36940	0.00000
128	N1	PY	-0.24013	0.00000	0.29609	-0.05895	0.00000
129	N1	PZ	0.00000	0.13284	0.00000	0.00000	0.01844
130	N1	DXX	-0.19436	0.00000	-0.17800	0.13175	0.00000
131	N1	DYY	0.08017	0.00000	-0.02444	-0.08241	0.00000
132	N1	DZZ	0.06770	0.00000	0.17996	-0.11237	0.00000
133	N1	DXY	0.05239	0.00000	0.35028	-0.22132	0.00000
134	N1	DXZ	0.00000	0.12263	0.00000	0.00000	0.08722
135	N1	DYZ	0.00000	0.33324	0.00000	0.00000	-0.09795
136	H6	S	0.15135	0.00000	0.03734	-0.00060	0.00000
137	H6	S	0.00780	0.00000	-0.06390	-0.09426	0.00000
138	H6	PX	-0.04478	0.00000	-0.06916	-0.07071	0.00000
139	H6	PY	-0.11390	0.00000	-0.39769	0.03534	0.00000
140	H6	PZ	0.00000	0.01303	0.00000	0.00000	0.45700
141	C8	S	-0.01486	0.00000	0.00589	0.06831	0.00000
142	C8	S	-0.03676	0.00000	0.14477	0.22126	0.00000
143	C8	PX	0.02245	0.00000	-0.23703	0.21460	0.00000
144	C8	PY	0.27604	0.00000	0.28778	0.11960	0.00000
145	C8	PZ	0.00000	0.04041	0.00000	0.00000	0.03853
146	C8	S	0.23398	0.00000	-0.16856	-2.80607	0.00000
147	C8	PX	0.85264	0.00000	-0.80599	-0.78280	0.00000
148	C8	PY	1.60478	0.00000	0.97952	-0.11731	0.00000
149	C8	PZ	0.00000	-0.05577	0.00000	0.00000	-0.02889
150	C8	DXX	0.25282	0.00000	0.13283	-0.17235	0.00000
151	C8	DYY	-0.20695	0.00000	-0.19904	-0.32876	0.00000
152	C8	DZZ	-0.02660	0.00000	0.08819	0.53304	0.00000
153	C8	DXY	0.00123	0.00000	0.00886	-0.21641	0.00000
154	C8	DXZ	0.00000	-0.01865	0.00000	0.00000	-0.05179
155	C8	DYZ	0.00000	-0.12817	0.00000	0.00000	-0.35551
156	H8	S	-0.03706	0.00000	-0.04622	0.05073	0.00000
157	H8	S	-0.10747	0.00000	-0.26485	0.03968	0.00000
158	H8	PX	-0.02095	0.00000	0.07214	0.22539	0.00000
159	H8	PY	-0.16453	0.00000	-0.11975	0.59832	0.00000
160	H8	PZ	0.00000	-0.22137	0.00000	0.00000	0.13582
161	C10	S	-0.02259	0.00000	-0.01991	-0.01669	0.00000
162	C10	S	-0.02366	0.00000	-0.02737	0.07094	0.00000
163	C10	PX	-0.02346	0.00000	0.15088	-0.09240	0.00000

164	C10	PY	0.18777	0.00000	0.15387	0.35362	0.00000
165	C10	PZ	0.00000	-0.00209	0.00000	0.00000	-0.03061
166	C10	S	1.40234	0.00000	0.95979	0.82983	0.00000
167	C10	PX	-0.21179	0.00000	0.57982	0.04295	0.00000
168	C10	PY	0.82486	0.00000	0.54967	0.37128	0.00000
169	C10	PZ	0.00000	0.03283	0.00000	0.00000	0.02418
170	C10	DXX	0.01631	0.00000	0.03127	-0.09997	0.00000
171	C10	DYY	0.19631	0.00000	0.14698	0.21835	0.00000
172	C10	DZZ	-0.20595	0.00000	-0.19667	-0.14982	0.00000
173	C10	DXY	-0.04894	0.00000	0.24314	-0.15876	0.00000
174	C10	DXZ	0.00000	-0.36593	0.00000	0.00000	0.07498
175	C10	DYZ	0.00000	-0.14830	0.00000	0.00000	-0.36230
176	H16	S	-0.06568	0.00000	-0.05572	-0.03034	0.00000
177	H16	S	0.23781	0.00000	-0.20415	0.05861	0.00000
178	H16	PX	-0.09401	0.00000	-0.04464	-0.13607	0.00000
179	H16	PY	-0.05543	0.00000	-0.26661	0.16838	0.00000
180	H16	PZ	0.00000	0.19413	0.00000	0.00000	-0.24464
181	H18	S	-0.07315	0.00000	-0.05205	0.03652	0.00000
182	H18	S	-0.00403	0.00000	0.39032	-0.12180	0.00000
183	H18	PX	0.05352	0.00000	0.13395	0.07423	0.00000
184	H18	PY	-0.14544	0.00000	0.13688	-0.24902	0.00000
185	H18	PZ	0.00000	-0.41611	0.00000	0.00000	-0.09047

MO:	151	152	153	154	155
Eigenvalues:	2.96574	2.96810	2.99339	3.03725	3.06360
(ev):	80.70196	80.76604	81.45435	82.64784	83.36496

			A	A	A	A	A
1	H1	S	0.00000	-0.10144	0.00000	0.04284	0.00000
2	H1	S	0.00000	-0.11324	0.00000	0.17261	0.00000
3	H1	PX	0.00000	-0.09024	0.00000	0.11166	0.00000
4	H1	PY	0.00000	0.40790	0.00000	0.05196	0.00000
5	H1	PZ	-0.15647	0.00000	-0.11844	0.00000	0.03771
6	C1	S	0.00000	-0.05191	0.00000	-0.04369	0.00000
7	C1	S	0.00000	-0.10363	0.00000	-0.00939	0.00000
8	C1	PX	0.00000	-0.10425	0.00000	-0.02531	0.00000
9	C1	PY	0.00000	0.10925	0.00000	0.12020	0.00000
10	C1	PZ	-0.02838	0.00000	-0.02798	0.00000	-0.00284
11	C1	S	0.00000	1.71595	0.00000	1.53881	0.00000
12	C1	PX	0.00000	0.16162	0.00000	-0.92773	0.00000
13	C1	PY	0.00000	-2.17107	0.00000	0.25103	0.00000
14	C1	PZ	0.02592	0.00000	-0.03000	0.00000	0.02778
15	C1	DXX	0.00000	-0.02236	0.00000	-0.06557	0.00000
16	C1	DYY	0.00000	0.25909	0.00000	0.36377	0.00000
17	C1	DZZ	0.00000	-0.38132	0.00000	-0.30895	0.00000
18	C1	DXY	0.00000	-0.27671	0.00000	-0.15871	0.00000
19	C1	DXZ	0.18877	0.00000	0.18216	0.00000	-0.04412
20	C1	DYZ	-0.23595	0.00000	-0.31624	0.00000	-0.33397
21	C2	S	0.00000	-0.01022	0.00000	-0.05875	0.00000
22	C2	S	0.00000	-0.05522	0.00000	-0.18888	0.00000
23	C2	PX	0.00000	0.18988	0.00000	0.04327	0.00000
24	C2	PY	0.00000	-0.11444	0.00000	0.07653	0.00000
25	C2	PZ	0.02393	0.00000	0.01196	0.00000	0.03006
26	C2	S	0.00000	0.52893	0.00000	2.70376	0.00000

27	C2	PX	0.00000	1.24496	0.00000	1.30402	0.00000
28	C2	PY	0.00000	1.86673	0.00000	-0.13977	0.00000
29	C2	PZ	-0.00583	0.00000	0.05621	0.00000	-0.04853
30	C2	DXX	0.00000	0.18905	0.00000	-0.08356	0.00000
31	C2	DYY	0.00000	-0.01558	0.00000	0.46878	0.00000
32	C2	DZZ	0.00000	-0.08034	0.00000	-0.36962	0.00000
33	C2	DXY	0.00000	-0.23079	0.00000	0.27140	0.00000
34	C2	DXZ	0.01751	0.00000	-0.15279	0.00000	0.27508
35	C2	DYZ	0.21857	0.00000	0.40058	0.00000	0.21049
36	C3	S	0.00000	-0.03275	0.00000	-0.00457	0.00000
37	C3	S	0.00000	-0.34128	0.00000	-0.09168	0.00000
38	C3	PX	0.00000	-0.11207	0.00000	-0.04710	0.00000
39	C3	PY	0.00000	0.17962	0.00000	0.00541	0.00000
40	C3	PZ	0.02410	0.00000	-0.01896	0.00000	0.06416
41	C3	S	0.00000	2.11260	0.00000	0.91562	0.00000
42	C3	PX	0.00000	-4.82807	0.00000	0.74212	0.00000
43	C3	PY	0.00000	-1.08913	0.00000	-1.74685	0.00000
44	C3	PZ	-0.00372	0.00000	0.05096	0.00000	-0.03779
45	C3	DXX	0.00000	0.44416	0.00000	-0.13317	0.00000
46	C3	DYY	0.00000	-0.38000	0.00000	0.08884	0.00000
47	C3	DZZ	0.00000	-0.09534	0.00000	-0.01270	0.00000
48	C3	DXY	0.00000	0.06614	0.00000	-0.19480	0.00000
49	C3	DXZ	0.03137	0.00000	-0.26892	0.00000	-0.22822
50	C3	DYZ	-0.21544	0.00000	-0.06126	0.00000	-0.37732
51	C4	S	0.00000	0.02872	0.00000	0.01229	0.00000
52	C4	S	0.00000	-0.13876	0.00000	-0.14923	0.00000
53	C4	PX	0.00000	0.03195	0.00000	-0.26108	0.00000
54	C4	PY	0.00000	0.22814	0.00000	0.14696	0.00000
55	C4	PZ	0.01822	0.00000	0.01947	0.00000	0.02708
56	C4	S	0.00000	0.19396	0.00000	-0.75450	0.00000
57	C4	PX	0.00000	1.16070	0.00000	-0.37138	0.00000
58	C4	PY	0.00000	-0.12232	0.00000	0.13414	0.00000
59	C4	PZ	-0.04182	0.00000	0.02323	0.00000	-0.01835
60	C4	DXX	0.00000	-0.33762	0.00000	-0.13492	0.00000
61	C4	DYY	0.00000	0.03980	0.00000	-0.05329	0.00000
62	C4	DZZ	0.00000	0.24775	0.00000	0.14327	0.00000
63	C4	DXY	0.00000	-0.01116	0.00000	0.23034	0.00000
64	C4	DXZ	0.08035	0.00000	0.29317	0.00000	0.17027
65	C4	DYZ	-0.37152	0.00000	-0.25675	0.00000	-0.16704
66	C5	S	0.00000	-0.00863	0.00000	0.00862	0.00000
67	C5	S	0.00000	0.10571	0.00000	-0.00114	0.00000
68	C5	PX	0.00000	0.14428	0.00000	0.23784	0.00000
69	C5	PY	0.00000	0.04240	0.00000	0.26828	0.00000
70	C5	PZ	-0.01240	0.00000	-0.02241	0.00000	-0.02698
71	C5	S	0.00000	-1.02078	0.00000	-1.33898	0.00000
72	C5	PX	0.00000	1.06245	0.00000	-0.07048	0.00000
73	C5	PY	0.00000	0.79549	0.00000	0.81322	0.00000
74	C5	PZ	0.03577	0.00000	-0.03929	0.00000	0.03701
75	C5	DXX	0.00000	0.44152	0.00000	-0.15202	0.00000
76	C5	DYY	0.00000	-0.28717	0.00000	-0.10911	0.00000
77	C5	DZZ	0.00000	-0.08350	0.00000	0.09974	0.00000
78	C5	DXY	0.00000	-0.12237	0.00000	-0.10523	0.00000
79	C5	DXZ	0.06405	0.00000	0.32563	0.00000	0.10034
80	C5	DYZ	0.27076	0.00000	0.12999	0.00000	0.30742

81	C6	S	0.00000	0.10305	0.00000	-0.00559	0.00000
82	C6	S	0.00000	0.56397	0.00000	0.34486	0.00000
83	C6	PX	0.00000	-0.05613	0.00000	0.01152	0.00000
84	C6	PY	0.00000	-0.23620	0.00000	-0.19959	0.00000
85	C6	PZ	-0.06014	0.00000	-0.02313	0.00000	0.01563
86	C6	S	0.00000	-3.58581	0.00000	-0.32536	0.00000
87	C6	PX	0.00000	-4.50515	0.00000	0.75300	0.00000
88	C6	PY	0.00000	-0.19446	0.00000	-1.28102	0.00000
89	C6	PZ	-0.03933	0.00000	-0.11830	0.00000	0.08571
90	C6	DXX	0.00000	-0.27285	0.00000	-0.03142	0.00000
91	C6	DYY	0.00000	-0.18120	0.00000	0.02864	0.00000
92	C6	DZZ	0.00000	0.53563	0.00000	-0.12846	0.00000
93	C6	DXY	0.00000	0.13179	0.00000	0.36253	0.00000
94	C6	DXZ	0.07812	0.00000	-0.27489	0.00000	-0.25148
95	C6	DYZ	0.35065	0.00000	0.39160	0.00000	-0.14895
96	C7	S	0.00000	-0.03662	0.00000	0.02820	0.00000
97	C7	S	0.00000	0.04462	0.00000	0.11934	0.00000
98	C7	PX	0.00000	-0.04877	0.00000	0.05715	0.00000
99	C7	PY	0.00000	0.13532	0.00000	-0.02290	0.00000
100	C7	PZ	0.00247	0.00000	-0.00689	0.00000	-0.03787
101	C7	S	0.00000	-0.22510	0.00000	-2.09646	0.00000
102	C7	PX	0.00000	1.46601	0.00000	0.79725	0.00000
103	C7	PY	0.00000	1.06762	0.00000	-1.31788	0.00000
104	C7	PZ	0.01222	0.00000	0.01396	0.00000	0.01458
105	C7	DXX	0.00000	-0.09703	0.00000	-0.18103	0.00000
106	C7	DYY	0.00000	0.33667	0.00000	-0.04162	0.00000
107	C7	DZZ	0.00000	-0.29153	0.00000	0.14290	0.00000
108	C7	DXY	0.00000	-0.05327	0.00000	-0.27058	0.00000
109	C7	DXZ	-0.06288	0.00000	-0.05128	0.00000	0.57538
110	C7	DYZ	-0.26491	0.00000	0.09523	0.00000	-0.18475
111	H3	S	0.00000	-0.05944	0.00000	0.04009	0.00000
112	H3	S	0.00000	-0.16897	0.00000	0.15083	0.00000
113	H3	PX	0.00000	0.12912	0.00000	0.06635	0.00000
114	H3	PY	0.00000	-0.00557	0.00000	-0.18536	0.00000
115	H3	PZ	0.28542	0.00000	0.07657	0.00000	0.05714
116	H4	S	0.00000	0.03677	0.00000	-0.01463	0.00000
117	H4	S	0.00000	-0.00869	0.00000	-0.16682	0.00000
118	H4	PX	0.00000	0.11944	0.00000	-0.20603	0.00000
119	H4	PY	0.00000	0.13334	0.00000	-0.14506	0.00000
120	H4	PZ	-0.19676	0.00000	0.07134	0.00000	-0.18163
121	N1	S	0.00000	0.01693	0.00000	0.05541	0.00000
122	N1	S	0.00000	0.16854	0.00000	0.52274	0.00000
123	N1	PX	0.00000	-0.02211	0.00000	-0.12490	0.00000
124	N1	PY	0.00000	0.16218	0.00000	-0.09806	0.00000
125	N1	PZ	0.01334	0.00000	0.02656	0.00000	-0.02219
126	N1	S	0.00000	-0.74065	0.00000	-3.07246	0.00000
127	N1	PX	0.00000	0.51101	0.00000	-1.30857	0.00000
128	N1	PY	0.00000	-1.14779	0.00000	0.57033	0.00000
129	N1	PZ	0.05277	0.00000	0.22610	0.00000	-0.09833
130	N1	DXX	0.00000	0.15558	0.00000	-0.20476	0.00000
131	N1	DYY	0.00000	-0.17958	0.00000	-0.33474	0.00000
132	N1	DZZ	0.00000	0.06813	0.00000	0.43451	0.00000
133	N1	DXY	0.00000	-0.04375	0.00000	0.35997	0.00000

134	N1	DXZ	-0.01015	0.00000	0.45485	0.00000	-0.12157
135	N1	DYZ	0.41492	0.00000	0.01900	0.00000	-0.21226
136	H6	S	0.00000	0.10623	0.00000	0.05143	0.00000
137	H6	S	0.00000	0.51394	0.00000	0.21081	0.00000
138	H6	PX	0.00000	0.14074	0.00000	-0.08697	0.00000
139	H6	PY	0.00000	-0.30450	0.00000	0.27370	0.00000
140	H6	PZ	0.01403	0.00000	-0.15292	0.00000	0.24045
141	C8	S	0.00000	-0.02702	0.00000	-0.07298	0.00000
142	C8	S	0.00000	-0.23954	0.00000	0.34454	0.00000
143	C8	PX	0.00000	0.05140	0.00000	-0.12440	0.00000
144	C8	PY	0.00000	-0.15670	0.00000	0.18281	0.00000
145	C8	PZ	0.01989	0.00000	0.01777	0.00000	-0.01743
146	C8	S	0.00000	1.21776	0.00000	2.60202	0.00000
147	C8	PX	0.00000	1.00556	0.00000	-1.29474	0.00000
148	C8	PY	0.00000	0.43033	0.00000	0.41593	0.00000
149	C8	PZ	0.00224	0.00000	-0.08052	0.00000	-0.00761
150	C8	DXX	0.00000	-0.11052	0.00000	0.28949	0.00000
151	C8	DYY	0.00000	0.23182	0.00000	0.12765	0.00000
152	C8	DZZ	0.00000	-0.14178	0.00000	-0.56500	0.00000
153	C8	DXY	0.00000	-0.11705	0.00000	-0.19037	0.00000
154	C8	DXZ	-0.37980	0.00000	0.27175	0.00000	0.17945
155	C8	DYZ	-0.03058	0.00000	-0.43575	0.00000	0.43524
156	H8	S	0.00000	-0.12214	0.00000	-0.06083	0.00000
157	H8	S	0.00000	-0.34744	0.00000	-0.24039	0.00000
158	H8	PX	0.00000	-0.02252	0.00000	0.07237	0.00000
159	H8	PY	0.00000	-0.06383	0.00000	0.34047	0.00000
160	H8	PZ	-0.04280	0.00000	0.06751	0.00000	-0.48019
161	C10	S	0.00000	0.00382	0.00000	0.02250	0.00000
162	C10	S	0.00000	-0.00751	0.00000	0.05040	0.00000
163	C10	PX	0.00000	-0.12974	0.00000	-0.00120	0.00000
164	C10	PY	0.00000	-0.14261	0.00000	-0.19090	0.00000
165	C10	PZ	-0.00752	0.00000	-0.03865	0.00000	0.05357
166	C10	S	0.00000	-0.02518	0.00000	-0.72831	0.00000
167	C10	PX	0.00000	-0.17086	0.00000	0.25212	0.00000
168	C10	PY	0.00000	-0.11269	0.00000	-0.46899	0.00000
169	C10	PZ	-0.00289	0.00000	0.02384	0.00000	0.00966
170	C10	DXX	0.00000	-0.05039	0.00000	0.06227	0.00000
171	C10	DYY	0.00000	-0.04216	0.00000	-0.12340	0.00000
172	C10	DZZ	0.00000	0.05897	0.00000	0.16063	0.00000
173	C10	DXY	0.00000	-0.13092	0.00000	-0.04720	0.00000
174	C10	DXZ	0.54568	0.00000	-0.32601	0.00000	-0.11700
175	C10	DYZ	-0.09663	0.00000	-0.34041	0.00000	0.37589
176	H16	S	0.00000	-0.02897	0.00000	-0.01474	0.00000
177	H16	S	0.00000	0.09915	0.00000	-0.12304	0.00000
178	H16	PX	0.00000	0.06655	0.00000	0.13063	0.00000
179	H16	PY	0.00000	0.18169	0.00000	0.05427	0.00000
180	H16	PZ	-0.44118	0.00000	0.07480	0.00000	0.22197
181	H18	S	0.00000	0.03815	0.00000	0.04505	0.00000
182	H18	S	0.00000	-0.15009	0.00000	-0.00462	0.00000
183	H18	PX	0.00000	-0.12762	0.00000	-0.09543	0.00000
184	H18	PY	0.00000	-0.01797	0.00000	-0.05951	0.00000
185	H18	PZ	0.40063	0.00000	-0.38140	0.00000	0.02721

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Eigenvalues:	3.10168	3.10809	3.11390	3.16425	3.24038
(ev):	84.40116	84.57542	84.73346	86.10363	88.17531

		A	A	A	A	A	
1	H1	S	-0.00322	0.00000	-0.04597	-0.01196	-0.09994
2	H1	S	-0.15890	0.00000	-0.16606	-0.24728	-0.30053
3	H1	PX	0.02673	0.00000	0.06031	-0.08548	0.22357
4	H1	PY	-0.30717	0.00000	-0.21101	-0.07393	0.17606
5	H1	PZ	0.00000	0.36050	0.00000	0.00000	0.00000
6	C1	S	0.04125	0.00000	0.01112	0.06330	0.02191
7	C1	S	0.07058	0.00000	0.15812	0.26671	0.26050
8	C1	PX	0.10409	0.00000	-0.03724	-0.01326	0.19840
9	C1	PY	0.13156	0.00000	0.24268	-0.01008	-0.20173
10	C1	PZ	0.00000	0.04923	0.00000	0.00000	0.00000
11	C1	S	-1.28251	0.00000	-0.02531	-2.66589	-1.04844
12	C1	PX	0.60734	0.00000	0.42022	1.41180	0.89961
13	C1	PY	0.97524	0.00000	0.19250	-0.33898	-0.46952
14	C1	PZ	0.00000	-0.08933	0.00000	0.00000	0.00000
15	C1	DXX	-0.02826	0.00000	0.00391	0.06583	0.04286
16	C1	DYY	-0.19698	0.00000	0.05079	-0.40344	-0.17438
17	C1	DZZ	0.23389	0.00000	0.00630	0.36397	0.12182
18	C1	DXY	0.10764	0.00000	-0.05254	0.09605	-0.08715
19	C1	DXZ	0.00000	-0.43738	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.09539	0.00000	0.00000	0.00000
21	C2	S	0.02293	0.00000	-0.05404	0.06037	-0.02617
22	C2	S	0.01676	0.00000	-0.19790	-0.02246	-0.27082
23	C2	PX	-0.08253	0.00000	0.13550	0.07686	0.11069
24	C2	PY	-0.16510	0.00000	-0.18715	-0.06714	0.21419
25	C2	PZ	0.00000	-0.03927	0.00000	0.00000	0.00000
26	C2	S	-0.81393	0.00000	1.73662	-1.67105	1.81534
27	C2	PX	-0.38890	0.00000	1.18042	0.18006	1.44266
28	C2	PY	-0.05239	0.00000	-0.38072	1.39754	1.25117
29	C2	PZ	0.00000	0.09654	0.00000	0.00000	0.00000
30	C2	DXX	0.00213	0.00000	0.00274	0.11343	-0.03517
31	C2	DYY	-0.19009	0.00000	0.18787	-0.42597	0.15909
32	C2	DZZ	0.17262	0.00000	-0.27975	0.39768	-0.13436
33	C2	DXY	-0.09044	0.00000	0.13370	0.08322	-0.01967
34	C2	DXZ	0.00000	-0.40548	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.01191	0.00000	0.00000	0.00000
36	C3	S	-0.04235	0.00000	-0.07093	-0.08090	-0.09009
37	C3	S	-0.17615	0.00000	-0.33415	-0.39548	-0.33235
38	C3	PX	-0.01254	0.00000	-0.06052	0.11433	0.11798
39	C3	PY	0.02019	0.00000	-0.09878	-0.06949	-0.11918
40	C3	PZ	0.00000	0.00768	0.00000	0.00000	0.00000
41	C3	S	2.09528	0.00000	4.08087	5.82234	6.45633
42	C3	PX	0.49522	0.00000	-1.84799	-1.66564	-1.54905
43	C3	PY	0.61423	0.00000	-0.50432	-0.43890	-2.74243
44	C3	PZ	0.00000	0.11095	0.00000	0.00000	0.00000
45	C3	DXX	-0.10352	0.00000	0.29947	0.35423	0.11113
46	C3	DYY	0.24893	0.00000	0.07236	0.11462	0.40470
47	C3	DZZ	-0.22275	0.00000	-0.37963	-0.41860	-0.46393
48	C3	DXY	0.37350	0.00000	0.12303	0.02405	-0.53749
49	C3	DXZ	0.00000	0.05878	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	-0.44161	0.00000	0.00000	0.00000

51	C4	S	0.01699	0.00000	0.04695	-0.00668	-0.05287
52	C4	S	0.01233	0.00000	0.01255	-0.14008	-0.11793
53	C4	PX	0.12411	0.00000	-0.01567	0.27153	-0.01992
54	C4	PY	-0.17368	0.00000	-0.03977	-0.15174	-0.00035
55	C4	PZ	0.00000	-0.03188	0.00000	0.00000	0.00000
56	C4	S	-0.33354	0.00000	-0.57012	1.38104	2.18715
57	C4	PX	-0.33354	0.00000	0.09424	0.49144	-0.24912
58	C4	PY	-0.11986	0.00000	0.07792	-1.15662	-1.31832
59	C4	PZ	0.00000	0.10216	0.00000	0.00000	0.00000
60	C4	DXX	-0.12745	0.00000	-0.17278	0.13662	0.14923
61	C4	DYY	0.13042	0.00000	-0.07085	0.02638	0.03269
62	C4	DZZ	0.08886	0.00000	0.32872	-0.06268	-0.27438
63	C4	DXY	-0.00190	0.00000	0.26265	-0.04613	-0.21354
64	C4	DXZ	0.00000	0.17304	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.35937	0.00000	0.00000	0.00000
66	C5	S	-0.02902	0.00000	-0.02830	-0.03205	0.05079
67	C5	S	0.06425	0.00000	-0.01662	-0.04290	0.06270
68	C5	PX	-0.06981	0.00000	0.11137	-0.20752	0.02193
69	C5	PY	-0.08972	0.00000	0.25504	-0.05078	0.01596
70	C5	PZ	0.00000	0.03668	0.00000	0.00000	0.00000
71	C5	S	0.57436	0.00000	-0.07607	0.04880	-3.04164
72	C5	PX	0.00183	0.00000	0.01575	0.49385	0.01201
73	C5	PY	-0.39285	0.00000	0.46330	0.14777	1.39279
74	C5	PZ	0.00000	-0.09728	0.00000	0.00000	0.00000
75	C5	DXX	0.07121	0.00000	0.18386	0.25499	-0.14874
76	C5	DYY	0.12105	0.00000	-0.11081	-0.04797	-0.07546
77	C5	DZZ	-0.21268	0.00000	-0.18496	-0.25533	0.26723
78	C5	DXY	0.21764	0.00000	0.11072	0.16587	-0.22383
79	C5	DXZ	0.00000	0.18686	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	-0.34047	0.00000	0.00000	0.00000
81	C6	S	-0.00908	0.00000	0.10178	0.00925	0.04947
82	C6	S	0.07951	0.00000	-0.04393	0.62688	0.12751
83	C6	PX	0.00846	0.00000	0.06759	-0.28121	0.11157
84	C6	PY	-0.01090	0.00000	0.50266	-0.20110	0.13432
85	C6	PZ	0.00000	-0.01967	0.00000	0.00000	0.00000
86	C6	S	0.58673	0.00000	-5.76230	-0.00973	-3.24897
87	C6	PX	-0.11432	0.00000	-1.09587	-3.37468	-2.05486
88	C6	PY	-0.11872	0.00000	0.14105	-0.09466	0.55783
89	C6	PZ	0.00000	-0.13925	0.00000	0.00000	0.00000
90	C6	DXX	-0.05376	0.00000	-0.21346	-0.17079	-0.15397
91	C6	DYY	0.05404	0.00000	-0.44723	0.14276	-0.20357
92	C6	DZZ	-0.04648	0.00000	0.73808	-0.13097	0.29166
93	C6	DXY	-0.00577	0.00000	0.05389	-0.04725	-0.49792
94	C6	DXZ	0.00000	0.08339	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.38642	0.00000	0.00000	0.00000
96	C7	S	0.01605	0.00000	0.03402	0.04915	0.09019
97	C7	S	0.23941	0.00000	0.23356	0.32288	0.36790
98	C7	PX	0.26477	0.00000	0.10023	0.00719	0.11069
99	C7	PY	-0.08866	0.00000	-0.10118	-0.01316	-0.27843
100	C7	PZ	0.00000	-0.04943	0.00000	0.00000	0.00000
101	C7	S	-0.83841	0.00000	-2.37353	-3.46258	-6.25763
102	C7	PX	0.36948	0.00000	1.72114	2.01881	2.97569
103	C7	PY	-0.20222	0.00000	0.00340	-0.76300	-1.31094
104	C7	PZ	0.00000	-0.03343	0.00000	0.00000	0.00000

105	C7	DXX	-0.05764	0.00000	-0.01128	0.00828	-0.09776
106	C7	DYY	0.15337	0.00000	-0.12721	-0.35403	-0.55861
107	C7	DZZ	0.05526	0.00000	0.17619	0.27660	0.49323
108	C7	DXY	0.06834	0.00000	0.00441	-0.10255	-0.17683
109	C7	DXZ	0.00000	0.22047	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	-0.33537	0.00000	0.00000	0.00000
111	H3	S	0.05756	0.00000	0.03369	0.03430	0.05916
112	H3	S	0.16952	0.00000	0.04692	0.20507	0.24678
113	H3	PX	-0.04403	0.00000	-0.15997	-0.28442	0.07163
114	H3	PY	-0.09571	0.00000	-0.05899	0.12869	0.02929
115	H3	PZ	0.00000	-0.34578	0.00000	0.00000	0.00000
116	H4	S	0.01783	0.00000	-0.05998	0.00408	0.02810
117	H4	S	0.03928	0.00000	-0.22584	-0.02261	-0.11353
118	H4	PX	-0.06636	0.00000	-0.18104	0.08906	0.06196
119	H4	PY	0.03660	0.00000	0.09539	0.15599	-0.12937
120	H4	PZ	0.00000	0.32986	0.00000	0.00000	0.00000
121	N1	S	0.00454	0.00000	-0.05960	0.05590	-0.01917
122	N1	S	0.18266	0.00000	-0.56776	0.66226	0.00088
123	N1	PX	0.00373	0.00000	0.08124	-0.15597	0.08372
124	N1	PY	-0.00546	0.00000	0.24194	0.10313	0.27558
125	N1	PZ	0.00000	0.02770	0.00000	0.00000	0.00000
126	N1	S	-0.72344	0.00000	3.10952	-3.41948	0.74553
127	N1	PX	-0.28230	0.00000	1.01652	-0.59193	0.17181
128	N1	PY	-0.09522	0.00000	0.64783	-0.97566	-0.02562
129	N1	PZ	0.00000	0.11492	0.00000	0.00000	0.00000
130	N1	DXX	-0.24318	0.00000	0.04700	-0.02675	-0.18554
131	N1	DYY	0.10829	0.00000	0.54385	-0.51917	0.42993
132	N1	DZZ	0.06965	0.00000	-0.51752	0.42630	-0.15170
133	N1	DXY	-0.04444	0.00000	0.37258	0.23637	-0.03138
134	N1	DXZ	0.00000	0.07056	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.30658	0.00000	0.00000	0.00000
136	H6	S	0.00298	0.00000	0.04950	0.17861	0.15467
137	H6	S	-0.10159	0.00000	0.35087	0.28963	0.43785
138	H6	PX	-0.01064	0.00000	0.09662	0.23647	0.18111
139	H6	PY	-0.00188	0.00000	0.33856	0.01263	-0.22004
140	H6	PZ	0.00000	-0.34321	0.00000	0.00000	0.00000
141	C8	S	-0.05967	0.00000	0.01364	-0.06436	-0.03949
142	C8	S	-0.09970	0.00000	-0.24738	0.04290	-0.32184
143	C8	PX	-0.03978	0.00000	0.08714	-0.11029	0.16807
144	C8	PY	0.07901	0.00000	-0.10270	-0.00720	0.08995
145	C8	PZ	0.00000	0.00448	0.00000	0.00000	0.00000
146	C8	S	2.42604	0.00000	-0.13320	2.39262	2.56910
147	C8	PX	0.06228	0.00000	1.50871	0.39479	1.75605
148	C8	PY	-0.60326	0.00000	1.04923	2.31403	1.67437
149	C8	PZ	0.00000	-0.01927	0.00000	0.00000	0.00000
150	C8	DXX	-0.35880	0.00000	0.12320	0.35817	0.15328
151	C8	DYY	0.46327	0.00000	-0.05137	0.03302	0.01193
152	C8	DZZ	-0.31850	0.00000	0.14309	-0.40734	-0.13484
153	C8	DXY	-0.00848	0.00000	0.13459	-0.22565	0.28424
154	C8	DXZ	0.00000	-0.07840	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.08896	0.00000	0.00000	0.00000
156	H8	S	-0.05925	0.00000	-0.09298	-0.07079	-0.04414
157	H8	S	-0.24367	0.00000	-0.47330	-0.45966	-0.66728
158	H8	PX	0.41702	0.00000	0.09157	-0.08755	-0.04037

159	H8	PY	-0.12922	0.00000	-0.14110	0.02542	0.15366
160	H8	PZ	0.00000	-0.21987	0.00000	0.00000	0.00000
161	C10	S	-0.00099	0.00000	-0.01047	0.02393	-0.01117
162	C10	S	0.17826	0.00000	-0.07830	-0.00965	0.21426
163	C10	PX	-0.05225	0.00000	0.02077	-0.07469	0.07284
164	C10	PY	-0.34341	0.00000	0.08186	-0.03435	-0.04373
165	C10	PZ	0.00000	0.01073	0.00000	0.00000	0.00000
166	C10	S	-1.20736	0.00000	0.98471	0.74886	0.61043
167	C10	PX	-0.13353	0.00000	-0.56742	-0.13367	-0.77235
168	C10	PY	-0.99874	0.00000	0.67954	0.31012	0.00806
169	C10	PZ	0.00000	0.00647	0.00000	0.00000	0.00000
170	C10	DXX	-0.28977	0.00000	0.10996	0.21716	-0.09622
171	C10	DYY	0.10114	0.00000	-0.05400	-0.22159	0.12323
172	C10	DZZ	0.02573	0.00000	-0.06537	0.15508	-0.07270
173	C10	DXY	-0.00460	0.00000	0.02189	-0.09338	0.06203
174	C10	DXZ	0.00000	0.06394	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.06004	0.00000	0.00000	0.00000
176	H16	S	0.04791	0.00000	0.04060	-0.01524	0.07862
177	H16	S	-0.17566	0.00000	0.30116	0.13444	0.07815
178	H16	PX	0.37724	0.00000	-0.15243	-0.08655	0.21017
179	H16	PY	0.32928	0.00000	-0.14818	-0.06172	-0.00707
180	H16	PZ	0.00000	-0.01993	0.00000	0.00000	0.00000
181	H18	S	0.05697	0.00000	-0.14609	-0.04314	-0.13272
182	H18	S	-0.28223	0.00000	-0.01586	-0.06191	-0.32399
183	H18	PX	-0.35839	0.00000	0.08820	0.00657	-0.20229
184	H18	PY	0.31383	0.00000	-0.05096	-0.23020	0.17741
185	H18	PZ	0.00000	0.05755	0.00000	0.00000	0.00000

MO:	161	162	163	164	165
Eigenvalues:	3.29653	3.32987	3.34927	3.43269	3.46974
(ev):	89.70315	90.61046	91.13834	93.40837	94.41652

		A	A	A	A	A	
1	H1	S	-0.15350	0.01250	0.08817	0.00796	0.06530
2	H1	S	-0.36332	-0.02323	0.24145	-0.01352	0.06404
3	H1	PX	0.31966	0.02270	-0.29923	-0.07341	-0.11664
4	H1	PY	-0.23776	0.03528	0.02582	0.14223	-0.38469
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02741	0.01585	0.04578	0.01242	0.01975
7	C1	S	0.08992	-0.02318	-0.23086	-0.15274	-0.24367
8	C1	PX	0.23780	0.13337	-0.06956	0.08287	0.10408
9	C1	PY	-0.11591	0.00457	-0.15211	0.07035	-0.25322
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.59282	-0.59426	-0.58915	0.20250	-0.20480
12	C1	PX	0.45979	0.11605	0.02477	0.11023	-0.01204
13	C1	PY	-0.20390	0.88140	-0.51450	-0.02954	0.86265
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.09553	-0.01958	0.06797	-0.01004	-0.11315
16	C1	DYY	0.17327	-0.13241	-0.30492	-0.14543	-0.06803
17	C1	DZZ	-0.16876	0.08830	0.31523	0.09489	0.15036
18	C1	DXY	0.35859	-0.15126	0.09781	-0.29773	0.58569
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02052	0.00496	-0.04218	-0.03023	-0.01386

22	C2	S	-0.13333	0.09227	0.20781	0.27321	0.08513
23	C2	PX	-0.15250	0.14006	-0.06023	0.06655	0.02196
24	C2	PY	-0.16866	0.03928	0.15293	0.11701	-0.16386
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.96541	-0.31572	0.79520	0.26396	0.19828
27	C2	PX	0.85092	-0.06667	0.06330	0.49551	0.15963
28	C2	PY	1.06183	-0.48785	0.69813	-0.40607	-0.12562
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.01956	0.05765	-0.09232	0.05267	0.11838
31	C2	DYY	0.06808	0.00128	0.32372	0.16484	0.06268
32	C2	DZZ	-0.09290	0.01310	-0.29108	-0.20682	-0.08278
33	C2	DXY	-0.33154	-0.09737	0.08121	0.32252	-0.49657
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03576	-0.00679	-0.02900	-0.06186	0.00114
37	C3	S	-0.11275	0.00455	0.00138	0.17992	-0.34157
38	C3	PX	-0.00864	0.10885	-0.02706	0.16854	-0.00132
39	C3	PY	-0.44068	0.07839	0.09708	-0.15075	-0.03355
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	3.04173	0.78799	1.57568	2.11372	1.48077
42	C3	PX	-2.06096	1.35193	-0.33333	-0.97750	0.80941
43	C3	PY	-0.57655	0.00349	-1.38563	-0.72389	-0.28917
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.10243	-0.44341	0.19850	-0.29826	0.06811
46	C3	DYY	0.17968	0.36485	-0.09008	0.52613	-0.09516
47	C3	DZZ	-0.17930	-0.02351	-0.13518	-0.33720	0.00559
48	C3	DXY	-0.31032	0.11829	0.25848	0.15830	0.13516
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01590	-0.01945	-0.06707	-0.03076	-0.01707
52	C4	S	0.09558	-0.11077	0.21917	-0.08680	0.18219
53	C4	PX	-0.03399	0.06377	0.06119	0.05502	0.17493
54	C4	PY	-0.19231	0.00928	0.01629	0.04645	-0.22744
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.35903	0.53529	1.37813	0.84599	0.14093
57	C4	PX	-0.00243	-0.81142	0.10658	-0.40801	-0.83880
58	C4	PY	-0.27256	-0.04688	-0.44526	0.01549	0.01393
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.27100	-0.06282	0.24549	-0.04807	-0.23275
61	C4	DYY	0.25093	0.09354	-0.00129	-0.01550	0.42150
62	C4	DZZ	0.10443	-0.10416	-0.42202	-0.15999	-0.13939
63	C4	DXY	-0.10333	-0.19037	-0.23745	-0.18198	-0.38278
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00927	0.01668	0.07296	0.01787	0.02310
67	C5	S	0.13383	0.06177	-0.17640	-0.23567	0.21174
68	C5	PX	0.07784	0.00760	0.07265	0.16726	0.00644
69	C5	PY	-0.11591	-0.01245	-0.00079	0.14539	-0.08595
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.12274	-0.44307	-1.67115	-0.44870	-0.95802
72	C5	PX	0.61914	-0.71979	0.14460	-0.57596	-0.46947
73	C5	PY	0.41292	-0.17076	0.58693	-0.20408	0.01447
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.16859	0.14086	-0.21494	0.22553	0.02055

76	C5	DYY	0.22376	-0.13786	-0.04598	-0.35021	0.10768
77	C5	DZZ	-0.06676	0.08269	0.45090	0.14632	0.09098
78	C5	DXY	0.12780	-0.15753	-0.27181	-0.26827	-0.11895
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.03560	-0.00397	0.02889	0.01568	0.03297
82	C6	S	0.52476	-0.02148	-0.25684	0.46219	-0.30892
83	C6	PX	-0.02330	0.16326	0.07921	-0.10495	0.05663
84	C6	PY	-0.40097	-0.04282	0.12638	-0.23903	-0.00011
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.95007	0.57949	-1.51037	-0.99512	-0.52507
87	C6	PX	-2.65540	0.85778	-0.22479	-1.04399	0.22076
88	C6	PY	-1.17200	0.20465	1.39559	-0.92208	0.32633
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.31399	0.39724	-0.20977	-0.07988	0.42165
91	C6	DYY	0.22681	-0.31841	-0.01152	0.20551	-0.48399
92	C6	DZZ	0.05143	0.00339	0.24512	-0.02832	0.19200
93	C6	DXY	0.16418	0.07943	0.06386	0.52308	0.41867
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.03160	0.01509	-0.01163	0.02560	0.02527
97	C7	S	0.11683	0.15291	0.29685	0.07942	0.02078
98	C7	PX	0.03170	0.41012	0.02209	0.23103	-0.13463
99	C7	PY	-0.30416	-0.12011	-0.07357	-0.27227	0.16294
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-2.39291	-0.99403	-1.31882	-1.82148	-1.20207
102	C7	PX	1.72229	0.34972	0.71644	1.18299	0.13798
103	C7	PY	0.33382	-0.62139	-0.89049	0.02997	-0.61554
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.29399	-0.09258	0.14452	0.30127	-0.19635
106	C7	DYY	-0.47797	0.09671	0.00377	-0.44644	0.05955
107	C7	DZZ	0.16134	0.04196	-0.10314	0.12287	0.12247
108	C7	DXY	0.35035	-0.18312	0.10827	0.32852	-0.11304
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.08444	0.02843	-0.07601	-0.00187	0.01423
112	H3	S	0.21282	0.07503	-0.14272	-0.04132	0.10277
113	H3	PX	0.12149	0.15995	0.11716	0.10307	0.32832
114	H3	PY	-0.21864	-0.07406	0.23478	-0.05667	-0.10061
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.06930	-0.00754	0.08485	0.04890	-0.03284
117	H4	S	0.12196	-0.03135	0.11489	0.07752	0.00439
118	H4	PX	-0.19353	0.19731	0.11151	0.31415	0.01347
119	H4	PY	-0.20095	0.11918	-0.22160	0.02106	0.09501
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.01447	-0.01202	0.00183	0.00615	0.00918
122	N1	S	0.13431	0.21212	-0.12057	-0.12232	-0.07086
123	N1	PX	-0.10501	0.13382	-0.06998	-0.06891	0.05901
124	N1	PY	-0.04973	-0.00269	0.07663	-0.13660	0.05185
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.21387	-0.20524	0.56860	-0.13166	0.03326
127	N1	PX	0.16704	-0.24063	-0.25106	0.42186	0.02039
128	N1	PY	-1.60835	0.12980	1.14930	-1.16450	0.51675
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

130	N1	DXX	0.05878	-0.02278	-0.37090	0.43144	0.29892
131	N1	DYY	-0.27040	0.01200	0.34185	-0.54677	-0.13572
132	N1	DZZ	0.09477	-0.00577	-0.00686	0.05066	-0.02417
133	N1	DXY	-0.42377	-0.01754	0.40234	-0.24028	0.50544
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.02994	0.01560	-0.05948	-0.04244	-0.05017
137	H6	S	0.16892	0.04075	-0.21190	0.09026	0.01045
138	H6	PX	-0.12559	0.07214	-0.25445	-0.19984	-0.10998
139	H6	PY	-0.22205	-0.04895	-0.09113	0.27789	-0.25362
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00963	-0.04106	-0.01918	0.03772	-0.00445
142	C8	S	-0.23524	0.32831	0.10703	-0.45811	-0.05951
143	C8	PX	-0.03187	0.05416	-0.16692	0.02955	-0.00482
144	C8	PY	-0.35682	-0.37166	-0.05181	0.03425	0.14501
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	1.26253	0.59943	0.77477	0.18426	0.01231
147	C8	PX	1.79922	-0.10886	-0.54972	1.30781	-0.37546
148	C8	PY	0.66722	0.61663	0.89622	0.09797	0.80932
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.17396	-0.27988	-0.09313	0.26459	0.38239
151	C8	DYY	0.31136	0.49460	0.23928	-0.31416	-0.32175
152	C8	DZZ	-0.07638	-0.30170	-0.12774	0.25559	-0.01243
153	C8	DXY	-0.08769	0.41237	-0.54034	0.10545	0.05318
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.07237	-0.15894	-0.13012	-0.12353	0.14036
157	H8	S	-0.37773	-0.33238	-0.38204	-0.34802	0.09030
158	H8	PX	-0.09386	0.50974	0.23870	0.07544	-0.23154
159	H8	PY	-0.35364	-0.00697	-0.07686	-0.40334	0.20059
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.03059	0.04314	0.00743	-0.01664	-0.02349
162	C10	S	-0.20512	-0.38286	-0.12624	0.25233	0.20270
163	C10	PX	-0.17032	0.25320	-0.33737	0.08754	0.18019
164	C10	PY	-0.11175	-0.23178	-0.02450	0.08453	0.05615
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.06988	-0.17063	0.30687	0.24374	0.80198
167	C10	PX	-0.66070	0.18803	-0.19731	-0.37685	0.18752
168	C10	PY	0.08631	0.15535	0.25173	-0.06297	0.21733
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.17769	0.29651	0.07036	-0.04717	0.03968
171	C10	DYY	-0.34047	-0.63107	-0.19185	0.27335	0.19792
172	C10	DZZ	0.21792	0.34571	0.07461	-0.16318	-0.18326
173	C10	DXY	-0.07733	-0.05894	-0.01310	-0.01545	-0.03749
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.12676	-0.02277	0.14841	-0.07009	-0.17748
177	H16	S	0.36952	0.02822	0.30165	-0.02791	-0.20534
178	H16	PX	-0.27041	-0.21083	-0.31556	0.25104	0.28307
179	H16	PY	0.03922	-0.29136	0.24491	-0.08649	-0.18474
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.04755	0.14403	-0.11938	-0.06214	-0.04428
182	H18	S	-0.21612	0.33750	-0.11315	-0.22557	0.04895
183	H18	PX	0.06885	0.49516	-0.10027	-0.15058	-0.06845

184	H18	PY	-0.18021	0.01090	-0.26191	0.05852	0.02625
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		166	167	168	169	170
Eigenvalues:		3.54727	3.62575	3.69588	3.72333	3.78343
(ev):		96.52618	98.66173	100.57002	101.31713	102.95245

			A	A	A	A	A
1	H1	S	0.19929	0.31260	0.37230	0.15946	-0.00208
2	H1	S	0.14116	0.24642	0.21759	0.16398	-0.00950
3	H1	PX	-0.42429	-0.49980	-0.56892	-0.21944	-0.00054
4	H1	PY	-0.00630	-0.03664	-0.04023	0.17623	0.24033
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.03496	0.01121	0.01578	0.00113	0.01121
7	C1	S	-0.03505	-0.23979	-0.22025	-0.00092	0.08178
8	C1	PX	-0.31594	-0.26166	-0.29377	-0.19065	-0.05725
9	C1	PY	0.01901	-0.10225	-0.12548	0.10104	0.23689
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.63181	0.00643	-0.26220	-0.18162	-0.24905
12	C1	PX	0.35182	-0.28212	-0.10134	-0.20973	0.13035
13	C1	PY	-0.96076	0.11780	0.22997	-0.32517	-0.71151
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.10523	-0.33369	-0.43654	-0.12306	0.08508
16	C1	DYY	0.00736	0.17356	0.22088	0.11572	-0.03551
17	C1	DZZ	0.19440	0.09957	0.13302	0.00093	0.02099
18	C1	DXY	-0.01677	0.05598	0.00634	-0.31369	-0.46100
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.04293	0.01436	-0.01050	-0.00275	-0.01414
22	C2	S	0.02680	-0.16649	0.24096	0.00538	-0.09589
23	C2	PX	-0.29112	0.27086	-0.33669	-0.17252	-0.05847
24	C2	PY	-0.13189	-0.03885	0.18035	-0.14951	-0.31280
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.87199	-0.22163	0.24772	0.12844	0.56538
27	C2	PX	0.67767	0.00834	-0.09036	-0.24127	0.34276
28	C2	PY	1.36433	-0.33763	-0.15434	0.32363	0.84374
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.05837	-0.28006	0.45278	0.16649	0.03517
31	C2	DYY	0.00431	0.12080	-0.21889	-0.15567	-0.05528
32	C2	DZZ	-0.23268	0.10525	-0.11598	-0.00870	-0.02902
33	C2	DXY	-0.14082	-0.03806	0.24193	-0.34671	-0.57960
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06065	0.01669	-0.02498	0.01253	-0.03615
37	C3	S	-0.40806	0.01497	-0.02656	0.13810	0.06888
38	C3	PX	-0.16093	-0.02596	-0.03724	0.14569	0.24625
39	C3	PY	0.20294	-0.04771	-0.09970	-0.04197	-0.00388
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	4.17211	-0.84778	0.86146	-0.76839	1.41301
42	C3	PX	-2.76744	0.42856	-0.02928	0.23215	-0.99482
43	C3	PY	-1.29753	0.12760	-0.13553	-0.03559	-0.89633
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.53988	-0.02537	-0.03605	-0.26409	-0.35432
46	C3	DYY	-0.36991	-0.00004	0.07181	0.22946	0.38132

47	C3	DZZ	-0.21003	0.05270	-0.13678	0.03766	-0.17464
48	C3	DXY	0.14459	-0.03596	-0.18655	-0.14509	0.08231
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.02329	0.03745	0.01467	0.01647	-0.00709
52	C4	S	0.02644	-0.34147	-0.22111	-0.17365	-0.08678
53	C4	PX	-0.10878	-0.17564	-0.14612	-0.27536	-0.22811
54	C4	PY	0.00754	-0.49872	-0.29661	-0.06461	0.13858
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.83767	-0.50604	0.02048	-0.31238	0.29034
57	C4	PX	0.56183	-0.22863	-0.42373	0.37640	0.60492
58	C4	PY	-0.72697	-0.12437	-0.27799	-0.28656	-0.51560
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.27319	0.06584	0.02047	0.26313	0.29188
61	C4	DYY	-0.21300	-0.31786	-0.16732	-0.40710	-0.36302
62	C4	DZZ	-0.12001	0.24004	0.12877	0.14115	0.00794
63	C4	DXY	0.14672	-0.42960	-0.37151	0.03688	0.26485
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02583	0.03076	-0.02467	-0.00843	0.01087
67	C5	S	-0.10727	-0.33205	0.23788	0.14348	0.06925
68	C5	PX	-0.09161	0.23462	-0.18968	-0.26449	-0.22718
69	C5	PY	-0.10581	-0.42795	0.41669	-0.02974	-0.20947
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.29631	-0.08167	0.03517	0.23514	-0.54784
72	C5	PX	0.72863	-0.02125	-0.44720	0.37371	0.64862
73	C5	PY	0.70797	-0.42198	0.27893	0.30643	0.58022
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.31144	0.10548	0.04116	-0.24986	-0.31649
76	C5	DYY	0.26958	-0.31890	0.09854	0.38330	0.42169
77	C5	DZZ	0.13157	0.20666	-0.17792	-0.09780	0.00302
78	C5	DXY	0.18737	0.38318	-0.49517	0.03614	0.25202
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.06913	0.00517	0.00068	-0.00258	0.01829
82	C6	S	0.46877	-0.13601	0.11234	-0.12774	-0.06467
83	C6	PX	-0.21107	0.03272	-0.03642	0.15715	0.17931
84	C6	PY	-0.41393	0.03436	0.11183	0.03295	-0.02282
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-2.10320	0.07274	-0.28463	0.43288	-0.75468
87	C6	PX	-3.40082	0.57973	-0.05225	0.18043	-1.11371
88	C6	PY	-0.20494	-0.04959	-0.12628	0.31209	0.14102
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.51797	0.06935	-0.06476	0.31289	0.38819
91	C6	DYY	0.43976	-0.02611	0.02890	-0.29982	-0.43817
92	C6	DZZ	0.19550	0.03601	0.01711	0.02648	0.08392
93	C6	DXY	0.26381	-0.01003	-0.28319	-0.04829	0.29077
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.02500	0.00203	0.03704	-0.04848	0.01372
97	C7	S	0.36116	-0.14235	-0.13561	0.07556	-0.02796
98	C7	PX	0.13167	-0.05748	-0.12692	0.17981	0.09664
99	C7	PY	0.19447	0.00054	-0.03257	-0.21284	-0.12537
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

101	C7	S	-2.95775	0.52761	-0.99876	0.98802	-1.11660
102	C7	PX	2.08368	-0.43144	0.31465	-0.25686	0.75910
103	C7	PY	0.10740	0.06396	-0.02317	-0.30635	-0.14160
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.24827	-0.00753	-0.09056	0.21784	0.11434
106	C7	DYY	0.17338	0.04987	-0.01529	-0.22031	-0.21121
107	C7	DZZ	0.04149	0.02669	0.21137	-0.23382	0.06821
108	C7	DXY	-0.43494	0.06041	0.11954	0.03340	0.16858
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.02048	0.54539	0.37102	0.24814	0.04926
112	H3	S	0.08450	0.40519	0.32970	0.17702	0.06765
113	H3	PX	-0.19687	-0.33972	-0.10980	-0.30026	-0.25063
114	H3	PY	0.09069	-0.83254	-0.54938	-0.26326	0.05860
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.09002	0.50698	-0.45953	-0.18032	-0.00524
117	H4	S	0.08449	0.40309	-0.39979	-0.13379	-0.00934
118	H4	PX	-0.15184	0.45008	-0.20691	-0.27156	-0.23244
119	H4	PY	-0.25618	-0.69774	0.67507	0.14957	-0.12953
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.00867	0.00525	-0.00190	-0.01432	0.04032
122	N1	S	-0.04785	-0.08667	0.09092	0.16837	-0.03542
123	N1	PX	-0.02964	0.00733	-0.00422	0.06359	0.03255
124	N1	PY	-0.15740	-0.00093	0.08664	0.07106	0.10700
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.15696	0.24117	-0.09068	-0.05567	-0.52834
127	N1	PX	0.60147	0.00264	-0.07990	-0.12925	0.07256
128	N1	PY	-1.54851	0.23525	-0.04485	0.26101	0.08527
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.27477	0.00884	-0.12465	-0.09344	0.28417
131	N1	DYY	-0.36522	0.09359	0.11420	0.01749	-0.06940
132	N1	DZZ	-0.02307	0.00207	0.00032	-0.04749	0.12026
133	N1	DXY	-0.53248	0.02839	-0.04816	0.19051	0.39847
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.11853	0.26492	-0.39071	-0.15597	0.00293
137	H6	S	0.02024	0.16395	-0.24530	-0.14821	0.09171
138	H6	PX	-0.35776	0.46542	-0.62525	-0.19180	-0.00874
139	H6	PY	-0.10921	0.05576	0.04389	-0.22171	-0.29369
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01281	0.00394	-0.02988	0.04906	-0.03066
142	C8	S	-0.22456	0.02008	-0.02205	0.12402	-0.22115
143	C8	PX	0.32005	-0.01506	-0.02188	-0.09536	-0.08344
144	C8	PY	-0.15121	0.00823	0.04720	-0.14264	0.22127
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.76611	-0.23245	0.91722	-1.30028	1.37025
147	C8	PX	1.86570	-0.23655	0.32899	-0.57046	0.08155
148	C8	PY	1.17629	-0.36989	-0.04426	0.51055	0.03199
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00778	-0.02722	-0.06968	0.01598	0.28781
151	C8	DYY	0.06687	0.00363	0.03658	0.10108	-0.31739
152	C8	DZZ	-0.00403	0.00767	-0.14330	0.21747	-0.12876
153	C8	DXY	0.51769	-0.02261	0.01682	-0.12069	-0.09119
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.13179	0.07691	0.17820	-0.23725	-0.03135
157	H8	S	-0.52537	0.14028	0.03733	-0.14474	-0.22992
158	H8	PX	0.16804	-0.08641	-0.25173	0.29484	-0.02498
159	H8	PY	0.09913	0.02785	0.07758	-0.14574	-0.13596
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00055	0.00384	0.03658	-0.08374	0.07049
162	C10	S	0.02612	-0.04401	-0.21470	0.46573	-0.32505
163	C10	PX	0.36630	-0.02407	-0.05531	-0.18136	0.03292
164	C10	PY	-0.06161	0.01805	0.13436	-0.38983	0.44107
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.69723	-0.23932	-0.61033	1.46613	-0.98182
167	C10	PX	-0.27519	0.05217	-0.17705	0.10389	-0.05229
168	C10	PY	0.21645	-0.05637	-0.11000	0.25074	-0.08473
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.03240	-0.03548	-0.22935	0.62584	-0.52658
171	C10	DYY	-0.06507	0.01704	0.07767	-0.34991	0.44732
172	C10	DZZ	0.02137	0.02515	0.23187	-0.51318	0.38636
173	C10	DXY	-0.20779	0.02623	0.09016	0.06524	0.08218
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.17989	0.03772	0.24128	-0.34319	0.34631
177	H16	S	-0.04822	0.00863	0.18129	-0.25153	0.25110
178	H16	PX	0.25739	-0.05010	-0.24295	0.30576	-0.31171
179	H16	PY	-0.27707	0.04511	0.23717	-0.41000	0.41411
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.12973	0.01688	0.12348	-0.51295	0.32499
182	H18	S	-0.00395	0.03630	0.04001	-0.28306	0.22572
183	H18	PX	0.24940	0.01640	0.15351	-0.61504	0.36059
184	H18	PY	0.16941	0.01452	0.15910	-0.50812	0.36662
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	171	172	173	174	175
Eigenvalues:	3.88398	3.98232	4.02097	4.25472	4.46388
(ev):	105.68842	108.36459	109.41620	115.77675	121.46844

		A	A	A	A	A	
1	H1	S	0.59034	0.05615	0.05647	0.42830	0.07508
2	H1	S	0.39235	-0.07394	-0.01733	0.28936	0.11206
3	H1	PX	-0.76336	-0.08529	-0.07023	-0.46160	-0.02514
4	H1	PY	-0.06689	0.10558	0.00531	-0.07468	-0.03939
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.06418	0.04317	0.03132	0.07110	-0.07626
7	C1	S	-0.34516	-0.09970	-0.07621	-0.36666	0.39465
8	C1	PX	-0.46223	-0.03457	-0.02877	-0.31267	-0.01946
9	C1	PY	0.01129	0.20484	0.11593	0.05771	-0.10133
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.62372	-0.79347	-0.54824	-0.28202	0.45218
12	C1	PX	-0.30999	0.41614	0.23188	-0.35629	-0.44302
13	C1	PY	0.02359	-0.19158	0.05157	0.08527	0.34701
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.63061	0.00177	-0.01493	-0.44538	-0.26257
16	C1	DYY	0.59294	0.06387	0.08342	0.82106	-0.20371
17	C1	DZZ	0.37581	0.17795	0.12727	0.32592	-0.28311

18	C1	DXY	-0.05641	-0.29967	-0.11061	-0.03350	0.11796
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.06603	-0.00960	-0.02362	-0.07581	-0.10285
22	C2	S	-0.37893	-0.02346	0.06421	0.38150	0.70404
23	C2	PX	0.47143	-0.00026	-0.06725	-0.31610	0.04109
24	C2	PY	0.05203	-0.05130	-0.08057	-0.10813	-0.07035
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.64883	0.30250	0.33791	0.45894	0.13882
27	C2	PX	0.30034	0.24266	0.23989	-0.25976	0.03217
28	C2	PY	-0.03625	0.37484	0.16118	-0.07416	-0.00899
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.63932	-0.03137	0.09317	0.43778	-0.42584
31	C2	DYY	0.59466	0.01699	-0.13671	-0.82421	-0.40407
32	C2	DZZ	0.38776	-0.02897	-0.10625	-0.34314	-0.40358
33	C2	DXY	-0.08102	-0.04900	-0.04400	0.05957	-0.08131
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.02014	-0.08595	-0.04896	0.02343	-0.23305
37	C3	S	0.06905	0.18835	-0.05620	-0.09635	1.56394
38	C3	PX	-0.04090	0.01142	-0.04680	0.02487	-0.03944
39	C3	PY	-0.11900	-0.01875	0.08525	-0.16670	-0.04418
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.23046	2.32965	1.99853	-0.13560	0.25003
42	C3	PX	0.13417	-0.52148	-0.35558	0.36216	0.52545
43	C3	PY	-0.05941	-0.58608	-0.36894	-0.21081	0.08535
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.14872	-0.41568	-0.16521	-0.11920	-0.82759
46	C3	DYY	0.09105	0.27408	0.04851	0.20472	-0.95089
47	C3	DZZ	-0.10848	-0.38913	-0.19068	0.08222	-0.92920
48	C3	DXY	-0.17410	0.28146	0.19780	-0.44109	-0.00883
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.05028	-0.02647	-0.02028	-0.04782	0.02433
52	C4	S	0.27790	0.00009	0.01389	0.20908	-0.00810
53	C4	PX	-0.03009	-0.03395	0.04568	0.12753	0.02620
54	C4	PY	0.27500	0.16671	0.14314	0.33746	-0.05693
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.36015	0.78649	0.53193	0.31824	-0.76093
57	C4	PX	0.10540	0.12401	-0.05612	0.03584	-0.04416
58	C4	PY	0.14098	-0.38512	-0.16387	0.33416	0.39589
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.28760	-0.01186	-0.08480	-0.59997	0.05103
61	C4	DYY	0.23842	-0.04272	0.08947	0.39016	0.07771
62	C4	DZZ	-0.26456	-0.10897	-0.10199	-0.24349	0.08540
63	C4	DXY	0.27674	0.20446	0.20279	0.59986	-0.04829
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.04957	0.00915	0.01832	0.04255	0.00110
67	C5	S	0.27709	0.01675	-0.06554	-0.15875	-0.02869
68	C5	PX	-0.00546	-0.01214	0.03572	0.15230	-0.02976
69	C5	PY	0.26320	-0.04591	-0.11770	-0.32178	-0.04637
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.38019	-0.59832	-0.55902	-0.41161	0.16381

72	C5	PX	-0.18784	0.10552	0.00668	0.08554	0.06845
73	C5	PY	0.10074	0.34149	0.08338	-0.28855	-0.20530
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.27194	-0.05049	0.07775	0.48639	0.03665
76	C5	DYY	0.22823	0.02425	-0.05683	-0.31855	0.07830
77	C5	DZZ	-0.26365	0.03848	0.09234	0.21941	0.00162
78	C5	DXY	-0.30605	0.08768	0.21125	0.68704	0.02356
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.02084	0.00504	0.01628	-0.01357	-0.17415
82	C6	S	0.06277	0.11397	0.15550	0.03019	1.05593
83	C6	PX	0.06151	0.10376	-0.04615	0.01617	0.11900
84	C6	PY	-0.11070	0.03590	-0.11035	0.16472	0.19743
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.34788	-0.96863	-0.57361	0.03931	2.10205
87	C6	PX	-0.06300	-0.72095	-0.71702	0.40513	0.02730
88	C6	PY	-0.13085	0.29444	-0.18641	0.15700	-1.01721
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.14449	-0.01576	0.04044	0.21402	-0.58775
91	C6	DYY	0.08675	-0.08555	0.01676	-0.24109	-0.83274
92	C6	DZZ	-0.11561	0.02508	0.01984	-0.02634	-0.68537
93	C6	DXY	0.12266	0.04862	0.15355	-0.37847	-0.11895
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00221	0.11860	0.09284	-0.04129	-0.16804
97	C7	S	-0.06143	-0.50894	-0.38771	0.19465	1.16955
98	C7	PX	0.09793	-0.51158	-0.09702	0.08760	-0.06287
99	C7	PY	-0.13547	0.02873	0.18409	-0.21577	0.14217
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.02249	-2.35246	-1.93986	0.01880	0.25270
102	C7	PX	-0.00130	0.54071	0.70653	0.08710	0.00926
103	C7	PY	-0.04627	-0.22219	-0.17838	-0.22583	-0.37670
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.14484	-0.38889	-0.35298	0.11943	-0.74651
106	C7	DYY	-0.13173	0.44292	0.45946	-0.39601	-0.56063
107	C7	DZZ	-0.01335	0.62636	0.42693	-0.17084	-0.66489
108	C7	DXY	0.00927	0.79797	0.11895	-0.04265	-0.01335
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.32588	-0.10895	-0.15600	-0.48800	0.00372
112	H3	S	-0.22466	-0.01452	-0.03977	-0.28079	-0.06119
113	H3	PX	0.25879	0.00043	0.06202	0.26245	0.01022
114	H3	PY	0.35099	0.17178	0.19649	0.45826	-0.01685
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.32844	0.04346	0.15978	0.49097	0.00057
117	H4	S	-0.22956	-0.02438	0.08295	0.27369	0.06636
118	H4	PX	-0.29476	-0.01747	0.08437	0.29150	-0.00226
119	H4	PY	0.32502	-0.08041	-0.17635	-0.43655	0.02172
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.01284	0.00508	-0.01174	0.00373	0.34116
122	N1	S	-0.12080	-0.03385	0.08131	0.11228	-0.28589
123	N1	PX	-0.02233	-0.02570	0.09055	0.02522	0.20610
124	N1	PY	-0.07838	0.04012	-0.09382	0.16536	0.13989
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

126	N1	S	-0.02228	0.07332	-0.03474	-0.03722	-4.34292
127	N1	PX	0.07847	-0.01978	0.18444	-0.15872	-0.94587
128	N1	PY	-0.16738	-0.03095	-0.47980	0.28956	-0.30025
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.09572	-0.18571	0.19715	-0.11058	1.02900
131	N1	DYY	-0.01607	0.21717	-0.20243	0.15281	1.13932
132	N1	DZZ	0.03688	0.01399	-0.02740	0.01662	1.08366
133	N1	DXY	-0.11962	0.02731	-0.17836	0.14863	0.00893
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.60353	0.02922	-0.07821	-0.42958	0.08036
137	H6	S	0.40042	0.05113	0.02885	-0.27004	-0.03173
138	H6	PX	0.79459	0.00799	-0.11685	-0.47491	0.05893
139	H6	PY	0.00574	-0.02948	-0.00335	0.00943	0.00655
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.01522	-0.02050	-0.02037	0.00141	-0.06109
142	C8	S	-0.08253	0.04808	-0.00522	-0.00330	0.50255
143	C8	PX	0.02085	-0.08420	0.00377	-0.03489	0.11977
144	C8	PY	-0.01722	-0.19453	-0.10216	0.04772	-0.05327
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.14649	0.75765	0.52804	0.11644	0.80602
147	C8	PX	0.13426	0.37708	0.83956	-0.21032	-0.84051
148	C8	PY	-0.21952	0.59195	0.47097	0.14438	0.65665
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.02192	-0.42340	-0.10368	0.08795	-0.32010
151	C8	DYY	-0.00865	0.43779	0.08416	-0.05339	-0.23515
152	C8	DZZ	0.07195	-0.11627	-0.08690	0.00420	-0.28104
153	C8	DXY	0.04375	-0.25231	0.66129	-0.15708	0.16768
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.08100	0.70495	0.31812	-0.14606	0.11677
157	H8	S	-0.05492	0.24695	-0.00644	-0.13622	-0.13297
158	H8	PX	0.10490	-0.89229	-0.36824	0.14730	-0.08586
159	H8	PY	-0.07810	0.23517	0.22412	-0.08769	0.06053
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00286	-0.02927	-0.00087	0.00187	-0.06292
162	C10	S	0.00094	0.02682	-0.02708	0.01746	0.38173
163	C10	PX	-0.04952	0.32397	-0.67028	0.08039	-0.00772
164	C10	PY	0.01891	-0.33768	-0.06290	0.04366	0.00063
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.13940	0.49656	0.25883	0.03086	0.40621
167	C10	PX	-0.10602	0.10427	-0.64659	0.05060	0.24562
168	C10	PY	-0.05041	0.04639	0.08032	0.02507	0.08804
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.01019	0.18573	0.23353	-0.05444	-0.20394
171	C10	DYY	0.01466	-0.27872	-0.24437	0.06244	-0.26946
172	C10	DZZ	0.01105	-0.12648	0.00439	0.00466	-0.25136
173	C10	DXY	0.07594	-0.61583	1.13621	-0.15819	0.07822
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.06164	-0.42027	0.60406	-0.06233	0.02846
177	H16	S	0.04650	-0.21493	0.31589	-0.01303	-0.10496
178	H16	PX	-0.05301	0.42632	-0.65728	0.07727	-0.04912
179	H16	PY	0.03735	-0.32898	0.24241	-0.00777	0.00458

180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.03844	0.17016	-0.67512	0.08783	-0.00067
182	H18	S	-0.05157	0.03839	-0.38174	0.03975	0.04448
183	H18	PX	-0.04677	0.25429	-0.74796	0.09871	-0.00529
184	H18	PY	-0.00718	-0.02941	-0.23735	0.03213	-0.02596
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	176	177	178	179	180
Eigenvalues:	4.53682	4.57047	4.59613	4.69338	4.75434
(ev):	123.45324	124.36886	125.06718	127.71346	129.37231

		A	A	A	A	A	
1	H1	S	-0.09646	0.10324	0.25826	0.14374	-0.03927
2	H1	S	0.10343	-0.09816	-0.03282	-0.07107	0.16213
3	H1	PX	0.07219	-0.08441	-0.21510	-0.14349	0.08311
4	H1	PY	0.01085	-0.00538	-0.04588	-0.00727	-0.00951
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.14675	-0.12126	-0.24252	-0.16089	0.02456
7	C1	S	-1.06979	0.82845	1.53514	0.98790	-0.23429
8	C1	PX	0.11204	-0.06672	-0.07989	-0.04067	0.01375
9	C1	PY	-0.05517	0.10726	-0.08857	-0.03914	0.18083
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.19065	0.16009	0.49313	0.65862	-0.16162
12	C1	PX	-0.05704	0.11019	-0.20112	-0.09429	-0.33667
13	C1	PY	0.05911	-0.12435	0.22780	-0.14008	0.22278
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.61192	-0.54553	-1.15482	-0.76776	0.26172
16	C1	DYY	0.56877	-0.42185	-0.84782	-0.62844	0.15974
17	C1	DZZ	0.56557	-0.47306	-0.91418	-0.59755	0.05830
18	C1	DXY	0.01522	-0.09719	0.10904	0.05077	-0.11352
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.17721	0.11847	0.19925	-0.02320	0.16455
22	C2	S	-1.20482	-0.68126	-1.28310	0.04546	-0.91281
23	C2	PX	-0.12227	-0.02044	-0.06950	-0.00392	-0.07676
24	C2	PY	-0.06186	0.11980	-0.06470	-0.12801	0.00367
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.44595	-0.50451	-0.37224	0.54517	-0.66376
27	C2	PX	0.06732	-0.01814	-0.22684	0.13763	-0.02069
28	C2	PY	0.17629	0.04831	-0.21131	-0.10321	0.38648
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.74395	0.54868	0.90563	-0.09054	0.80462
31	C2	DYY	0.60840	0.40777	0.70097	-0.08283	0.51304
32	C2	DZZ	0.67781	0.44168	0.77076	-0.06617	0.59088
33	C2	DXY	0.00134	0.12411	-0.00444	-0.10993	0.07461
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03012	-0.00086	-0.20616	0.01662	0.12411
37	C3	S	-0.25626	0.01436	1.33267	-0.12099	-0.78958
38	C3	PX	0.04068	0.11113	0.03568	-0.03189	-0.01608
39	C3	PY	-0.15051	-0.06493	0.06708	0.18067	0.01403
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.28159	0.31725	0.02027	-0.66372	0.31757
42	C3	PX	-0.33093	-0.61602	0.44105	0.03015	0.67873

43	C3	PY	0.22401	0.13430	0.24372	-0.08322	-0.08444
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.07940	-0.08300	-0.85898	0.14214	0.46020
46	C3	DYY	0.20890	0.19249	-0.81878	-0.05530	0.49797
47	C3	DZZ	0.10116	-0.01716	-0.80062	0.07089	0.46913
48	C3	DXY	-0.06975	0.00951	0.03365	0.03860	-0.02131
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.23452	-0.20900	-0.02781	0.00259	-0.20533
52	C4	S	-1.53175	1.30500	0.25072	0.03482	1.25910
53	C4	PX	0.07090	-0.01294	0.14961	0.09268	-0.00406
54	C4	PY	0.10789	-0.03563	-0.09012	-0.07213	0.03570
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.61983	0.60094	-0.01096	0.14973	0.16723
57	C4	PX	0.03543	-0.00615	-0.17221	-0.05696	-0.03600
58	C4	PY	0.11244	-0.11586	0.11001	0.00466	0.01713
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.80192	-0.79007	-0.22560	-0.06386	-0.90411
61	C4	DYY	1.02454	-0.87390	0.05489	0.11896	-0.98016
62	C4	DZZ	0.89552	-0.80324	-0.12758	0.00079	-0.76481
63	C4	DXY	0.07825	-0.00922	-0.00966	-0.02583	-0.00378
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.24109	-0.11128	0.18517	0.15616	0.01224
67	C5	S	-1.66554	0.61856	-1.11946	-0.86677	-0.37327
68	C5	PX	-0.06445	0.11895	0.07138	-0.01325	0.07757
69	C5	PY	0.11620	0.05202	0.05154	-0.02974	0.12352
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.41257	0.32642	-0.43963	-0.74807	0.10037
72	C5	PX	0.09537	0.01506	-0.22168	-0.17742	0.32364
73	C5	PY	-0.07233	-0.12947	0.05867	0.29240	-0.43067
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.89924	-0.32994	0.75947	0.62104	0.28193
76	C5	DYY	1.06339	-0.57035	0.65706	0.67945	0.06465
77	C5	DZZ	0.92432	-0.41176	0.72195	0.58116	0.04852
78	C5	DXY	-0.08777	0.02982	0.01050	0.01247	-0.01484
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.11157	0.21541	0.02355	-0.13067	0.05387
82	C6	S	-0.68331	-1.15261	-0.25327	0.73657	-0.35716
83	C6	PX	0.02439	0.00886	0.08082	-0.01432	0.04908
84	C6	PY	-0.06831	-0.07241	-0.06460	0.03899	0.05050
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.24850	-0.94401	-0.28638	-0.09879	3.43723
87	C6	PX	-0.51715	-0.78531	0.60220	0.47812	-0.45773
88	C6	PY	-0.33285	-0.15847	0.33571	0.14062	-2.00711
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.36610	0.77994	0.25647	-0.48859	0.13149
91	C6	DYY	0.44826	0.86930	0.05532	-0.57892	0.17671
92	C6	DZZ	0.40256	0.80167	0.11450	-0.47437	0.17117
93	C6	DXY	0.05472	0.08959	0.04421	-0.01659	-0.06792
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.09248	-0.14115	-0.02591	0.23406	0.12455

97	C7	S	0.60747	0.91248	0.12828	-1.49879	-0.60281
98	C7	PX	-0.03551	-0.07649	-0.00719	0.05606	0.08950
99	C7	PY	-0.06194	-0.07699	0.13806	-0.02003	0.00705
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00615	0.02154	0.62715	-0.43901	-1.07655
102	C7	PX	0.30350	0.10049	-0.54417	-0.13811	0.87506
103	C7	PY	0.19750	0.50579	-0.12662	0.17331	-0.93742
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.39286	-0.58446	-0.10847	1.16403	0.40173
106	C7	DYY	-0.43187	-0.62263	0.01122	0.96977	0.40238
107	C7	DZZ	-0.34714	-0.51654	-0.09428	0.87581	0.44407
108	C7	DXY	0.09379	0.17392	-0.07896	-0.12125	-0.10114
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.20534	0.14297	-0.04290	-0.03834	0.19215
112	H3	S	0.09488	-0.07922	-0.03785	-0.01238	-0.05794
113	H3	PX	0.07913	-0.06295	0.02816	0.01894	-0.08738
114	H3	PY	0.14211	-0.09327	0.05175	0.03363	-0.15771
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.19754	0.12483	-0.09171	-0.12562	0.03320
117	H4	S	0.17226	-0.00821	0.03543	-0.02645	0.23660
118	H4	PX	-0.09275	0.05806	-0.03282	-0.06048	-0.00244
119	H4	PY	0.13879	-0.09532	0.04218	0.08182	0.00973
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.09750	-0.03737	-0.10463	-0.05350	0.42714
122	N1	S	-0.10825	-0.01838	0.09944	-0.00382	0.03316
123	N1	PX	0.04087	-0.00435	-0.06340	0.01412	0.09877
124	N1	PY	-0.06291	-0.14105	-0.01494	0.05080	0.07676
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.34729	0.46832	1.42741	0.98601	-7.45202
127	N1	PX	-0.22781	0.32543	0.18176	0.22912	-1.90282
128	N1	PY	-0.38098	-0.46593	0.34556	0.31769	-0.76575
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.33214	0.01877	-0.38181	-0.09565	1.01913
131	N1	DYY	0.23381	-0.21646	-0.31315	-0.08047	1.10704
132	N1	DZZ	0.31604	-0.12033	-0.32783	-0.18792	1.37750
133	N1	DXY	-0.10283	-0.16550	0.05146	0.07077	0.04110
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.12205	-0.11276	-0.20411	0.01306	-0.15321
137	H6	S	0.14034	0.06845	-0.00081	0.00630	0.09052
138	H6	PX	-0.09824	-0.10749	-0.15430	0.02680	-0.17614
139	H6	PY	0.01388	0.01322	0.01075	-0.00111	-0.00377
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.11737	-0.23710	0.11829	-0.02599	0.16283
142	C8	S	0.70204	1.46049	-0.72003	0.31437	-1.02233
143	C8	PX	0.03685	0.01645	-0.01890	-0.07688	0.01627
144	C8	PY	-0.04748	-0.05757	0.11132	-0.19928	-0.07200
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.73946	0.54671	-0.84897	-0.31634	1.32489
147	C8	PX	0.17772	0.78505	-0.22347	0.08524	-1.41885
148	C8	PY	0.39701	-0.11390	-0.50348	-0.39783	2.05031
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.46638	-0.90228	0.49914	-0.15656	0.57231

151	C8	DYY	-0.41684	-0.91846	0.41230	-0.06981	0.81696
152	C8	DZZ	-0.45562	-0.89968	0.45993	-0.12166	0.56807
153	C8	DXY	0.08023	0.08635	-0.05392	-0.10460	0.01099
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.07619	0.18680	0.02914	-0.23466	-0.20060
157	H8	S	-0.11536	0.01148	0.12320	0.19759	-0.35687
158	H8	PX	-0.09251	-0.16221	0.01522	0.22777	0.10780
159	H8	PY	-0.01097	-0.01186	0.03447	-0.09573	0.01496
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.08014	-0.14746	0.15507	-0.30794	-0.00734
162	C10	S	0.56024	1.07811	-1.02702	1.96607	-0.07654
163	C10	PX	-0.00128	0.00287	-0.00174	0.01060	-0.02292
164	C10	PY	0.06015	0.16225	-0.07283	0.07021	-0.15474
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.29898	0.18037	-0.58047	0.73985	1.09728
167	C10	PX	-0.05004	-0.28503	0.04943	-0.00520	0.64915
168	C10	PY	0.02405	-0.10034	-0.07518	0.02021	0.33854
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.35381	-0.71155	0.70280	-1.47805	0.07542
171	C10	DYY	-0.32299	-0.56167	0.64545	-1.33227	-0.17315
172	C10	DZZ	-0.30351	-0.54988	0.58037	-1.12627	-0.02902
173	C10	DXY	0.02089	0.02209	-0.01630	-0.03279	0.02512
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.06503	0.15520	-0.11933	0.23648	-0.08920
177	H16	S	-0.02420	-0.00668	0.06113	-0.16586	-0.21073
178	H16	PX	-0.04901	-0.09081	0.09648	-0.19269	-0.00665
179	H16	PY	0.02128	0.04950	-0.04986	0.12946	-0.00741
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.04497	0.09874	-0.10251	0.26991	0.00896
182	H18	S	-0.07461	-0.21323	0.10409	-0.15885	0.20361
183	H18	PX	0.03348	0.07378	-0.09074	0.24256	-0.00760
184	H18	PY	0.00978	0.03840	-0.03536	0.10963	-0.03015
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	181	182	183	184	185
Eigenvalues:	4.86203	4.88576	5.04654	5.28033	0.00000
(ev):	132.30270	132.94838	137.32340	143.68525	0.00000

		A	A	A	A	A	
1	H1	S	-0.00313	0.25367	0.06797	-0.21258	0.00000
2	H1	S	0.04847	0.04260	-0.11924	0.04590	0.00000
3	H1	PX	0.01114	-0.24467	-0.09210	0.22936	0.00000
4	H1	PY	-0.02417	-0.01295	-0.00890	-0.01060	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.04057	-0.23752	-0.04869	0.17493	0.00000
7	C1	S	-0.27385	1.33181	0.37159	-1.07533	0.00000
8	C1	PX	0.01476	0.04918	0.00108	-0.06938	0.00000
9	C1	PY	-0.15118	-0.02790	-0.09380	-0.03666	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.37526	1.41893	-0.28652	-0.91727	0.00000
12	C1	PX	0.00558	-0.54508	0.32339	0.26349	0.00000
13	C1	PY	0.29788	0.07785	0.01723	-0.13797	0.00000

14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.15572	-1.18125	-0.34653	1.01811	0.00000
16	C1	DYY	0.21248	-1.05767	-0.26480	1.00925	0.00000
17	C1	DZZ	0.15770	-0.85104	-0.16517	0.57101	0.00000
18	C1	DXY	0.14458	-0.00038	0.09100	0.07709	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.06772	-0.23027	0.14392	-0.13268	0.00000
22	C2	S	-0.35772	1.38673	-0.93128	0.82945	0.00000
23	C2	PX	-0.00872	-0.05196	0.01059	-0.05380	0.00000
24	C2	PY	0.16324	0.02600	0.08611	-0.01730	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.16015	1.53411	-0.44593	0.71019	0.00000
27	C2	PX	0.05007	0.70403	0.16539	0.36744	0.00000
28	C2	PY	-0.01483	0.32703	0.05195	0.41553	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.40911	-1.12560	0.87688	-0.75043	0.00000
31	C2	DYY	0.26025	-1.12767	0.72188	-0.78444	0.00000
32	C2	DZZ	0.22318	-0.83381	0.48424	-0.43466	0.00000
33	C2	DXY	0.15873	0.05973	0.05644	0.00520	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.20263	0.09926	-0.03300	-0.24852	0.00000
37	C3	S	1.19534	-0.69620	0.06703	1.34366	0.00000
38	C3	PX	0.03086	0.10038	-0.02462	-0.00731	0.00000
39	C3	PY	0.04209	0.03028	0.11750	0.11288	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.41304	0.50046	0.89614	3.53678	0.00000
42	C3	PX	0.02412	-0.17882	-0.36204	-0.86575	0.00000
43	C3	PY	0.39903	-0.22782	0.50537	-0.98022	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.90452	0.29572	-0.03939	-1.04713	0.00000
46	C3	DYY	-0.97493	0.67450	-0.26120	-1.43542	0.00000
47	C3	DZZ	-0.74281	0.36468	-0.10141	-0.83969	0.00000
48	C3	DXY	-0.05959	0.02773	-0.01143	-0.11698	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.15826	0.13547	0.12173	-0.13827	0.00000
52	C4	S	-0.98363	-0.77670	-0.82036	0.86294	0.00000
53	C4	PX	-0.02621	0.12689	0.01880	-0.05605	0.00000
54	C4	PY	0.02358	-0.05919	-0.01897	0.05410	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-1.00805	-1.16812	-0.34896	1.04117	0.00000
57	C4	PX	0.12690	0.06877	0.08030	-0.05654	0.00000
58	C4	PY	0.20703	0.35696	-0.08654	-0.31856	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.77445	0.56486	0.66701	-0.77045	0.00000
61	C4	DYY	0.74126	0.78377	0.68658	-0.81867	0.00000
62	C4	DZZ	0.56990	0.46371	0.42153	-0.44981	0.00000
63	C4	DXY	0.03222	-0.03327	0.01845	0.00580	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.22184	0.03586	-0.16331	0.12009	0.00000
67	C5	S	1.30153	-0.28080	1.01789	-0.77289	0.00000

68	C5	PX	0.01932	-0.12750	0.05468	-0.04095	0.00000
69	C5	PY	0.03215	-0.05939	0.05374	-0.04185	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	1.10151	-0.50032	0.66645	-1.14590	0.00000
72	C5	PX	0.27718	0.31229	0.09328	0.02565	0.00000
73	C5	PY	-0.33332	0.09208	-0.08073	0.27012	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-1.00610	0.15372	-0.82428	0.69928	0.00000
76	C5	DYY	-1.07997	0.37082	-0.92607	0.71734	0.00000
77	C5	DZZ	-0.79822	0.10266	-0.56097	0.38810	0.00000
78	C5	DXY	0.02374	0.03582	0.01653	0.00411	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.17013	0.26217	-0.03969	0.17596	0.00000
82	C6	S	-1.03366	-1.48003	0.40761	-0.96418	0.00000
83	C6	PX	0.05146	-0.04931	0.07236	0.02296	0.00000
84	C6	PY	-0.05442	0.01955	0.04275	-0.04008	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.07785	0.24556	0.38298	-1.73173	0.00000
87	C6	PX	-0.28095	-0.82911	-0.60168	-1.23639	0.00000
88	C6	PY	-0.96370	-1.61530	-0.82374	0.14888	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.83159	0.99258	-0.24438	0.83462	0.00000
91	C6	DYY	0.75634	1.31575	-0.40814	0.90714	0.00000
92	C6	DZZ	0.61082	0.91663	-0.14713	0.59339	0.00000
93	C6	DXY	-0.00568	-0.08317	-0.02080	-0.06601	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.05846	0.04544	0.22163	0.19461	0.00000
97	C7	S	-0.24707	-0.17701	-1.37586	-0.89381	0.00000
98	C7	PX	0.03850	0.03332	-0.00837	-0.03366	0.00000
99	C7	PY	0.16866	-0.07107	-0.01960	0.13767	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.15862	-1.00633	-1.01258	-3.04260	0.00000
102	C7	PX	0.13555	0.79838	0.42604	1.30880	0.00000
103	C7	PY	-0.26203	-0.38683	0.10776	-0.38530	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.21180	0.10673	1.29698	1.04895	0.00000
106	C7	DYY	0.31180	0.06151	0.97812	0.90205	0.00000
107	C7	DZZ	0.19487	0.17645	0.77058	0.61991	0.00000
108	C7	DXY	-0.21544	0.07098	-0.06610	-0.23490	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.13743	-0.15941	-0.13881	0.17994	0.00000
112	H3	S	0.03333	-0.00770	0.07809	0.00335	0.00000
113	H3	PX	0.06801	0.07946	0.06219	-0.07709	0.00000
114	H3	PY	0.12818	0.15029	0.14419	-0.18022	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.22772	-0.05769	0.19583	-0.13888	0.00000
117	H4	S	0.02822	0.08872	-0.03784	0.04240	0.00000
118	H4	PX	0.11558	-0.05562	0.10976	-0.08166	0.00000
119	H4	PY	-0.18582	0.07004	-0.18590	0.14738	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.04920	0.19371	0.11360	-0.00700	0.00000

122	N1	S	0.20026	0.09766	-0.13615	-0.00499	0.00000
123	N1	PX	-0.09423	-0.02345	0.13465	-0.04264	0.00000
124	N1	PY	-0.04509	-0.10365	0.05577	-0.07893	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.64116	-4.00911	-1.74496	-0.01352	0.00000
127	N1	PX	-0.52122	-0.99044	-0.14603	0.09288	0.00000
128	N1	PY	-0.23040	-0.76611	-0.41672	-0.37291	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.08313	0.40982	0.53266	-0.00762	0.00000
131	N1	DYY	-0.09393	0.31997	0.47186	-0.13917	0.00000
132	N1	DZZ	0.21708	0.65931	0.27643	0.00453	0.00000
133	N1	DXY	0.05586	-0.11671	-0.06808	-0.10717	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.09881	0.24340	-0.18538	0.17624	0.00000
137	H6	S	0.03868	0.07839	0.14597	0.03417	0.00000
138	H6	PX	-0.12112	0.20935	-0.21430	0.16453	0.00000
139	H6	PY	-0.00432	0.00562	-0.00388	-0.00126	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.20104	-0.00143	-0.23473	-0.11992	0.00000
142	C8	S	-1.20376	-0.07961	1.48166	0.61555	0.00000
143	C8	PX	-0.05542	-0.00884	-0.00156	-0.02494	0.00000
144	C8	PY	-0.12113	0.01588	0.08119	0.01526	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.53717	1.22147	1.57225	1.34958	0.00000
147	C8	PX	-0.42589	-0.36816	0.19320	0.81979	0.00000
148	C8	PY	0.50031	1.33811	0.25965	0.88479	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.87956	-0.02404	-1.13088	-0.48419	0.00000
151	C8	DYY	1.05073	0.04558	-1.35618	-0.66673	0.00000
152	C8	DZZ	0.71376	-0.00932	-0.82714	-0.39590	0.00000
153	C8	DXY	-0.05602	-0.00966	-0.07904	-0.09133	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.11675	-0.05438	-0.30948	-0.30118	0.00000
157	H8	S	-0.06051	-0.25349	0.01688	-0.22109	0.00000
158	H8	PX	0.10451	-0.01136	0.26973	0.26994	0.00000
159	H8	PY	-0.00246	-0.00033	-0.12496	-0.09187	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.17714	0.06308	0.15128	0.05280	0.00000
162	C10	S	1.04887	-0.40904	-0.87231	-0.25962	0.00000
163	C10	PX	-0.01469	-0.01284	0.01351	0.01602	0.00000
164	C10	PY	-0.11327	-0.02687	0.17490	0.12488	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	1.02964	0.41767	-0.68464	0.13520	0.00000
167	C10	PX	0.23955	0.25656	-0.01149	-0.25174	0.00000
168	C10	PY	0.18239	0.14806	-0.09156	0.09552	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.86353	0.35620	0.77480	0.25097	0.00000
171	C10	DYY	-0.95991	0.25482	0.93492	0.37078	0.00000
172	C10	DZZ	-0.60740	0.21925	0.47818	0.15830	0.00000
173	C10	DXY	-0.00864	-0.00258	-0.04170	-0.05519	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

176	H16	S	0.12646	-0.10467	-0.17749	-0.05409	0.00000
177	H16	S	-0.18393	-0.06110	0.09690	0.10788	0.00000
178	H16	PX	-0.14189	0.05672	0.16302	0.07216	0.00000
179	H16	PY	0.10084	-0.04215	-0.10881	-0.04117	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.18276	-0.04689	-0.13611	-0.05442	0.00000
182	H18	S	-0.03400	0.09450	0.09712	-0.06220	0.00000
183	H18	PX	0.15962	-0.06151	-0.13698	-0.04004	0.00000
184	H18	PY	0.07652	-0.04122	-0.08140	-0.01938	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

Mulliken Population Analysis

AO	atom type		Occupancy
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1	H1	S	0.534227
2	H1	S	0.293930
3	H1	PX	0.010027
4	H1	PY	0.001556
5	H1	PZ	0.002424
6	C1	S	1.996538
7	C1	S	0.673068
8	C1	PX	0.731242
9	C1	PY	0.741701
10	C1	PZ	0.520173
11	C1	S	0.451915
12	C1	PX	0.308437
13	C1	PY	0.165618
14	C1	PZ	0.451393
15	C1	DXX	0.018907
16	C1	DYY	0.020693
17	C1	DZZ	-0.018414
18	C1	DXY	0.013999
19	C1	DXZ	0.003430
20	C1	DYZ	0.008192
21	C2	S	1.996536
22	C2	S	0.672240
23	C2	PX	0.730798
24	C2	PY	0.744021
25	C2	PZ	0.532194
26	C2	S	0.467023
27	C2	PX	0.306340
28	C2	PY	0.159501
29	C2	PZ	0.465732
30	C2	DXX	0.018030
31	C2	DYY	0.020448
32	C2	DZZ	-0.017929
33	C2	DXY	0.014807
34	C2	DXZ	0.003257
35	C2	DYZ	0.006821
36	C3	S	1.996655
37	C3	S	0.671935
38	C3	PX	0.714603

39	C3	PY	0.760397
40	C3	PZ	0.544646
41	C3	S	0.440812
42	C3	PX	0.210980
43	C3	PY	0.233561
44	C3	PZ	0.466911
45	C3	DXX	0.019466
46	C3	DYY	0.030938
47	C3	DZZ	-0.017152
48	C3	DXY	0.013298
49	C3	DXZ	0.003656
50	C3	DYZ	0.010067
51	C4	S	1.996540
52	C4	S	0.669391
53	C4	PX	0.718668
54	C4	PY	0.746079
55	C4	PZ	0.524657
56	C4	S	0.489691
57	C4	PX	0.199828
58	C4	PY	0.294507
59	C4	PZ	0.474817
60	C4	DXX	0.020150
61	C4	DYY	0.019471
62	C4	DZZ	-0.018519
63	C4	DXY	0.014098
64	C4	DXZ	0.005439
65	C4	DYZ	0.005240
66	C5	S	1.996582
67	C5	S	0.674128
68	C5	PX	0.722416
69	C5	PY	0.754860
70	C5	PZ	0.499870
71	C5	S	0.499096
72	C5	PX	0.212127
73	C5	PY	0.293392
74	C5	PZ	0.453126
75	C5	DXX	0.019682
76	C5	DYY	0.019518
77	C5	DZZ	-0.018988
78	C5	DXY	0.014776
79	C5	DXZ	0.005484
80	C5	DYZ	0.005965
81	C6	S	1.996741
82	C6	S	0.693344
83	C6	PX	0.723360
84	C6	PY	0.756907
85	C6	PZ	0.480469
86	C6	S	0.345409
87	C6	PX	0.184739
88	C6	PY	0.130464
89	C6	PZ	0.365449
90	C6	DXX	0.021562
91	C6	DYY	0.034517
92	C6	DZZ	-0.020076

93	C6	DXY	0.024653
94	C6	DXZ	0.006464
95	C6	DYZ	0.015544
96	C7	S	1.996678
97	C7	S	0.676646
98	C7	PX	0.724481
99	C7	PY	0.751110
100	C7	PZ	0.511160
101	C7	S	0.445210
102	C7	PX	0.309117
103	C7	PY	0.200439
104	C7	PZ	0.458662
105	C7	DXX	0.021581
106	C7	DYY	0.016439
107	C7	DZZ	-0.017967
108	C7	DXY	0.016389
109	C7	DXZ	0.002856
110	C7	DYZ	0.008651
111	H3	S	0.535714
112	H3	S	0.297733
113	H3	PX	0.003041
114	H3	PY	0.008358
115	H3	PZ	0.002458
116	H4	S	0.536095
117	H4	S	0.294211
118	H4	PX	0.003646
119	H4	PY	0.007816
120	H4	PZ	0.002259
121	N1	S	1.996235
122	N1	S	0.785459
123	N1	PX	0.913388
124	N1	PY	0.778246
125	N1	PZ	0.672021
126	N1	S	0.964114
127	N1	PX	0.571462
128	N1	PY	0.314826
129	N1	PZ	0.552948
130	N1	DXX	-0.000187
131	N1	DYY	0.013831
132	N1	DZZ	-0.011239
133	N1	DXY	0.017646
134	N1	DXZ	0.006469
135	N1	DYZ	0.009289
136	H6	S	0.531044
137	H6	S	0.282647
138	H6	PX	0.010177
139	H6	PY	0.001499
140	H6	PZ	0.002415
141	C8	S	1.996653
142	C8	S	0.680637
143	C8	PX	0.667464
144	C8	PY	0.769201
145	C8	PZ	0.537599
146	C8	S	0.375689

147	C8	PX	0.126334
148	C8	PY	0.093261
149	C8	PZ	0.429449
150	C8	DXX	0.019140
151	C8	DYY	0.030685
152	C8	DZZ	-0.019127
153	C8	DXY	0.025934
154	C8	DXZ	0.009133
155	C8	DYZ	0.010716
156	H8	S	0.530976
157	H8	S	0.287277
158	H8	PX	0.009214
159	H8	PY	0.002740
160	H8	PZ	0.002486
161	C10	S	1.996645
162	C10	S	0.679880
163	C10	PX	0.726621
164	C10	PY	0.770854
165	C10	PZ	0.463199
166	C10	S	0.565019
167	C10	PX	0.369295
168	C10	PY	0.236050
169	C10	PZ	0.444426
170	C10	DXX	0.011825
171	C10	DYY	0.018859
172	C10	DZZ	-0.020377
173	C10	DXY	0.013621
174	C10	DXZ	0.000145
175	C10	DYZ	0.007897
176	H16	S	0.533171
177	H16	S	0.306004
178	H16	PX	0.007270
179	H16	PY	0.004369
180	H16	PZ	0.002240
181	H18	S	0.529085
182	H18	S	0.288122
183	H18	PX	0.008764
184	H18	PY	0.003094
185	H18	PZ	0.002105

Atom	Occupancy	Charge
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H1	0.842164	0.157836
C1	6.086893	-0.086893
C2	6.119819	-0.119819
C3	6.100773	-0.100773
C4	6.160057	-0.160057
C5	6.152032	-0.152032
C6	5.759546	0.240454
C7	6.121452	-0.121452
H3	0.847304	0.152696
H4	0.844027	0.155973
N1	7.584508	-0.584508

H6	0.827782	0.172218
C8	5.752768	0.247232
H8	0.832693	0.167307
C10	6.283960	-0.283960
H16	0.853054	0.146946
H18	0.831169	0.168831

Total Charge = 0.000000

Natural Atomic Orbital Populations

Nao	Atom	Type	Basis	Occupancy
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1	H1	S	MIN	0.762232
2	H1	S	RYD	0.000660
3	H1	PX	RYD	0.000584
4	H1	PY	RYD	0.000022
5	H1	PZ	RYD	0.000084
6	C1	S	MIN	1.999001
7	C1	S	MIN	0.946432
8	C1	S	RYD	0.000872
9	C1	S	RYD	0.000017
10	C1	PX	MIN	1.202635
11	C1	PX	RYD	0.005762
12	C1	PY	MIN	1.048784
13	C1	PY	RYD	0.006172
14	C1	PZ	MIN	0.978641
15	C1	PZ	RYD	0.001737
16	C1	DXY	RYD	0.001645
17	C1	DXZ	RYD	0.000736
18	C1	DYZ	RYD	0.000962
19	C1	DXX-YY	RYD	0.001647
20	C1	D3ZZ-RR	RYD	0.001200
21	C2	S	MIN	1.998979
22	C2	S	MIN	0.958145
23	C2	S	RYD	0.001101
24	C2	S	RYD	0.000030
25	C2	PX	MIN	1.208579
26	C2	PX	RYD	0.005767
27	C2	PY	MIN	1.052169
28	C2	PY	RYD	0.007106
29	C2	PZ	MIN	1.005452
30	C2	PZ	RYD	0.001993
31	C2	DXY	RYD	0.001815
32	C2	DXZ	RYD	0.000747
33	C2	DYZ	RYD	0.000851
34	C2	DXX-YY	RYD	0.001530
35	C2	D3ZZ-RR	RYD	0.001217
36	C3	S	MIN	1.998972
37	C3	S	MIN	0.885307
38	C3	S	RYD	0.001378
39	C3	S	RYD	0.000049

40	C3	PX	MIN	1.074367
41	C3	PX	RYD	0.008200
42	C3	PY	MIN	1.115619
43	C3	PY	RYD	0.004436
44	C3	PZ	MIN	1.037130
45	C3	PZ	RYD	0.001083
46	C3	DXY	RYD	0.001228
47	C3	DXZ	RYD	0.000292
48	C3	DYZ	RYD	0.001438
49	C3	DXX-YY	RYD	0.001830
50	C3	D3ZZ-RR	RYD	0.001064
51	C4	S	MIN	1.999075
52	C4	S	MIN	0.958946
53	C4	S	RYD	0.000696
54	C4	S	RYD	0.000025
55	C4	PX	MIN	1.067538
56	C4	PX	RYD	0.005994
57	C4	PY	MIN	1.183150
58	C4	PY	RYD	0.006385
59	C4	PZ	MIN	1.008590
60	C4	PZ	RYD	0.001893
61	C4	DXY	RYD	0.001657
62	C4	DXZ	RYD	0.000548
63	C4	DYZ	RYD	0.001053
64	C4	DXX-YY	RYD	0.001705
65	C4	D3ZZ-RR	RYD	0.001256
66	C5	S	MIN	1.999086
67	C5	S	MIN	0.962389
68	C5	S	RYD	0.000636
69	C5	S	RYD	0.000028
70	C5	PX	MIN	1.077615
71	C5	PX	RYD	0.005832
72	C5	PY	MIN	1.176961
73	C5	PY	RYD	0.006360
74	C5	PZ	MIN	0.961742
75	C5	PZ	RYD	0.001598
76	C5	DXY	RYD	0.001718
77	C5	DXZ	RYD	0.000546
78	C5	DYZ	RYD	0.001159
79	C5	DXX-YY	RYD	0.001678
80	C5	D3ZZ-RR	RYD	0.001280
81	C6	S	MIN	1.999157
82	C6	S	MIN	0.838809
83	C6	S	RYD	0.003640
84	C6	S	RYD	0.000105
85	C6	PX	MIN	1.009691
86	C6	PX	RYD	0.010802
87	C6	PY	MIN	0.972122
88	C6	PY	RYD	0.007625
89	C6	PZ	MIN	0.864754
90	C6	PZ	RYD	0.001134
91	C6	DXY	RYD	0.002288
92	C6	DXZ	RYD	0.000670
93	C6	DYZ	RYD	0.002295

94	C6	DXX-YY	RYD	0.002404
95	C6	D3ZZ-RR	RYD	0.001021
96	C7	S	MIN	1.998878
97	C7	S	MIN	0.958603
98	C7	S	RYD	0.000707
99	C7	S	RYD	0.000040
100	C7	PX	MIN	1.176245
101	C7	PX	RYD	0.004635
102	C7	PY	MIN	1.069483
103	C7	PY	RYD	0.005020
104	C7	PZ	MIN	0.959855
105	C7	PZ	RYD	0.001440
106	C7	DXY	RYD	0.001665
107	C7	DXZ	RYD	0.000509
108	C7	DYZ	RYD	0.001260
109	C7	DXX-YY	RYD	0.001580
110	C7	D3ZZ-RR	RYD	0.001232
111	H3	S	MIN	0.763667
112	H3	S	RYD	0.000525
113	H3	PX	RYD	0.000134
114	H3	PY	RYD	0.000474
115	H3	PZ	RYD	0.000083
116	H4	S	MIN	0.763460
117	H4	S	RYD	0.000544
118	H4	PX	RYD	0.000181
119	H4	PY	RYD	0.000442
120	H4	PZ	RYD	0.000072
121	N1	S	MIN	1.999380
122	N1	S	MIN	1.378795
123	N1	S	RYD	0.000485
124	N1	S	RYD	0.000015
125	N1	PX	MIN	1.623516
126	N1	PX	RYD	0.004276
127	N1	PY	MIN	1.254374
128	N1	PY	RYD	0.003891
129	N1	PZ	MIN	1.246202
130	N1	PZ	RYD	0.001303
131	N1	DXY	RYD	0.003892
132	N1	DXZ	RYD	0.002985
133	N1	DYZ	RYD	0.001751
134	N1	DXX-YY	RYD	0.002990
135	N1	D3ZZ-RR	RYD	0.002863
136	H6	S	MIN	0.751460
137	H6	S	RYD	0.000765
138	H6	PX	RYD	0.000571
139	H6	PY	RYD	0.000022
140	H6	PZ	RYD	0.000077
141	C8	S	MIN	1.999041
142	C8	S	MIN	0.865816
143	C8	S	RYD	0.002880
144	C8	S	RYD	0.000109
145	C8	PX	MIN	0.937354
146	C8	PX	RYD	0.009642
147	C8	PY	MIN	1.062377

148	C8	PY	RVD	0.007632
149	C8	PZ	MIN	1.009711
150	C8	PZ	RVD	0.001605
151	C8	DXY	RVD	0.002139
152	C8	DXZ	RVD	0.001079
153	C8	DYZ	RVD	0.001641
154	C8	DXX-YY	RVD	0.002298
155	C8	D3ZZ-RR	RVD	0.001107
156	H8	S	MIN	0.760888
157	H8	S	RVD	0.000440
158	H8	PX	RVD	0.000538
159	H8	PY	RVD	0.000083
160	H8	PZ	RVD	0.000088
161	C10	S	MIN	1.998994
162	C10	S	MIN	1.046941
163	C10	S	RVD	0.001135
164	C10	S	RVD	0.000016
165	C10	PX	MIN	1.220922
166	C10	PX	RVD	0.004335
167	C10	PY	MIN	1.127537
168	C10	PY	RVD	0.003594
169	C10	PZ	MIN	0.889253
170	C10	PZ	RVD	0.002249
171	C10	DXY	RVD	0.001857
172	C10	DXZ	RVD	0.000047
173	C10	DYZ	RVD	0.001501
174	C10	DXX-YY	RVD	0.002020
175	C10	D3ZZ-RR	RVD	0.001518
176	H16	S	MIN	0.782447
177	H16	S	RVD	0.000416
178	H16	PX	RVD	0.000420
179	H16	PY	RVD	0.000203
180	H16	PZ	RVD	0.000087
181	H18	S	MIN	0.764824
182	H18	S	RVD	0.000813
183	H18	PX	RVD	0.000526
184	H18	PY	RVD	0.000101
185	H18	PZ	RVD	0.000072

Total MIN occupancy: 67.762094
Total RVD occupancy: 0.237906
Total occupancy: 68.000000

Natural Atomic Populations and Charges

Atom	Occupancy	Charge
-----	-----	-----
H1	0.763582	0.236418
C1	6.196243	-0.196243
C2	6.245483	-0.245483
C3	6.132393	-0.132393
C4	6.238510	-0.238510

C5	6.198625	-0.198625
C6	5.716518	0.283482
C7	6.181153	-0.181153
H3	0.764883	0.235117
H4	0.764701	0.235299
N1	7.526719	-0.526719
H6	0.752895	0.247105
C8	5.904430	0.095570
H8	0.762037	0.237963
C10	6.301918	-0.301918
H16	0.783574	0.216426
H18	0.766336	0.233664

Total Charge = 0.000000

Q-minus(NAO) = -0.5267

Q-plus(NAO) = 0.2471

Reason for exit: Normal completion

Wall Time: 000:00:00

CPU Time: 000:00:00

TITAN Properties Program: (PC/x86)

Release 6.0.2

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-15.53909	-11.27106	-11.26094	-11.24910	-11.24814
(ev):		-422.84044	-306.70126	-306.42581	-306.10379	-306.07750

		A	A	A	A	A	
1	H1	S	-0.00005	-0.00006	0.00008	0.00000	-0.00006
2	H1	S	-0.00035	-0.00056	0.00066	0.00003	-0.00076
3	H1	PX	0.00000	0.00000	-0.00001	0.00000	0.00000
4	H1	PY	0.00000	0.00004	-0.00002	0.00000	-0.00002
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00002	0.00077	-0.00006	0.00007	-0.00833
7	C1	S	0.00010	0.00030	-0.00015	-0.00005	0.00015
8	C1	PX	-0.00003	-0.00010	0.00005	0.00000	-0.00005
9	C1	PY	-0.00001	-0.00004	0.00003	0.00000	0.00003
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.00114	-0.00198	0.00172	0.00041	-0.00364
12	C1	PX	0.00106	0.00145	-0.00190	-0.00019	0.00231
13	C1	PY	-0.00015	0.00003	0.00072	-0.00010	0.00025
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	-0.00004	-0.00001	-0.00001	-0.00006
16	C1	DYY	0.00002	-0.00006	-0.00006	0.00001	-0.00009
17	C1	DZZ	0.00005	0.00013	-0.00007	-0.00002	0.00015
18	C1	DXY	0.00000	0.00000	-0.00001	0.00000	0.00004
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

21	C2	S	-0.00002	-0.01105	0.00015	0.00003	-0.05698
22	C2	S	-0.00004	-0.00053	0.00013	0.00000	-0.00147
23	C2	PX	0.00000	0.00014	0.00001	0.00001	0.00008
24	C2	PY	0.00005	-0.00005	-0.00007	-0.00002	0.00013
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00041	-0.00160	-0.00068	-0.00003	-0.00082
27	C2	PX	0.00003	-0.00109	-0.00103	-0.00013	0.00037
28	C2	PY	-0.00076	-0.00088	-0.00039	-0.00020	-0.00124
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00013	0.00042	0.00001	0.00000	0.00051
31	C2	DYY	0.00002	0.00066	0.00002	0.00002	0.00046
32	C2	DZZ	-0.00002	0.00010	0.00006	0.00001	0.00016
33	C2	DXY	0.00003	-0.00022	0.00004	-0.00001	-0.00004
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00001	-0.01158	0.00000	0.00041	0.00038
37	C3	S	0.00003	-0.00025	0.00010	0.00007	0.00000
38	C3	PX	-0.00004	-0.00006	-0.00006	0.00002	-0.00001
39	C3	PY	-0.00002	0.00000	-0.00003	0.00004	-0.00004
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00002	-0.00764	-0.00269	-0.00153	-0.00001
42	C3	PX	-0.00080	0.00282	0.00300	-0.00004	-0.00020
43	C3	PY	0.00101	0.00218	-0.00071	0.00043	0.00387
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00056	-0.00004	0.00000	0.00003
46	C3	DYY	-0.00007	0.00028	0.00021	-0.00004	0.00002
47	C3	DZZ	0.00001	0.00019	0.00008	0.00000	0.00002
48	C3	DXY	0.00002	0.00013	0.00000	-0.00001	0.00002
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00001	0.00013	0.00007	-0.00001	-0.07202
52	C4	S	-0.00005	-0.00011	0.00012	0.00004	-0.00224
53	C4	PX	0.00000	-0.00004	0.00000	-0.00001	-0.00005
54	C4	PY	-0.00002	-0.00006	0.00002	-0.00001	-0.00001
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00141	0.00238	-0.00255	-0.00032	-0.00020
57	C4	PX	-0.00027	-0.00057	0.00021	0.00013	0.00083
58	C4	PY	-0.00054	-0.00101	0.00133	0.00027	-0.00116
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00001	0.00005	0.00000	0.00000	0.00081
61	C4	DYY	0.00000	0.00004	0.00000	0.00000	0.00041
62	C4	DZZ	-0.00001	-0.00001	0.00004	0.00002	0.00024
63	C4	DXY	0.00000	0.00001	0.00000	0.00000	-0.00005
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00002	0.00143	-0.00011	-0.00046	-0.99130
67	C5	S	0.00007	0.00043	-0.00016	-0.00003	-0.02725
68	C5	PX	0.00002	0.00006	-0.00001	0.00001	-0.00015
69	C5	PY	-0.00004	-0.00013	0.00005	0.00000	0.00002
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.00031	-0.00039	0.00178	0.00037	0.00998
72	C5	PX	-0.00073	-0.00156	0.00062	0.00005	0.00014
73	C5	PY	0.00039	0.00106	-0.00122	-0.00018	-0.00005
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

75	C5	DXX	0.00000	-0.00005	-0.00001	0.00000	0.00165
76	C5	DYY	0.00003	-0.00013	-0.00002	0.00000	0.00146
77	C5	DZZ	0.00005	0.00015	-0.00007	-0.00001	0.00245
78	C5	DXY	-0.00001	-0.00002	-0.00001	0.00000	-0.00014
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00005	-0.99556	-0.00040	-0.00004	-0.00071
82	C6	S	-0.00030	-0.02754	-0.00038	-0.00006	0.00023
83	C6	PX	-0.00005	-0.00006	-0.00007	-0.00003	0.00001
84	C6	PY	-0.00009	0.00022	-0.00007	0.00005	0.00009
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.00424	0.00877	0.00480	0.00002	-0.00015
87	C6	PX	0.00018	0.00460	0.00276	0.00037	-0.00039
88	C6	PY	0.00160	0.00281	-0.00122	-0.00010	-0.00316
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00009	0.00177	0.00006	0.00000	0.00003
91	C6	DYY	0.00059	0.00094	0.00017	-0.00002	-0.00010
92	C6	DZZ	0.00003	0.00241	-0.00009	-0.00003	0.00006
93	C6	DXY	0.00019	-0.00008	-0.00001	0.00003	0.00002
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00002	0.00154	0.02231	0.00586	-0.00010
97	C7	S	-0.00005	-0.00027	0.00078	0.00020	-0.00015
98	C7	PX	-0.00005	0.00005	0.00006	0.00002	0.00001
99	C7	PY	-0.00003	-0.00005	0.00005	-0.00006	0.00004
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00160	0.00610	0.00335	0.00129	0.00360
102	C7	PX	-0.00097	-0.00416	-0.00120	-0.00073	-0.00147
103	C7	PY	0.00105	0.00112	-0.00258	0.00063	0.00105
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00006	-0.00072	-0.00010	0.00002
106	C7	DYY	-0.00002	-0.00009	-0.00034	-0.00007	0.00001
107	C7	DZZ	-0.00001	-0.00017	-0.00015	-0.00002	-0.00005
108	C7	DXY	0.00002	0.00008	-0.00013	-0.00007	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	0.00000	-0.00001	-0.00001	0.00010
112	H3	S	0.00010	0.00023	-0.00029	-0.00010	0.00021
113	H3	PX	0.00000	0.00001	0.00001	0.00000	0.00002
114	H3	PY	0.00001	0.00002	-0.00001	0.00000	0.00006
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00006	-0.00012	0.00006	0.00000	0.00025
117	H4	S	-0.00027	-0.00079	0.00043	0.00004	-0.00186
118	H4	PX	0.00001	0.00003	0.00000	0.00000	0.00014
119	H4	PY	0.00002	0.00001	0.00000	0.00000	-0.00021
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.99524	0.00031	-0.00011	-0.00004	0.00004
122	N1	S	-0.02515	-0.00072	0.00073	0.00001	0.00015
123	N1	PX	-0.00197	0.00006	0.00002	-0.00003	-0.00001
124	N1	PY	-0.00078	-0.00009	-0.00011	-0.00003	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00731	0.00539	-0.00350	0.00086	-0.00201
127	N1	PX	0.00294	0.00164	-0.00208	0.00018	-0.00006
128	N1	PY	0.00070	0.00204	0.00046	0.00006	-0.00076

129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00282	0.00015	-0.00040	-0.00010	0.00012
131	N1	DYY	0.00262	0.00013	-0.00011	-0.00016	0.00003
132	N1	DZZ	0.00306	-0.00047	0.00041	-0.00002	0.00007
133	N1	DXY	-0.00021	0.00004	0.00023	0.00009	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.00002	-0.00009	-0.00004	-0.00001	0.00001
137	H6	S	-0.00001	-0.00031	-0.00037	-0.00004	0.00017
138	H6	PX	0.00003	-0.00010	0.00000	0.00000	-0.00013
139	H6	PY	0.00004	0.00003	-0.00001	0.00000	-0.00004
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00002	-0.00036	0.99275	0.07266	-0.00008
142	C8	S	-0.00039	0.00031	0.02727	0.00233	0.00010
143	C8	PX	0.00013	0.00011	-0.00014	-0.00005	-0.00003
144	C8	PY	-0.00011	0.00003	0.00033	-0.00020	0.00003
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.00284	-0.00345	-0.01032	-0.00573	-0.00104
147	C8	PX	0.00160	-0.00116	-0.00387	0.00015	-0.00044
148	C8	PY	-0.00214	-0.00501	0.00107	0.00116	-0.00113
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00023	-0.00013	-0.00169	0.00024	-0.00001
151	C8	DYY	0.00017	-0.00014	-0.00103	0.00021	0.00001
152	C8	DZZ	0.00008	0.00006	-0.00237	-0.00007	0.00004
153	C8	DXY	-0.00019	0.00010	-0.00010	-0.00001	-0.00001
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00007	0.00017	-0.00008	0.00004	0.00002
157	H8	S	0.00039	0.00123	-0.00038	0.00031	0.00042
158	H8	PX	-0.00001	-0.00002	-0.00005	-0.00002	0.00000
159	H8	PY	-0.00002	0.00002	0.00013	-0.00003	-0.00001
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00001	0.00000	0.07207	-0.99301	0.00045
162	C10	S	0.00001	-0.00002	0.00172	-0.02741	0.00002
163	C10	PX	0.00001	0.00003	-0.00002	-0.00011	-0.00002
164	C10	PY	0.00000	-0.00009	-0.00025	-0.00001	-0.00001
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.00064	-0.00264	0.00318	0.01172	-0.00056
167	C10	PX	-0.00076	-0.00002	0.00166	0.00011	0.00029
168	C10	PY	-0.00008	-0.00080	0.00138	0.00105	-0.00024
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00007	-0.00006	-0.00055	0.00168	-0.00001
171	C10	DYY	0.00000	0.00001	-0.00057	0.00141	-0.00001
172	C10	DZZ	0.00001	-0.00003	-0.00026	0.00256	0.00000
173	C10	DXY	-0.00010	0.00005	0.00008	0.00001	0.00001
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00006	0.00006	-0.00011	0.00027	-0.00002
177	H16	S	0.00029	0.00006	-0.00050	-0.00197	-0.00012
178	H16	PX	0.00001	-0.00002	-0.00008	-0.00027	0.00000
179	H16	PY	0.00000	0.00001	0.00011	0.00010	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.00003	-0.00001	0.00011	0.00022	0.00004
182	H18	S	-0.00020	0.00010	0.00068	-0.00194	0.00010

183	H18	PX	0.00004	0.00001	0.00009	0.00022	0.00000
184	H18	PY	0.00002	-0.00001	0.00011	0.00005	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-11.24548	-11.24411	-11.24241	-11.23867	-11.23421
(ev):		-306.00533	-305.96782	-305.92176	-305.81997	-305.69865

		A	A	A	A	A	
1	H1	S	0.00028	0.00004	0.00007	0.00001	-0.00003
2	H1	S	-0.00175	0.00057	-0.00106	-0.00018	-0.00070
3	H1	PX	-0.00022	0.00002	-0.00022	-0.00013	-0.00002
4	H1	PY	-0.00004	-0.00001	0.00003	0.00002	-0.00001
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.95337	0.03077	-0.27760	-0.06524	-0.00041
7	C1	S	-0.02630	0.00067	-0.00767	-0.00173	0.00029
8	C1	PX	0.00015	0.00001	0.00013	0.00014	0.00002
9	C1	PY	0.00024	-0.00007	-0.00003	0.00020	0.00007
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00840	0.00260	0.00266	0.00377	-0.00490
12	C1	PX	-0.00007	-0.00181	0.00104	-0.00069	0.00263
13	C1	PY	0.00014	-0.00002	0.00144	-0.00103	0.00079
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00158	0.00001	0.00000	-0.00040	-0.00009
16	C1	DYY	0.00160	-0.00003	0.00007	-0.00058	-0.00006
17	C1	DZZ	0.00237	-0.00011	0.00071	0.00002	0.00008
18	C1	DXY	0.00013	-0.00001	0.00002	-0.00026	-0.00002
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00327	-0.00002	-0.00995	-0.00583	0.99383
22	C2	S	-0.00003	0.00019	-0.00070	-0.00030	0.02758
23	C2	PX	0.00005	0.00001	-0.00002	-0.00004	0.00030
24	C2	PY	-0.00005	0.00003	-0.00001	0.00001	-0.00010
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00287	-0.00316	0.00463	0.00032	-0.00969
27	C2	PX	0.00126	-0.00212	0.00270	0.00016	-0.00009
28	C2	PY	-0.00069	-0.00040	-0.00073	-0.00017	-0.00049
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00002	-0.00007	0.00015	0.00008	-0.00153
31	C2	DYY	-0.00002	0.00002	0.00018	0.00010	-0.00151
32	C2	DZZ	-0.00003	0.00006	-0.00012	-0.00003	-0.00249
33	C2	DXY	-0.00002	0.00000	0.00003	-0.00003	0.00014
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06061	-0.14358	-0.03720	0.98259	0.00548
37	C3	S	-0.00163	-0.00364	-0.00118	0.02765	0.00007
38	C3	PX	0.00006	-0.00001	0.00005	-0.00014	0.00003
39	C3	PY	0.00003	-0.00019	-0.00012	-0.00002	-0.00016
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00488	-0.00538	-0.00244	-0.01646	-0.00156
42	C3	PX	0.00039	0.00017	-0.00048	0.00126	0.00053
43	C3	PY	0.00238	-0.00009	0.00563	0.00150	0.00590
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00045	0.00058	0.00021	-0.00175	0.00007

46	C3	DYY	0.00060	0.00059	0.00035	-0.00099	0.00002
47	C3	DZZ	0.00029	0.00047	0.00012	-0.00229	-0.00003
48	C3	DXY	0.00020	0.00007	0.00008	0.00012	0.00003
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.27703	0.02303	0.95303	0.02234	0.00638
52	C4	S	-0.00749	0.00084	0.02627	0.00045	-0.00011
53	C4	PX	0.00015	-0.00004	-0.00012	0.00002	0.00008
54	C4	PY	-0.00010	0.00000	-0.00012	0.00002	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00074	-0.00273	-0.01004	-0.00071	0.00211
57	C4	PX	-0.00115	0.00058	-0.00012	-0.00001	-0.00057
58	C4	PY	0.00063	0.00169	-0.00002	-0.00002	-0.00161
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00079	-0.00004	-0.00139	0.00006	0.00014
61	C4	DYY	0.00077	-0.00010	-0.00127	0.00014	0.00006
62	C4	DZZ	0.00071	0.00001	-0.00234	-0.00010	-0.00009
63	C4	DXY	0.00007	0.00000	-0.00014	-0.00003	0.00003
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02813	-0.00194	-0.06663	-0.00035	-0.05820
67	C5	S	0.00095	-0.00016	-0.00148	-0.00001	-0.00170
68	C5	PX	0.00010	0.00000	-0.00004	-0.00002	0.00011
69	C5	PY	-0.00001	-0.00002	-0.00001	0.00003	0.00014
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.00220	0.00282	0.00110	0.00017	0.00292
72	C5	PX	-0.00099	0.00043	0.00030	0.00006	-0.00112
73	C5	PY	0.00086	-0.00137	0.00161	0.00000	-0.00065
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00004	0.00000	-0.00058	-0.00007	-0.00031
76	C5	DYY	0.00001	0.00001	-0.00021	-0.00005	-0.00035
77	C5	DZZ	0.00002	-0.00002	0.00014	-0.00003	0.00012
78	C5	DXY	0.00007	0.00000	-0.00008	0.00001	0.00001
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00004	0.00010	0.00046	-0.01203	-0.01154
82	C6	S	0.00011	-0.00009	0.00019	-0.00025	-0.00018
83	C6	PX	0.00004	-0.00001	0.00000	-0.00006	0.00008
84	C6	PY	0.00012	-0.00001	0.00009	0.00005	0.00001
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00031	0.00046	-0.00148	0.00528	0.00431
87	C6	PX	0.00115	0.00097	0.00060	0.00226	-0.00003
88	C6	PY	-0.00301	0.00322	-0.00469	-0.00096	-0.00275
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00001	-0.00008	0.00003	-0.00059	-0.00033
91	C6	DYY	0.00000	-0.00006	-0.00004	-0.00028	-0.00051
92	C6	DZZ	0.00004	-0.00005	0.00003	-0.00012	-0.00008
93	C6	DXY	0.00000	0.00003	-0.00001	0.00006	0.00018
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.02747	-0.98415	0.01912	-0.14547	-0.00065
97	C7	S	-0.00091	-0.02740	0.00025	-0.00438	-0.00024
98	C7	PX	0.00006	0.00020	0.00000	0.00016	-0.00002
99	C7	PY	0.00008	-0.00003	0.00007	-0.00021	0.00009

100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00449	0.01233	0.00615	0.00820	0.00575
102	C7	PX	-0.00221	-0.00237	-0.00233	-0.00188	-0.00234
103	C7	PY	0.00081	0.00057	0.00195	0.00178	0.00158
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00004	0.00145	-0.00002	-0.00032	0.00004
106	C7	DYY	0.00003	0.00160	-0.00001	-0.00016	0.00003
107	C7	DZZ	0.00004	0.00236	-0.00014	0.00023	-0.00006
108	C7	DXY	0.00005	0.00030	0.00003	0.00024	-0.00002
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00005	-0.00005	-0.00025	-0.00001	0.00006
112	H3	S	-0.00042	-0.00045	0.00188	0.00019	0.00057
113	H3	PX	-0.00001	0.00000	0.00013	0.00002	-0.00003
114	H3	PY	0.00008	-0.00002	0.00027	0.00003	0.00003
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00004	0.00002	-0.00010	0.00001	0.00003
117	H4	S	-0.00034	0.00026	-0.00068	0.00001	-0.00028
118	H4	PX	-0.00003	0.00000	0.00004	0.00000	0.00006
119	H4	PY	0.00000	0.00001	-0.00009	-0.00002	-0.00017
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00003	-0.00011	0.00003	0.00007	0.00007
122	N1	S	0.00013	-0.00029	0.00011	0.00019	0.00014
123	N1	PX	-0.00001	-0.00002	0.00000	0.00005	0.00005
124	N1	PY	-0.00005	-0.00002	-0.00004	-0.00001	-0.00004
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.00175	0.00408	-0.00204	-0.00220	-0.00278
127	N1	PX	-0.00038	0.00092	-0.00024	-0.00075	-0.00036
128	N1	PY	-0.00019	0.00083	-0.00041	-0.00001	-0.00064
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00006	-0.00027	0.00008	0.00016	0.00018
131	N1	DYY	0.00005	-0.00017	0.00006	0.00016	0.00017
132	N1	DZZ	0.00005	-0.00019	0.00004	0.00014	0.00005
133	N1	DXY	-0.00003	0.00002	-0.00002	0.00004	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.00002	-0.00006	0.00004	0.00000	-0.00028
137	H6	S	0.00023	-0.00059	0.00078	0.00013	0.00191
138	H6	PX	-0.00001	0.00002	-0.00003	0.00000	-0.00027
139	H6	PY	0.00002	0.00001	0.00003	-0.00001	0.00002
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00066	0.02278	-0.00047	0.00339	-0.00009
142	C8	S	0.00016	0.00054	0.00015	0.00005	0.00015
143	C8	PX	-0.00004	0.00008	-0.00005	0.00001	-0.00005
144	C8	PY	0.00002	0.00001	0.00006	0.00007	0.00008
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.00155	-0.00480	-0.00138	-0.00123	-0.00118
147	C8	PX	-0.00121	-0.00094	-0.00092	-0.00158	-0.00098
148	C8	PY	-0.00148	-0.00170	-0.00207	-0.00073	-0.00168
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00001	0.00040	-0.00002	0.00014	-0.00002
151	C8	DYY	0.00002	0.00041	0.00001	0.00024	0.00005
152	C8	DZZ	0.00004	0.00007	0.00005	0.00006	0.00006
153	C8	DXY	-0.00004	0.00021	-0.00004	0.00009	-0.00002

154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00008	0.00048	0.00000	0.00010	0.00001
157	H8	S	0.00059	-0.00121	0.00070	-0.00003	0.00062
158	H8	PX	-0.00001	-0.00031	0.00000	-0.00019	0.00001
159	H8	PY	0.00002	0.00009	-0.00003	0.00006	-0.00002
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00023	-0.00425	0.00005	-0.00023	0.00004
162	C10	S	-0.00001	-0.00004	0.00000	0.00001	0.00001
163	C10	PX	-0.00002	0.00006	-0.00004	-0.00002	-0.00003
164	C10	PY	-0.00002	-0.00002	-0.00004	-0.00004	-0.00004
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.00066	-0.00001	-0.00113	-0.00030	-0.00095
167	C10	PX	0.00052	-0.00029	0.00052	0.00070	0.00049
168	C10	PY	-0.00030	-0.00008	-0.00041	-0.00014	-0.00039
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00001	-0.00004	-0.00002	0.00000	-0.00001
171	C10	DYY	-0.00001	-0.00013	-0.00001	-0.00008	-0.00003
172	C10	DZZ	0.00000	0.00005	-0.00001	0.00001	0.00000
173	C10	DXY	0.00002	0.00002	0.00001	0.00005	0.00002
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.00004	0.00008	-0.00004	-0.00005	-0.00004
177	H16	S	-0.00022	0.00007	-0.00016	-0.00021	-0.00017
178	H16	PX	0.00000	-0.00001	-0.00001	-0.00001	0.00000
179	H16	PY	0.00000	0.00003	0.00000	0.00001	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00005	-0.00004	0.00007	0.00006	0.00006
182	H18	S	0.00016	-0.00024	0.00021	0.00025	0.00017
183	H18	PX	0.00000	0.00001	0.00001	0.00000	0.00000
184	H18	PY	0.00000	-0.00001	0.00000	0.00000	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	11	12	13	14	15
Eigenvalues:	-1.27357	-1.13269	-1.07025	-1.03312	-0.99958
(ev):	-34.65549	-30.82212	-29.12296	-28.11256	-27.20010

		A	A	A	A	A	
1	H1	S	0.00508	0.04286	-0.03663	0.01218	-0.06232
2	H1	S	-0.00659	0.00783	-0.01223	0.00554	-0.01052
3	H1	PX	-0.00056	-0.00474	0.00373	-0.00106	0.00637
4	H1	PY	0.00007	-0.00008	0.00052	-0.00051	-0.00063
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.01704	-0.10122	0.06278	-0.01742	0.10159
7	C1	S	0.03515	0.19254	-0.11923	0.03329	-0.19743
8	C1	PX	-0.01380	-0.06328	0.01518	0.00202	0.03112
9	C1	PY	-0.01048	0.02228	0.02771	-0.05775	-0.09198
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00014	0.12411	-0.09381	0.03294	-0.12199
12	C1	PX	0.01674	-0.00861	0.00974	-0.00553	-0.02028
13	C1	PY	-0.00405	0.00374	0.00297	-0.01056	-0.01688
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00039	0.00323	-0.00048	-0.00005	-0.00250
16	C1	DYY	0.00237	0.00761	-0.00732	0.00388	-0.00386

17	C1	DZZ	-0.00110	-0.00879	0.00572	-0.00196	0.00720
18	C1	DXY	0.00111	-0.00303	-0.00176	0.00572	0.00805
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02843	-0.08173	-0.08158	0.04291	-0.09962
22	C2	S	0.05266	0.15673	0.15473	-0.08095	0.19269
23	C2	PX	0.01858	0.05640	0.02697	-0.01484	0.03094
24	C2	PY	-0.02189	0.03667	-0.00290	-0.06621	0.02991
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.03640	0.08409	0.12102	-0.05828	0.12680
27	C2	PX	0.00244	-0.00816	0.00794	-0.00480	-0.01208
28	C2	PY	-0.01578	0.00280	-0.00156	-0.01531	0.00757
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00008	0.00281	0.00094	-0.00032	0.00260
31	C2	DYY	0.00514	0.00528	0.00885	-0.00168	0.00556
32	C2	DZZ	-0.00308	-0.00648	-0.00684	0.00312	-0.00740
33	C2	DXY	-0.00249	0.00342	0.00015	-0.00676	0.00133
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06210	-0.06494	0.09229	-0.08166	-0.04395
37	C3	S	0.11552	0.12555	-0.17551	0.15746	0.08500
38	C3	PX	-0.03852	0.00348	-0.05756	-0.01045	-0.02326
39	C3	PY	-0.03599	0.05348	0.04817	-0.02863	-0.11117
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.05414	0.06134	-0.13372	0.10388	0.06914
42	C3	PX	-0.01472	0.00884	-0.00452	0.00197	0.00210
43	C3	PY	0.01019	0.01746	0.00622	-0.00936	-0.05975
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00731	0.00241	0.00532	0.00486	0.00152
46	C3	DYY	0.00450	0.00831	-0.01490	0.00508	0.00000
47	C3	DZZ	-0.00592	-0.00547	0.00695	-0.00623	-0.00269
48	C3	DXY	0.00217	0.00232	0.00041	0.00068	-0.00808
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.01115	-0.10899	0.01557	0.04274	0.10134
52	C4	S	0.02007	0.20724	-0.03067	-0.08134	-0.19282
53	C4	PX	-0.00247	-0.01578	-0.04421	0.04096	-0.07867
54	C4	PY	-0.01027	-0.06254	0.02813	-0.00849	0.05598
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.03508	0.12516	-0.00970	-0.06477	-0.17700
57	C4	PX	-0.00476	-0.00317	-0.00784	0.00914	-0.00326
58	C4	PY	-0.00998	-0.00379	-0.00730	0.00430	0.01316
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00103	0.00828	0.00440	-0.00741	0.00129
61	C4	DYY	0.00082	0.00483	-0.00350	0.00115	-0.00814
62	C4	DZZ	-0.00110	-0.00940	0.00076	0.00398	0.00775
63	C4	DXY	-0.00036	-0.00385	0.00367	-0.00109	0.00799
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.01295	-0.10306	-0.05186	0.07778	-0.04746
67	C5	S	0.02730	0.19488	0.10120	-0.14998	0.08939
68	C5	PX	0.00136	0.02733	-0.03222	-0.00091	-0.09624
69	C5	PY	-0.01364	-0.05246	-0.04201	0.02209	-0.06857
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

71	C5	S	0.00686	0.13990	0.05912	-0.10381	0.09140
72	C5	PX	-0.01354	0.01121	-0.00713	-0.00240	-0.00568
73	C5	PY	0.00881	-0.01635	0.00732	-0.00225	-0.01476
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00040	0.00859	-0.00148	-0.00467	-0.00830
76	C5	DYY	0.00108	0.00445	0.00505	-0.00322	0.00881
77	C5	DZZ	-0.00056	-0.00942	-0.00365	0.00642	-0.00340
78	C5	DXY	0.00067	0.00358	0.00388	-0.00306	0.00611
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.11142	-0.02696	-0.06497	-0.04975	-0.02426
82	C6	S	0.21497	0.05202	0.12958	0.09830	0.04650
83	C6	PX	-0.00405	0.02770	-0.10777	0.04491	0.03034
84	C6	PY	-0.10745	0.09706	-0.02603	-0.04404	0.11721
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.04237	0.05241	0.06301	0.06853	0.05741
87	C6	PX	0.01862	0.01628	-0.00106	0.02695	0.00986
88	C6	PY	0.02472	0.02468	0.01534	-0.00791	0.04176
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00004	0.00770	-0.00958	0.00803	0.00875
91	C6	DYY	0.01759	-0.00145	0.01448	-0.00183	-0.00199
92	C6	DZZ	-0.01220	-0.00247	-0.00617	-0.00484	-0.00181
93	C6	DXY	0.00446	-0.00517	0.00290	0.00358	-0.01190
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.05479	-0.00837	0.11160	-0.02793	-0.08464
97	C7	S	0.10131	0.01407	-0.21525	0.05265	0.16412
98	C7	PX	-0.05311	0.01217	0.04029	0.00294	-0.02446
99	C7	PY	0.01620	0.03771	-0.03702	0.09495	0.03157
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.06529	0.03244	-0.13974	0.04620	0.08859
102	C7	PX	-0.01327	-0.01100	-0.00470	-0.00022	0.01487
103	C7	PY	0.01731	0.00261	0.00139	0.00839	-0.01426
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00568	-0.00345	-0.00326	-0.00361	0.00222
106	C7	DYY	0.00369	0.00243	-0.00873	0.00351	0.00544
107	C7	DZZ	-0.00570	-0.00052	0.00878	-0.00198	-0.00654
108	C7	DXY	0.00036	-0.00308	-0.00003	-0.00907	-0.00348
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00307	0.04711	-0.00758	-0.02638	-0.06569
112	H3	S	0.00169	0.00817	0.00171	-0.00993	-0.02078
113	H3	PX	-0.00011	-0.00211	0.00001	0.00139	0.00189
114	H3	PY	-0.00025	-0.00476	0.00105	0.00215	0.00631
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00301	0.04505	0.02704	-0.04672	0.02899
117	H4	S	-0.00654	0.01227	0.00189	-0.01215	0.00982
118	H4	PX	0.00031	0.00241	0.00105	-0.00223	0.00050
119	H4	PY	-0.00027	-0.00431	-0.00274	0.00415	-0.00327
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.14422	0.05226	-0.06921	-0.00221	0.07083
122	N1	S	0.28540	-0.10838	0.14253	0.00393	-0.14880
123	N1	PX	0.10533	-0.03781	-0.00114	-0.00205	-0.02521
124	N1	PY	0.05565	0.01227	0.08376	0.08944	-0.00065

125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.32801	-0.10545	0.17242	-0.00303	-0.16263
127	N1	PX	0.06128	-0.01864	0.00923	-0.00751	-0.01621
128	N1	PY	0.02279	0.01197	0.03252	0.03653	0.00455
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00583	-0.00405	-0.00621	-0.00293	-0.00070
131	N1	DYY	0.00608	-0.00117	0.00607	0.00102	-0.00195
132	N1	DZZ	-0.01353	0.00362	-0.00332	-0.00023	0.00361
133	N1	DXY	0.00259	0.00279	0.00627	0.01155	0.00079
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.01021	0.03125	0.04482	-0.02299	0.05826
137	H6	S	0.00074	-0.00106	0.01154	-0.00736	0.01027
138	H6	PX	0.00132	0.00352	0.00476	-0.00247	0.00581
139	H6	PY	0.00025	0.00044	0.00001	-0.00071	0.00069
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.08826	0.04637	0.06712	0.10125	-0.00594
142	C8	S	0.16846	-0.09040	-0.13103	-0.19849	0.00996
143	C8	PX	-0.04358	0.03327	-0.07860	0.02159	0.09741
144	C8	PY	0.06687	-0.00300	0.03594	0.13992	-0.00773
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.04461	-0.05447	-0.09646	-0.13342	0.02587
147	C8	PX	0.02993	-0.01586	-0.01592	-0.01459	0.01350
148	C8	PY	-0.00505	-0.00122	-0.01380	0.01365	0.01864
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00795	-0.00264	-0.00047	0.00434	-0.00079
151	C8	DYY	0.01224	-0.00436	-0.00597	-0.00822	0.00118
152	C8	DZZ	-0.00993	0.00440	0.00516	0.00721	-0.00003
153	C8	DXY	-0.00910	0.00502	-0.01305	0.00014	0.01304
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.01512	0.00456	-0.05839	0.00728	0.04888
157	H8	S	0.00498	0.00389	-0.01031	-0.00114	0.00734
158	H8	PX	-0.00146	-0.00042	0.00540	-0.00036	-0.00409
159	H8	PY	0.00025	0.00068	-0.00225	0.00136	0.00195
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.02546	0.02737	0.05883	0.13573	-0.00705
162	C10	S	0.04820	-0.05287	-0.11293	-0.26146	0.01321
163	C10	PX	-0.00158	0.00198	-0.01455	-0.00419	0.01684
164	C10	PY	0.03175	-0.02668	-0.04463	-0.08784	0.00185
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.03321	-0.03605	-0.09138	-0.20180	0.01996
167	C10	PX	-0.01366	0.00630	-0.00082	0.00029	0.00147
168	C10	PY	0.00650	-0.00198	-0.00588	-0.00783	0.00323
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00228	0.00136	0.00148	0.00274	0.00033
171	C10	DYY	0.00304	-0.00311	-0.00511	-0.01228	-0.00007
172	C10	DZZ	-0.00191	0.00210	0.00480	0.01137	-0.00057
173	C10	DXY	-0.00136	0.00059	-0.00247	-0.00090	0.00201
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00892	-0.01196	-0.03506	-0.07744	0.01033
177	H16	S	0.00489	-0.00319	-0.00814	-0.01848	0.00470
178	H16	PX	-0.00071	0.00094	0.00296	0.00625	-0.00080

179	H16	PY	0.00052	-0.00092	-0.00273	-0.00551	0.00079
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00944	-0.01359	-0.02685	-0.07738	-0.00159
182	H18	S	-0.00397	0.00043	-0.00219	-0.01651	-0.00259
183	H18	PX	0.00136	-0.00137	-0.00241	-0.00706	-0.00014
184	H18	PY	0.00078	-0.00106	-0.00146	-0.00460	-0.00037
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	16	17	18	19	20
Eigenvalues:	-0.90918	-0.80562	-0.79464	-0.75492	-0.68891
(ev):	-24.74003	-21.92213	-21.62336	-20.54253	-18.74617

		A	A	A	A	A	
1	H1	S	-0.04160	-0.12145	0.00323	0.05688	-0.06736
2	H1	S	-0.01017	-0.05224	0.01110	0.03304	-0.04468
3	H1	PX	0.00365	0.00918	-0.00050	-0.00351	0.00419
4	H1	PY	0.00081	0.00096	0.00218	-0.00145	-0.00167
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.05775	0.08513	0.00938	-0.01010	-0.00133
7	C1	S	-0.11573	-0.17100	-0.02332	0.02053	0.00611
8	C1	PX	0.00710	-0.09298	0.01550	0.09237	-0.11945
9	C1	PY	0.06789	0.02496	0.18373	-0.06510	-0.11735
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.06845	-0.14148	0.03355	0.02456	-0.02407
12	C1	PX	-0.01697	-0.05352	-0.02600	0.03131	-0.03181
13	C1	PY	0.01212	0.00887	0.04166	-0.01756	-0.03582
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00283	-0.00463	-0.00152	0.00037	0.00039
16	C1	DYY	-0.00327	-0.00103	-0.00223	0.00204	0.00091
17	C1	DZZ	0.00460	0.00585	0.00089	-0.00070	0.00012
18	C1	DXY	-0.00724	-0.00092	-0.01249	0.00262	0.00364
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.04350	0.07420	-0.03920	0.01662	0.03760
22	C2	S	-0.08703	-0.14631	0.08207	-0.03424	-0.07515
23	C2	PX	-0.01126	0.08051	-0.03454	-0.07343	0.16026
24	C2	PY	0.12115	-0.07770	-0.16856	0.03158	-0.04769
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.06684	-0.13397	0.04277	-0.00450	-0.07966
27	C2	PX	0.00491	0.03374	-0.03445	-0.00780	0.08162
28	C2	PY	0.02475	-0.02157	-0.03089	0.01386	-0.00879
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00357	-0.00222	0.00403	-0.00315	-0.00534
31	C2	DYY	-0.00338	-0.00042	0.00156	0.00319	0.00500
32	C2	DZZ	0.00383	0.00475	-0.00276	0.00129	0.00208
33	C2	DXY	0.01108	-0.00667	-0.01027	0.00333	-0.00130
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03808	-0.03418	0.07748	-0.00916	0.01713
37	C3	S	-0.07750	0.06855	-0.15457	0.01859	-0.03461
38	C3	PX	0.03273	-0.16396	-0.01726	0.15777	0.06922
39	C3	PY	-0.13504	-0.05792	-0.08410	-0.06009	0.17632
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.05057	0.04554	-0.14254	0.03376	0.00087

42	C3	PX	-0.00081	-0.04004	-0.00716	0.05432	0.01684
43	C3	PY	-0.05841	-0.02267	-0.07335	-0.02976	0.05808
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00898	0.01101	-0.00229	-0.00553	-0.00013
46	C3	DYY	0.00177	-0.00785	-0.00301	0.00309	0.00094
47	C3	DZZ	0.00292	-0.00263	0.00521	0.00055	0.00122
48	C3	DXY	-0.00499	-0.00448	-0.00735	-0.00217	-0.00062
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.06019	-0.05636	-0.06729	0.01110	0.01646
52	C4	S	0.11904	0.11326	0.13538	-0.02204	-0.03331
53	C4	PX	-0.08377	-0.10407	0.11259	-0.02642	-0.17111
54	C4	PY	0.06968	0.08345	0.02454	0.07067	-0.11192
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.08897	0.09334	0.09205	-0.01122	-0.02255
57	C4	PX	-0.01544	-0.02359	0.04149	-0.00810	-0.06591
58	C4	PY	0.02639	0.04149	0.04615	0.01376	-0.06440
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.01100	0.00615	-0.00428	0.00359	0.00610
61	C4	DYY	-0.00325	-0.00052	0.00496	-0.00228	-0.00487
62	C4	DZZ	-0.00498	-0.00450	-0.00405	0.00075	0.00079
63	C4	DXY	0.00355	0.00618	-0.00086	0.00038	-0.00026
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.08796	-0.01045	0.07223	-0.03450	-0.02427
67	C5	S	0.17246	0.02146	-0.14566	0.07086	0.05172
68	C5	PX	0.04460	0.15524	0.06255	-0.03717	0.13116
69	C5	PY	0.06428	0.08617	-0.02383	0.10429	-0.03240
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.15077	0.02723	-0.11528	0.05742	0.02725
72	C5	PX	0.01072	0.04103	0.03473	-0.01619	0.03684
73	C5	PY	0.02056	0.01847	-0.03962	0.05438	0.00374
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.01002	0.00931	0.00244	0.00112	0.00310
76	C5	DYY	-0.00091	-0.00463	-0.00447	0.00081	-0.00141
77	C5	DZZ	-0.00729	-0.00158	0.00490	-0.00215	-0.00145
78	C5	DXY	-0.00050	-0.00522	0.00204	-0.00245	-0.00471
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.07157	-0.07266	-0.04705	0.00784	-0.01064
82	C6	S	-0.14644	0.14981	0.09828	-0.01466	0.02337
83	C6	PX	0.01391	0.11485	-0.15118	-0.13225	-0.09436
84	C6	PY	-0.10589	-0.01234	0.04628	-0.16102	0.03599
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.12706	0.13253	0.10678	-0.02242	0.00900
87	C6	PX	-0.00951	0.04892	-0.04696	-0.03250	-0.04201
88	C6	PY	-0.03098	-0.00265	0.03807	-0.05677	0.01374
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00705	0.01075	-0.00445	-0.00643	-0.00827
91	C6	DYY	0.00048	-0.00623	0.00502	0.00169	0.00423
92	C6	DZZ	0.00497	-0.00536	-0.00334	-0.00044	-0.00040
93	C6	DXY	0.00139	0.00345	-0.00612	0.01257	0.01106
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

96	C7	S	-0.07287	0.02533	-0.07196	-0.03984	-0.02519
97	C7	S	0.14539	-0.05308	0.14459	0.08058	0.05014
98	C7	PX	-0.03317	-0.04423	0.03498	0.15496	0.20404
99	C7	PY	-0.01619	0.05328	-0.12489	0.09959	-0.14194
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.08401	-0.04537	0.10262	0.06671	0.06998
102	C7	PX	0.01642	-0.01871	0.03777	0.06366	0.08637
103	C7	PY	-0.01213	0.01143	-0.05470	0.00905	-0.05467
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00753	-0.00341	0.00915	-0.00603	0.00603
106	C7	DYY	-0.00034	0.00131	-0.00355	0.00415	-0.00466
107	C7	DZZ	-0.00563	0.00146	-0.00508	-0.00174	-0.00142
108	C7	DXY	0.00041	-0.00634	0.00288	-0.01012	0.00114
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.06002	0.06581	0.09444	0.01757	-0.11496
112	H3	S	0.02149	0.02696	0.03606	0.01339	-0.06681
113	H3	PX	-0.00310	-0.00352	-0.00205	-0.00100	0.00177
114	H3	PY	-0.00404	-0.00379	-0.00729	-0.00026	0.00696
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.08449	0.00901	-0.08978	0.08953	-0.02741
117	H4	S	0.03200	0.00588	-0.03307	0.04377	-0.02477
118	H4	PX	0.00422	0.00212	-0.00314	0.00316	0.00035
119	H4	PY	-0.00588	0.00081	0.00642	-0.00505	0.00183
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.02368	0.03648	0.02404	-0.04288	-0.03197
122	N1	S	0.05000	-0.07984	-0.05061	0.09645	0.07032
123	N1	PX	0.05352	-0.00064	-0.05283	-0.08713	-0.08173
124	N1	PY	-0.04912	0.10794	0.12745	0.16277	0.02407
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.05351	-0.10848	-0.07332	0.09284	0.10369
127	N1	PX	0.02230	-0.00620	-0.02380	-0.05139	-0.04127
128	N1	PY	-0.02575	0.05482	0.04624	0.06420	0.00851
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00840	-0.00295	-0.00709	-0.01352	-0.01005
131	N1	DYY	-0.00540	0.00274	0.00606	0.00884	0.00517
132	N1	DZZ	-0.00249	0.00054	0.00186	0.00131	0.00175
133	N1	DXY	-0.00376	0.01334	0.00720	0.01260	-0.00146
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.03166	-0.10256	0.05580	0.02188	-0.12510
137	H6	S	-0.00820	-0.04558	0.01919	0.01775	-0.06567
138	H6	PX	-0.00277	-0.00812	0.00401	0.00126	-0.00776
139	H6	PY	0.00120	-0.00147	-0.00220	-0.00012	-0.00168
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.02072	0.04113	-0.00115	0.09331	-0.00193
142	C8	S	0.04332	-0.08510	0.00053	-0.19212	0.00295
143	C8	PX	0.02338	0.03998	0.16493	-0.00140	0.01329
144	C8	PY	0.15596	-0.04921	-0.00631	-0.03376	-0.08864
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.03849	-0.06912	0.01776	-0.16223	0.00794
147	C8	PX	0.02304	-0.00655	0.04675	-0.01709	0.00158
148	C8	PY	0.04305	-0.01924	0.01621	-0.01318	-0.02109
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

150	C8	DXX	0.01268	-0.01001	0.00126	-0.00281	0.00351
151	C8	DYY	-0.00375	0.00664	-0.00150	-0.00012	-0.00750
152	C8	DZZ	-0.00307	0.00344	0.00102	0.00683	0.00063
153	C8	DXY	0.00045	0.00398	0.01079	-0.00139	-0.00295
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.04832	-0.05290	0.10594	0.09624	0.16300
157	H8	S	0.01033	-0.02615	0.04537	0.04826	0.09888
158	H8	PX	-0.00383	0.00398	-0.00761	-0.00590	-0.00987
159	H8	PY	0.00118	-0.00125	0.00149	0.00447	0.00259
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.09445	-0.05475	0.00771	-0.05990	0.01537
162	C10	S	-0.18396	0.10722	-0.01637	0.11823	-0.03042
163	C10	PX	0.00340	0.01052	0.06352	-0.00340	0.03452
164	C10	PY	0.00500	-0.07564	0.00299	-0.17732	0.08893
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.15079	0.10223	-0.00658	0.12502	-0.04243
167	C10	PX	-0.00814	0.00847	0.01621	0.00271	0.01467
168	C10	PY	0.01177	-0.02760	0.00735	-0.05955	0.03432
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00286	0.00636	-0.00019	0.01307	-0.00573
171	C10	DYY	-0.00393	-0.00262	-0.00012	-0.00695	0.00472
172	C10	DZZ	0.00814	-0.00475	0.00059	-0.00538	0.00131
173	C10	DXY	0.00015	-0.00031	0.00145	-0.00229	-0.00004
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.07487	0.07389	0.01869	0.11048	-0.02693
177	H16	S	-0.02463	0.03526	0.01412	0.06284	-0.01429
178	H16	PX	0.00557	-0.00493	-0.00053	-0.00676	0.00223
179	H16	PY	-0.00403	0.00266	0.00123	0.00288	0.00044
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.07680	0.06022	-0.03548	0.10033	-0.05492
182	H18	S	-0.03074	0.02962	-0.01838	0.05674	-0.03035
183	H18	PX	-0.00638	0.00472	-0.00203	0.00711	-0.00325
184	H18	PY	-0.00317	0.00098	-0.00161	0.00122	-0.00025
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	21	22	23	24	25
Eigenvalues:	-0.67123	-0.65389	-0.61355	-0.58253	-0.56450
(ev):	-18.26519	-17.79316	-16.69552	-15.85157	-15.36080

		A	A	A	A	A	
1	H1	S	0.09914	-0.06272	0.19193	0.05053	0.02053
2	H1	S	0.05294	-0.04437	0.13799	0.04307	0.02247
3	H1	PX	-0.00609	0.00284	-0.00983	-0.00190	-0.00053
4	H1	PY	0.00017	0.00277	-0.00023	-0.00240	-0.00197
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.04593	-0.00460	-0.00298	0.01268	-0.00418
7	C1	S	0.09435	0.00913	0.00366	-0.02752	0.00648
8	C1	PX	0.08584	-0.12195	0.29704	0.10707	0.02828
9	C1	PY	0.02406	0.16915	0.04593	-0.13632	-0.14112
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.06670	0.00498	0.00700	-0.01337	0.03634
12	C1	PX	0.06892	-0.04625	0.14247	0.03288	0.00042

13	C1	PY	0.00665	0.04849	0.01160	-0.04246	-0.05948
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00875	-0.00211	0.01300	0.00292	0.00317
16	C1	DYY	-0.00862	-0.00135	-0.01177	0.00011	-0.00041
17	C1	DZZ	-0.00273	0.00015	-0.00102	0.00000	-0.00091
18	C1	DXY	0.00058	-0.01262	0.00034	0.00393	0.01200
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.03518	-0.01448	0.00771	-0.02183	-0.00793
22	C2	S	-0.07343	0.02996	-0.01461	0.04702	0.01310
23	C2	PX	0.04273	0.07812	0.29080	0.07795	-0.04459
24	C2	PY	0.08906	0.17501	0.00365	-0.01006	-0.12356
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.04112	-0.00050	-0.01376	0.02979	0.04300
27	C2	PX	0.04679	0.00926	0.14261	0.01060	-0.00939
28	C2	PY	0.02599	0.04099	-0.00350	-0.01148	-0.04503
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00721	-0.00126	-0.01172	0.00163	0.00530
31	C2	DYY	0.00550	-0.00222	0.01042	-0.00217	-0.00375
32	C2	DZZ	0.00196	-0.00033	0.00107	-0.00047	-0.00127
33	C2	DXY	0.00335	0.01291	-0.00232	0.00530	-0.01005
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03549	0.02848	0.03357	-0.01322	0.01301
37	C3	S	-0.07232	-0.05906	-0.06912	0.02869	-0.02733
38	C3	PX	-0.09585	-0.03096	-0.05484	0.16789	-0.07960
39	C3	PY	0.07678	-0.07000	-0.09928	-0.06001	0.22369
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.07230	-0.08014	-0.06293	-0.00912	-0.02721
42	C3	PX	-0.03340	-0.01543	-0.03904	0.09099	-0.04637
43	C3	PY	0.04376	-0.03315	-0.03295	-0.00706	0.06729
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00591	-0.00516	0.00990	-0.01080	0.00886
46	C3	DYY	-0.00265	0.00453	-0.01144	0.00632	-0.00602
47	C3	DZZ	0.00100	0.00099	0.00134	-0.00017	-0.00024
48	C3	DXY	0.01209	-0.00395	-0.00441	0.00121	0.00712
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.04335	-0.00936	0.02374	-0.00910	0.01176
52	C4	S	-0.09009	0.01980	-0.05002	0.02044	-0.02583
53	C4	PX	0.01619	0.05530	0.01180	-0.15378	-0.02969
54	C4	PY	-0.09009	-0.22369	0.10907	0.11449	0.13738
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.06172	0.00155	-0.02427	0.01708	-0.02264
57	C4	PX	-0.00996	0.01677	0.00338	-0.05083	-0.00876
58	C4	PY	-0.07238	-0.07695	0.01919	0.05802	0.05812
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00283	-0.00225	0.00791	0.00816	-0.00182
61	C4	DYY	-0.00428	-0.00080	-0.00620	-0.00467	0.00336
62	C4	DZZ	0.00256	0.00014	0.00081	-0.00050	-0.00022
63	C4	DXY	-0.00834	-0.00520	0.00508	0.01218	0.00431
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.03934	0.00015	-0.02265	-0.00101	0.01635

67	C5	S	0.08164	-0.00133	0.04728	0.00323	-0.03466
68	C5	PX	-0.10343	-0.02773	-0.01842	0.17112	0.02088
69	C5	PY	0.05472	-0.24525	-0.09786	-0.16425	0.12537
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.05317	0.00766	0.02798	0.01805	-0.03963
72	C5	PX	-0.05362	-0.00346	-0.01269	0.08014	0.00637
73	C5	PY	0.05942	-0.10888	-0.01504	-0.09244	0.05357
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00591	-0.00138	-0.01018	0.00576	-0.00041
76	C5	DYY	0.00530	-0.00166	0.00815	-0.00652	0.00159
77	C5	DZZ	-0.00223	0.00049	-0.00093	0.00054	0.00021
78	C5	DXY	-0.00624	0.00720	0.00383	0.01226	-0.00304
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.03316	0.03487	-0.03637	0.03747	0.00118
82	C6	S	0.07362	-0.07564	0.07738	-0.08314	-0.00565
83	C6	PX	0.03259	0.04865	0.01585	-0.11372	0.08778
84	C6	PY	-0.14090	-0.06554	0.11083	0.04023	0.17581
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.03556	-0.09038	0.06001	-0.06146	-0.00679
87	C6	PX	0.02366	0.02782	-0.00086	-0.03298	0.03365
88	C6	PY	-0.05442	-0.01280	0.02745	0.01235	0.06165
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00306	-0.00569	-0.00535	-0.00638	0.00251
91	C6	DYY	0.00186	0.00678	0.00699	0.00759	0.00046
92	C6	DZZ	-0.00321	0.00095	-0.00106	0.00152	0.00104
93	C6	DXY	0.00945	0.00067	-0.00679	-0.00480	-0.01032
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01874	-0.02671	-0.01122	0.01068	0.00461
97	C7	S	-0.03881	0.05337	0.02313	-0.02043	-0.01100
98	C7	PX	-0.11690	-0.00234	0.03775	-0.12838	0.05266
99	C7	PY	-0.17279	-0.00649	0.00412	0.12769	-0.22707
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.01352	0.06399	0.01404	-0.00795	0.01358
102	C7	PX	-0.06256	-0.00190	0.03152	-0.08128	0.02098
103	C7	PY	-0.05313	-0.00477	0.00813	0.05116	-0.08427
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00722	0.00570	0.00295	-0.01004	0.01675
106	C7	DYY	-0.00406	-0.00526	-0.00221	0.00930	-0.01384
107	C7	DZZ	0.00015	-0.00194	-0.00080	0.00094	-0.00067
108	C7	DXY	0.01158	-0.00397	-0.00504	0.00682	0.00392
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.08933	-0.09744	0.03752	0.03677	0.06181
112	H3	S	-0.04488	-0.07110	0.03676	0.02372	0.05361
113	H3	PX	0.00299	0.00420	-0.00097	-0.00290	-0.00253
114	H3	PY	0.00454	0.00321	-0.00130	-0.00014	-0.00165
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.09844	-0.11972	-0.02145	-0.14894	0.04695
117	H4	S	0.05095	-0.07927	-0.02484	-0.11161	0.04145
118	H4	PX	0.00235	-0.00507	-0.00092	-0.00279	0.00223
119	H4	PY	-0.00579	0.00403	0.00024	0.00664	-0.00086
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

121	N1	S	0.02667	-0.01707	0.01178	-0.02490	-0.00247
122	N1	S	-0.06010	0.03454	-0.02655	0.05571	0.00333
123	N1	PX	0.05150	0.05837	0.02204	-0.03491	0.10959
124	N1	PY	0.20152	-0.03140	-0.04329	-0.05757	-0.22395
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.10040	0.06772	-0.03141	0.08120	0.03874
127	N1	PX	0.02851	0.03286	0.01658	-0.02270	0.06800
128	N1	PY	0.09581	-0.00855	-0.02060	-0.03055	-0.10591
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00158	0.00654	0.00157	-0.00095	0.01530
131	N1	DYY	0.00137	-0.00766	-0.00049	-0.00245	-0.01468
132	N1	DZZ	-0.00200	-0.00234	-0.00009	0.00082	-0.00180
133	N1	DXY	0.01778	0.00076	-0.00306	-0.00794	-0.01428
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.06387	-0.03403	-0.18801	-0.02272	0.04082
137	H6	S	-0.03234	-0.02935	-0.12633	-0.02433	0.03411
138	H6	PX	-0.00396	-0.00143	-0.00993	-0.00105	0.00197
139	H6	PY	0.00102	0.00262	-0.00046	-0.00053	-0.00101
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01391	0.04034	0.00296	-0.00614	-0.00422
142	C8	S	0.02944	-0.08157	-0.00652	0.01337	0.01229
143	C8	PX	0.21140	-0.01477	-0.04969	0.00946	-0.04597
144	C8	PY	0.02567	0.19287	0.01378	0.05309	0.28481
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.01456	-0.07689	0.00535	0.00509	0.03872
147	C8	PX	0.05749	-0.00846	-0.00048	-0.02436	-0.02043
148	C8	PY	0.00175	0.04255	0.00687	0.00488	0.06865
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00483	0.00989	0.00158	0.00182	0.02229
151	C8	DYY	0.00607	-0.00357	-0.00105	-0.00052	-0.01584
152	C8	DZZ	0.00011	0.00101	-0.00022	-0.00056	-0.00228
153	C8	DXY	0.00247	-0.00321	0.00355	-0.00849	-0.01187
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.04588	0.03129	0.03607	-0.12134	0.08608
157	H8	S	-0.02067	0.02127	0.02468	-0.08496	0.07630
158	H8	PX	0.00212	-0.00165	-0.00147	0.00601	-0.00420
159	H8	PY	-0.00382	0.00027	0.00116	-0.00095	-0.00182
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00015	-0.01351	-0.00073	0.00283	0.01965
162	C10	S	-0.00207	0.02536	0.00198	-0.00665	-0.04177
163	C10	PX	0.20343	-0.02694	-0.14042	0.25234	0.04706
164	C10	PY	-0.01749	-0.25779	-0.00872	-0.05388	-0.26461
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00153	0.04061	0.00419	-0.01365	-0.05492
167	C10	PX	0.08799	-0.00955	-0.07029	0.12988	0.02887
168	C10	PY	-0.00171	-0.09457	-0.00562	-0.02029	-0.11082
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00012	0.01586	0.00161	0.00043	0.01382
171	C10	DYY	-0.00022	-0.01120	-0.00147	0.00014	-0.00907
172	C10	DZZ	-0.00019	-0.00207	-0.00004	-0.00015	-0.00005
173	C10	DXY	-0.00487	-0.00247	0.00615	-0.01499	-0.00742
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.10169	0.09149	-0.06809	0.15274	0.10975
177	H16	S	0.06775	0.06634	-0.04817	0.11593	0.09676
178	H16	PX	-0.00382	-0.00535	0.00224	-0.00553	-0.00479
179	H16	PY	0.00417	-0.00012	-0.00285	0.00484	-0.00007
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.09941	0.09849	0.08001	-0.13111	0.03112
182	H18	S	-0.05999	0.06781	0.05133	-0.08794	0.03307
183	H18	PX	-0.00418	0.00589	0.00343	-0.00526	0.00204
184	H18	PY	-0.00406	-0.00071	0.00221	-0.00416	-0.00284
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	26	27	28	29	30
Eigenvalues:	-0.56064	-0.55853	-0.51793	-0.49062	-0.45735
(ev):	-15.25576	-15.19827	-14.09354	-13.35042	-12.44505

		A	A	A	A	A	
1	H1	S	0.05829	0.00000	-0.00809	-0.12105	0.00000
2	H1	S	0.04003	0.00000	-0.01195	-0.10928	0.00000
3	H1	PX	-0.00266	0.00000	-0.00042	0.00439	0.00000
4	H1	PY	-0.00059	0.00000	0.00321	-0.00066	0.00000
5	H1	PZ	0.00000	0.00219	0.00000	0.00000	0.00451
6	C1	S	-0.02196	0.00000	-0.00557	-0.00958	0.00000
7	C1	S	0.04314	0.00000	0.01073	0.02144	0.00000
8	C1	PX	0.04630	0.00000	-0.02997	-0.16550	0.00000
9	C1	PY	-0.01424	0.00000	0.22327	-0.09963	0.00000
10	C1	PZ	0.00000	0.10483	0.00000	0.00000	0.21403
11	C1	S	0.06425	0.00000	-0.00771	0.03228	0.00000
12	C1	PX	0.03164	0.00000	-0.00245	-0.10987	0.00000
13	C1	PY	-0.00641	0.00000	0.09655	-0.03278	0.00000
14	C1	PZ	0.00000	0.05797	0.00000	0.00000	0.15122
15	C1	DXX	0.00901	0.00000	-0.00125	-0.01726	0.00000
16	C1	DYY	-0.00867	0.00000	-0.00287	0.01628	0.00000
17	C1	DZZ	-0.00140	0.00000	-0.00010	-0.00020	0.00000
18	C1	DXY	-0.00499	0.00000	-0.01313	0.00560	0.00000
19	C1	DXZ	0.00000	-0.00683	0.00000	0.00000	-0.01216
20	C1	DYZ	0.00000	-0.00171	0.00000	0.00000	0.01004
21	C2	S	0.00449	0.00000	0.00927	-0.00469	0.00000
22	C2	S	-0.00961	0.00000	-0.01582	0.01303	0.00000
23	C2	PX	-0.07440	0.00000	0.07198	0.18641	0.00000
24	C2	PY	-0.19696	0.00000	-0.19589	-0.00046	0.00000
25	C2	PZ	0.00000	0.11756	0.00000	0.00000	0.16070
26	C2	S	0.02005	0.00000	-0.02342	-0.00414	0.00000
27	C2	PX	-0.02488	0.00000	0.05233	0.10952	0.00000
28	C2	PY	-0.06950	0.00000	-0.08117	-0.01101	0.00000
29	C2	PZ	0.00000	0.06362	0.00000	0.00000	0.11706
30	C2	DXX	0.00596	0.00000	-0.00547	-0.01669	0.00000
31	C2	DYY	-0.00212	0.00000	0.00769	0.01495	0.00000
32	C2	DZZ	-0.00024	0.00000	0.00064	0.00027	0.00000
33	C2	DXY	-0.00606	0.00000	-0.01507	-0.00345	0.00000
34	C2	DXZ	0.00000	0.00787	0.00000	0.00000	0.00945
35	C2	DYZ	0.00000	-0.00179	0.00000	0.00000	0.01136
36	C3	S	0.02831	0.00000	0.00339	-0.00907	0.00000
37	C3	S	-0.05998	0.00000	-0.00778	0.01785	0.00000

38	C3	PX	0.08458	0.00000	-0.00741	0.17297	0.00000
39	C3	PY	-0.03965	0.00000	-0.19147	0.10262	0.00000
40	C3	PZ	0.00000	0.19514	0.00000	0.00000	0.05714
41	C3	S	-0.08891	0.00000	-0.00617	0.00576	0.00000
42	C3	PX	0.02928	0.00000	-0.00657	0.10094	0.00000
43	C3	PY	-0.01709	0.00000	-0.05574	0.05322	0.00000
44	C3	PZ	0.00000	0.11756	0.00000	0.00000	0.04332
45	C3	DXX	-0.01067	0.00000	-0.00350	-0.01682	0.00000
46	C3	DYY	0.00981	0.00000	0.00230	0.01664	0.00000
47	C3	DZZ	0.00080	0.00000	0.00055	0.00013	0.00000
48	C3	DXY	0.00436	0.00000	-0.01617	0.00526	0.00000
49	C3	DXZ	0.00000	-0.00500	0.00000	0.00000	0.00283
50	C3	DYZ	0.00000	-0.00707	0.00000	0.00000	0.01042
51	C4	S	0.00265	0.00000	0.00428	0.00931	0.00000
52	C4	S	-0.00193	0.00000	-0.00543	-0.02036	0.00000
53	C4	PX	-0.21685	0.00000	0.09085	0.19138	0.00000
54	C4	PY	-0.14112	0.00000	-0.18845	0.08258	0.00000
55	C4	PZ	0.00000	0.08454	0.00000	0.00000	0.25580
56	C4	S	-0.00716	0.00000	-0.02943	-0.04693	0.00000
57	C4	PX	-0.09783	0.00000	0.02840	0.09174	0.00000
58	C4	PY	-0.07822	0.00000	-0.08724	0.06689	0.00000
59	C4	PZ	0.00000	0.05075	0.00000	0.00000	0.18018
60	C4	DXX	0.01328	0.00000	-0.00029	-0.01578	0.00000
61	C4	DYY	-0.01359	0.00000	-0.00427	0.01573	0.00000
62	C4	DZZ	0.00094	0.00000	0.00113	0.00015	0.00000
63	C4	DXY	-0.00936	0.00000	-0.01723	0.00539	0.00000
64	C4	DXZ	0.00000	-0.00033	0.00000	0.00000	-0.00165
65	C4	DYZ	0.00000	-0.00617	0.00000	0.00000	-0.01362
66	C5	S	-0.00983	0.00000	-0.00128	0.00510	0.00000
67	C5	S	0.02117	0.00000	-0.00246	-0.01297	0.00000
68	C5	PX	0.21564	0.00000	-0.06148	-0.20592	0.00000
69	C5	PY	0.12382	0.00000	0.20056	-0.00885	0.00000
70	C5	PZ	0.00000	0.09004	0.00000	0.00000	0.22646
71	C5	S	0.02713	0.00000	0.01739	-0.01508	0.00000
72	C5	PX	0.08291	0.00000	-0.04089	-0.09978	0.00000
73	C5	PY	0.05391	0.00000	0.09943	0.00478	0.00000
74	C5	PZ	0.00000	0.05546	0.00000	0.00000	0.15770
75	C5	DXX	0.01139	0.00000	-0.00595	-0.01482	0.00000
76	C5	DYY	-0.00749	0.00000	0.01003	0.01376	0.00000
77	C5	DZZ	-0.00068	0.00000	-0.00135	-0.00020	0.00000
78	C5	DXY	-0.00966	0.00000	-0.01940	-0.00172	0.00000
79	C5	DXZ	0.00000	0.00036	0.00000	0.00000	0.00504
80	C5	DYZ	0.00000	-0.00682	0.00000	0.00000	-0.01075
81	C6	S	0.00356	0.00000	-0.00454	0.01715	0.00000
82	C6	S	-0.00613	0.00000	0.00540	-0.03986	0.00000
83	C6	PX	-0.15160	0.00000	-0.04462	-0.19586	0.00000
84	C6	PY	0.03784	0.00000	0.23242	0.07613	0.00000
85	C6	PZ	0.00000	0.24032	0.00000	0.00000	-0.02349
86	C6	S	-0.01836	0.00000	0.04079	-0.02772	0.00000
87	C6	PX	-0.06038	0.00000	-0.04129	-0.08901	0.00000
88	C6	PY	0.00422	0.00000	0.06529	0.00960	0.00000
89	C6	PZ	0.00000	0.13965	0.00000	0.00000	-0.01787
90	C6	DXX	-0.00395	0.00000	0.00491	-0.00749	0.00000
91	C6	DYY	0.00215	0.00000	-0.00378	0.00682	0.00000

92	C6	DZZ	-0.00030	0.00000	0.00185	0.00043	0.00000
93	C6	DXY	-0.00987	0.00000	-0.01398	0.00447	0.00000
94	C6	DXZ	0.00000	0.00115	0.00000	0.00000	0.00240
95	C6	DYZ	0.00000	-0.01304	0.00000	0.00000	0.01697
96	C7	S	-0.01716	0.00000	-0.01521	-0.01672	0.00000
97	C7	S	0.03965	0.00000	0.03138	0.03879	0.00000
98	C7	PX	-0.20006	0.00000	-0.00184	-0.19425	0.00000
99	C7	PY	-0.02472	0.00000	0.16704	-0.05704	0.00000
100	C7	PZ	0.00000	0.15928	0.00000	0.00000	-0.04209
101	C7	S	0.03062	0.00000	0.05772	0.06857	0.00000
102	C7	PX	-0.08877	0.00000	-0.00303	-0.11325	0.00000
103	C7	PY	0.00549	0.00000	0.06253	-0.02389	0.00000
104	C7	PZ	0.00000	0.09337	0.00000	0.00000	-0.03138
105	C7	DXX	-0.00031	0.00000	-0.00613	-0.00443	0.00000
106	C7	DYY	0.00047	0.00000	0.00464	0.00362	0.00000
107	C7	DZZ	-0.00050	0.00000	-0.00006	0.00027	0.00000
108	C7	DXY	0.01221	0.00000	-0.00732	0.01848	0.00000
109	C7	DXZ	0.00000	-0.01091	0.00000	0.00000	0.00565
110	C7	DYZ	0.00000	0.00748	0.00000	0.00000	0.00604
111	H3	S	-0.15372	0.00000	-0.10339	0.10834	0.00000
112	H3	S	-0.12257	0.00000	-0.09106	0.09730	0.00000
113	H3	PX	0.00148	0.00000	0.00389	-0.00034	0.00000
114	H3	PY	0.00718	0.00000	0.00229	-0.00443	0.00000
115	H3	PZ	0.00000	0.00164	0.00000	0.00000	0.00546
116	H4	S	0.01319	0.00000	0.15271	0.06630	0.00000
117	H4	S	0.00868	0.00000	0.13340	0.06095	0.00000
118	H4	PX	0.00308	0.00000	0.00390	-0.00051	0.00000
119	H4	PY	0.00163	0.00000	-0.00452	-0.00342	0.00000
120	H4	PZ	0.00000	0.00169	0.00000	0.00000	0.00477
121	N1	S	0.02446	0.00000	-0.02256	-0.02007	0.00000
122	N1	S	-0.05466	0.00000	0.05164	0.04389	0.00000
123	N1	PX	0.00851	0.00000	-0.11151	-0.14990	0.00000
124	N1	PY	0.04498	0.00000	-0.20840	0.02951	0.00000
125	N1	PZ	0.00000	0.25471	0.00000	0.00000	-0.15802
126	N1	S	-0.08113	0.00000	0.07619	0.07823	0.00000
127	N1	PX	0.01248	0.00000	-0.07738	-0.09635	0.00000
128	N1	PY	0.01555	0.00000	-0.11727	0.00234	0.00000
129	N1	PZ	0.00000	0.16143	0.00000	0.00000	-0.11548
130	N1	DXX	0.00263	0.00000	-0.00460	-0.00948	0.00000
131	N1	DYY	0.00097	0.00000	-0.00195	0.00154	0.00000
132	N1	DZZ	-0.00093	0.00000	0.00383	0.00307	0.00000
133	N1	DXY	-0.00065	0.00000	-0.01762	-0.00477	0.00000
134	N1	DXZ	0.00000	0.02153	0.00000	0.00000	-0.01360
135	N1	DYZ	0.00000	0.01218	0.00000	0.00000	-0.00076
136	H6	S	0.04970	0.00000	-0.05718	-0.13294	0.00000
137	H6	S	0.03908	0.00000	-0.03741	-0.10872	0.00000
138	H6	PX	0.00183	0.00000	-0.00259	-0.00497	0.00000
139	H6	PY	-0.00293	0.00000	-0.00292	-0.00061	0.00000
140	H6	PZ	0.00000	0.00248	0.00000	0.00000	0.00315
141	C8	S	-0.01855	0.00000	0.00869	-0.01342	0.00000
142	C8	S	0.03872	0.00000	-0.01937	0.02600	0.00000
143	C8	PX	0.11073	0.00000	-0.10584	0.16921	0.00000
144	C8	PY	0.13116	0.00000	0.00133	0.09508	0.00000
145	C8	PZ	0.00000	0.19254	0.00000	0.00000	-0.19895

146	C8	S	0.06815	0.00000	-0.02123	0.05862	0.00000
147	C8	PX	0.07272	0.00000	-0.07879	0.06991	0.00000
148	C8	PY	0.02958	0.00000	0.00064	0.00758	0.00000
149	C8	PZ	0.00000	0.11214	0.00000	0.00000	-0.13502
150	C8	DXX	0.00395	0.00000	0.00541	0.00837	0.00000
151	C8	DYY	-0.00086	0.00000	-0.00638	-0.00879	0.00000
152	C8	DZZ	-0.00056	0.00000	-0.00032	0.00045	0.00000
153	C8	DXY	0.01712	0.00000	-0.00701	0.01551	0.00000
154	C8	DXZ	0.00000	-0.00381	0.00000	0.00000	0.00415
155	C8	DYZ	0.00000	0.00558	0.00000	0.00000	0.00365
156	H8	S	-0.10085	0.00000	-0.02222	-0.10413	0.00000
157	H8	S	-0.08221	0.00000	-0.02230	-0.09943	0.00000
158	H8	PX	0.00390	0.00000	0.00162	0.00297	0.00000
159	H8	PY	-0.00260	0.00000	0.00176	-0.00295	0.00000
160	H8	PZ	0.00000	0.00330	0.00000	0.00000	-0.00081
161	C10	S	0.00350	0.00000	0.00396	0.00948	0.00000
162	C10	S	-0.00739	0.00000	-0.00821	-0.02022	0.00000
163	C10	PX	-0.19241	0.00000	0.14582	-0.07739	0.00000
164	C10	PY	-0.08475	0.00000	-0.02419	-0.07573	0.00000
165	C10	PZ	0.00000	0.09743	0.00000	0.00000	-0.14133
166	C10	S	-0.01034	0.00000	-0.01650	-0.04513	0.00000
167	C10	PX	-0.10955	0.00000	0.08730	-0.04752	0.00000
168	C10	PY	-0.04444	0.00000	-0.00620	-0.04258	0.00000
169	C10	PZ	0.00000	0.05719	0.00000	0.00000	-0.10163
170	C10	DXX	0.00637	0.00000	-0.00051	0.00480	0.00000
171	C10	DYY	-0.00564	0.00000	0.00131	-0.00347	0.00000
172	C10	DZZ	0.00015	0.00000	-0.00015	0.00025	0.00000
173	C10	DXY	0.01341	0.00000	-0.01258	0.00962	0.00000
174	C10	DXZ	0.00000	0.00078	0.00000	0.00000	-0.00083
175	C10	DYZ	0.00000	0.01065	0.00000	0.00000	-0.01250
176	H16	S	-0.08138	0.00000	0.09337	-0.03159	0.00000
177	H16	S	-0.06429	0.00000	0.08066	-0.02869	0.00000
178	H16	PX	0.00177	0.00000	-0.00315	0.00017	0.00000
179	H16	PY	-0.00429	0.00000	0.00273	-0.00196	0.00000
180	H16	PZ	0.00000	0.00208	0.00000	0.00000	-0.00307
181	H18	S	0.13603	0.00000	-0.08726	0.06799	0.00000
182	H18	S	0.09760	0.00000	-0.06089	0.06597	0.00000
183	H18	PX	0.00565	0.00000	-0.00360	0.00238	0.00000
184	H18	PY	0.00193	0.00000	-0.00174	0.00044	0.00000
185	H18	PZ	0.00000	0.00210	0.00000	0.00000	-0.00306

MO: 31 32 33 34 35
Eigenvalues: -0.41260 -0.39954 -0.33330 -0.29083 0.03440
(ev): -11.22740 -10.87203 -9.06956 -7.91387 0.93598

			A	A	A	A	A
1	H1	S	0.06571	0.00000	0.00000	0.00000	0.00000
2	H1	S	0.07175	0.00000	0.00000	0.00000	0.00000
3	H1	PX	-0.00207	0.00000	0.00000	0.00000	0.00000
4	H1	PY	0.00015	0.00000	0.00000	0.00000	0.00000
5	H1	PZ	0.00000	0.00454	-0.00020	-0.00557	0.00466
6	C1	S	0.00887	0.00000	0.00000	0.00000	0.00000
7	C1	S	-0.02022	0.00000	0.00000	0.00000	0.00000
8	C1	PX	0.08865	0.00000	0.00000	0.00000	0.00000

9	C1	PY	0.02576	0.00000	0.00000	0.00000	0.00000
10	C1	PZ	0.00000	0.19553	-0.01614	-0.22352	0.15014
11	C1	S	-0.04265	0.00000	0.00000	0.00000	0.00000
12	C1	PX	0.05610	0.00000	0.00000	0.00000	0.00000
13	C1	PY	0.03714	0.00000	0.00000	0.00000	0.00000
14	C1	PZ	0.00000	0.14677	-0.02277	-0.20082	0.21567
15	C1	DXX	0.01015	0.00000	0.00000	0.00000	0.00000
16	C1	DYY	-0.01047	0.00000	0.00000	0.00000	0.00000
17	C1	DZZ	-0.00024	0.00000	0.00000	0.00000	0.00000
18	C1	DXY	0.00287	0.00000	0.00000	0.00000	0.00000
19	C1	DXZ	0.00000	-0.00770	0.00135	0.00775	-0.00104
20	C1	DYZ	0.00000	-0.00226	-0.01321	-0.01687	-0.01223
21	C2	S	0.01846	0.00000	0.00000	0.00000	0.00000
22	C2	S	-0.03742	0.00000	0.00000	0.00000	0.00000
23	C2	PX	-0.08753	0.00000	0.00000	0.00000	0.00000
24	C2	PY	0.10429	0.00000	0.00000	0.00000	0.00000
25	C2	PZ	0.00000	-0.23336	-0.06465	0.22514	0.13652
26	C2	S	-0.10344	0.00000	0.00000	0.00000	0.00000
27	C2	PX	-0.05512	0.00000	0.00000	0.00000	0.00000
28	C2	PY	0.04402	0.00000	0.00000	0.00000	0.00000
29	C2	PZ	0.00000	-0.17535	-0.06012	0.20282	0.20857
30	C2	DXX	0.00905	0.00000	0.00000	0.00000	0.00000
31	C2	DYY	-0.00948	0.00000	0.00000	0.00000	0.00000
32	C2	DZZ	0.00064	0.00000	0.00000	0.00000	0.00000
33	C2	DXY	0.00411	0.00000	0.00000	0.00000	0.00000
34	C2	DXZ	0.00000	-0.01004	-0.00210	0.00776	0.00263
35	C2	DYZ	0.00000	-0.00319	-0.01416	0.01156	-0.01480
36	C3	S	-0.02061	0.00000	0.00000	0.00000	0.00000
37	C3	S	0.04186	0.00000	0.00000	0.00000	0.00000
38	C3	PX	-0.22022	0.00000	0.00000	0.00000	0.00000
39	C3	PY	0.00175	0.00000	0.00000	0.00000	0.00000
40	C3	PZ	0.00000	0.21952	0.20608	0.13945	0.12177
41	C3	S	0.11754	0.00000	0.00000	0.00000	0.00000
42	C3	PX	-0.11418	0.00000	0.00000	0.00000	0.00000
43	C3	PY	0.04406	0.00000	0.00000	0.00000	0.00000
44	C3	PZ	0.00000	0.16011	0.18065	0.13713	0.15114
45	C3	DXX	0.00905	0.00000	0.00000	0.00000	0.00000
46	C3	DYY	-0.00628	0.00000	0.00000	0.00000	0.00000
47	C3	DZZ	-0.00013	0.00000	0.00000	0.00000	0.00000
48	C3	DXY	0.00046	0.00000	0.00000	0.00000	0.00000
49	C3	DXZ	0.00000	0.01200	-0.00546	0.00201	-0.00757
50	C3	DYZ	0.00000	-0.00619	-0.00757	-0.02184	0.02205
51	C4	S	0.00255	0.00000	0.00000	0.00000	0.00000
52	C4	S	-0.00474	0.00000	0.00000	0.00000	0.00000
53	C4	PX	-0.05758	0.00000	0.00000	0.00000	0.00000
54	C4	PY	0.02256	0.00000	0.00000	0.00000	0.00000
55	C4	PZ	0.00000	0.09067	-0.13757	-0.21480	-0.14883
56	C4	S	-0.01744	0.00000	0.00000	0.00000	0.00000
57	C4	PX	-0.03743	0.00000	0.00000	0.00000	0.00000
58	C4	PY	0.01236	0.00000	0.00000	0.00000	0.00000
59	C4	PZ	0.00000	0.07254	-0.11277	-0.20805	-0.19642
60	C4	DXX	0.00474	0.00000	0.00000	0.00000	0.00000
61	C4	DYY	-0.00432	0.00000	0.00000	0.00000	0.00000
62	C4	DZZ	-0.00003	0.00000	0.00000	0.00000	0.00000

63	C4	DXY	0.00128	0.00000	0.00000	0.00000	0.00000
64	C4	DXZ	0.00000	0.01122	0.00504	-0.01376	0.01263
65	C4	DYZ	0.00000	-0.00883	0.00244	0.01220	-0.00861
66	C5	S	-0.00528	0.00000	0.00000	0.00000	0.00000
67	C5	S	0.00762	0.00000	0.00000	0.00000	0.00000
68	C5	PX	0.04338	0.00000	0.00000	0.00000	0.00000
69	C5	PY	-0.03246	0.00000	0.00000	0.00000	0.00000
70	C5	PZ	0.00000	-0.16043	-0.16691	0.15793	-0.16803
71	C5	S	0.03668	0.00000	0.00000	0.00000	0.00000
72	C5	PX	0.02753	0.00000	0.00000	0.00000	0.00000
73	C5	PY	-0.04794	0.00000	0.00000	0.00000	0.00000
74	C5	PZ	0.00000	-0.12586	-0.13788	0.15760	-0.22436
75	C5	DXX	0.00518	0.00000	0.00000	0.00000	0.00000
76	C5	DYY	-0.00552	0.00000	0.00000	0.00000	0.00000
77	C5	DZZ	-0.00098	0.00000	0.00000	0.00000	0.00000
78	C5	DXY	0.00506	0.00000	0.00000	0.00000	0.00000
79	C5	DXZ	0.00000	0.00932	-0.00284	-0.01505	-0.01048
80	C5	DYZ	0.00000	0.01250	0.00449	-0.01316	-0.00895
81	C6	S	0.02069	0.00000	0.00000	0.00000	0.00000
82	C6	S	-0.05790	0.00000	0.00000	0.00000	0.00000
83	C6	PX	0.18981	0.00000	0.00000	0.00000	0.00000
84	C6	PY	0.04432	0.00000	0.00000	0.00000	0.00000
85	C6	PZ	0.00000	-0.18085	0.19332	-0.05641	0.15857
86	C6	S	0.03068	0.00000	0.00000	0.00000	0.00000
87	C6	PX	0.05040	0.00000	0.00000	0.00000	0.00000
88	C6	PY	-0.03691	0.00000	0.00000	0.00000	0.00000
89	C6	PZ	0.00000	-0.12806	0.15415	-0.06280	0.16019
90	C6	DXX	0.02499	0.00000	0.00000	0.00000	0.00000
91	C6	DYY	-0.02425	0.00000	0.00000	0.00000	0.00000
92	C6	DZZ	0.00184	0.00000	0.00000	0.00000	0.00000
93	C6	DXY	0.02102	0.00000	0.00000	0.00000	0.00000
94	C6	DXZ	0.00000	0.01726	0.00646	0.00858	0.00436
95	C6	DYZ	0.00000	0.00447	-0.00958	0.02476	0.02188
96	C7	S	-0.01306	0.00000	0.00000	0.00000	0.00000
97	C7	S	0.02640	0.00000	0.00000	0.00000	0.00000
98	C7	PX	-0.09657	0.00000	0.00000	0.00000	0.00000
99	C7	PY	-0.11827	0.00000	0.00000	0.00000	0.00000
100	C7	PZ	0.00000	0.22243	0.06792	0.24861	-0.23108
101	C7	S	0.09656	0.00000	0.00000	0.00000	0.00000
102	C7	PX	-0.05538	0.00000	0.00000	0.00000	0.00000
103	C7	PY	-0.08417	0.00000	0.00000	0.00000	0.00000
104	C7	PZ	0.00000	0.17787	0.05418	0.22947	-0.29281
105	C7	DXX	0.00302	0.00000	0.00000	0.00000	0.00000
106	C7	DYY	0.00025	0.00000	0.00000	0.00000	0.00000
107	C7	DZZ	0.00026	0.00000	0.00000	0.00000	0.00000
108	C7	DXY	0.00002	0.00000	0.00000	0.00000	0.00000
109	C7	DXZ	0.00000	-0.00739	0.00138	-0.00623	0.00492
110	C7	DYZ	0.00000	0.01117	0.01905	0.00900	0.00545
111	H3	S	-0.00821	0.00000	0.00000	0.00000	0.00000
112	H3	S	-0.00686	0.00000	0.00000	0.00000	0.00000
113	H3	PX	-0.00047	0.00000	0.00000	0.00000	0.00000
114	H3	PY	0.00042	0.00000	0.00000	0.00000	0.00000
115	H3	PZ	0.00000	0.00205	-0.00340	-0.00523	-0.00534
116	H4	S	-0.03803	0.00000	0.00000	0.00000	0.00000

117	H4	S	-0.03275	0.00000	0.00000	0.00000	0.00000
118	H4	PX	-0.00031	0.00000	0.00000	0.00000	0.00000
119	H4	PY	0.00089	0.00000	0.00000	0.00000	0.00000
120	H4	PZ	0.00000	-0.00358	-0.00402	0.00370	-0.00587
121	N1	S	-0.06370	0.00000	0.00000	0.00000	0.00000
122	N1	S	0.13749	0.00000	0.00000	0.00000	0.00000
123	N1	PX	-0.45341	0.00000	0.00000	0.00000	0.00000
124	N1	PY	-0.10426	0.00000	0.00000	0.00000	0.00000
125	N1	PZ	0.00000	-0.20217	0.08992	-0.27021	-0.17580
126	N1	S	0.24774	0.00000	0.00000	0.00000	0.00000
127	N1	PX	-0.35810	0.00000	0.00000	0.00000	0.00000
128	N1	PY	-0.08874	0.00000	0.00000	0.00000	0.00000
129	N1	PZ	0.00000	-0.16244	0.08295	-0.24417	-0.19485
130	N1	DXX	-0.02542	0.00000	0.00000	0.00000	0.00000
131	N1	DYY	-0.00297	0.00000	0.00000	0.00000	0.00000
132	N1	DZZ	0.01062	0.00000	0.00000	0.00000	0.00000
133	N1	DXY	-0.00376	0.00000	0.00000	0.00000	0.00000
134	N1	DXZ	0.00000	-0.01086	0.00311	-0.01518	-0.01141
135	N1	DYZ	0.00000	-0.01422	0.01795	-0.00886	0.00453
136	H6	S	0.05200	0.00000	0.00000	0.00000	0.00000
137	H6	S	0.07985	0.00000	0.00000	0.00000	0.00000
138	H6	PX	0.00181	0.00000	0.00000	0.00000	0.00000
139	H6	PY	0.00063	0.00000	0.00000	0.00000	0.00000
140	H6	PZ	0.00000	-0.00526	-0.00137	0.00538	0.00395
141	C8	S	0.02869	0.00000	0.00000	0.00000	0.00000
142	C8	S	-0.07019	0.00000	0.00000	0.00000	0.00000
143	C8	PX	0.17716	0.00000	0.00000	0.00000	0.00000
144	C8	PY	-0.05369	0.00000	0.00000	0.00000	0.00000
145	C8	PZ	0.00000	0.06863	-0.26226	0.00570	-0.08309
146	C8	S	-0.05674	0.00000	0.00000	0.00000	0.00000
147	C8	PX	0.02008	0.00000	0.00000	0.00000	0.00000
148	C8	PY	-0.03286	0.00000	0.00000	0.00000	0.00000
149	C8	PZ	0.00000	0.04250	-0.20817	-0.00429	-0.12808
150	C8	DXX	0.01314	0.00000	0.00000	0.00000	0.00000
151	C8	DYY	-0.01763	0.00000	0.00000	0.00000	0.00000
152	C8	DZZ	0.00175	0.00000	0.00000	0.00000	0.00000
153	C8	DXY	0.01688	0.00000	0.00000	0.00000	0.00000
154	C8	DXZ	0.00000	0.01431	-0.00113	0.01973	-0.00260
155	C8	DYZ	0.00000	-0.00522	0.02647	-0.00332	-0.02745
156	H8	S	-0.01773	0.00000	0.00000	0.00000	0.00000
157	H8	S	-0.02505	0.00000	0.00000	0.00000	0.00000
158	H8	PX	0.00065	0.00000	0.00000	0.00000	0.00000
159	H8	PY	-0.00278	0.00000	0.00000	0.00000	0.00000
160	H8	PZ	0.00000	0.00515	0.00142	0.00638	-0.00793
161	C10	S	0.00825	0.00000	0.00000	0.00000	0.00000
162	C10	S	-0.01906	0.00000	0.00000	0.00000	0.00000
163	C10	PX	-0.02188	0.00000	0.00000	0.00000	0.00000
164	C10	PY	-0.02298	0.00000	0.00000	0.00000	0.00000
165	C10	PZ	0.00000	0.06425	-0.30721	0.01696	0.26557
166	C10	S	-0.05537	0.00000	0.00000	0.00000	0.00000
167	C10	PX	0.00103	0.00000	0.00000	0.00000	0.00000
168	C10	PY	-0.00055	0.00000	0.00000	0.00000	0.00000
169	C10	PZ	0.00000	0.05398	-0.26954	0.01980	0.37242
170	C10	DXX	0.00237	0.00000	0.00000	0.00000	0.00000

171	C10	DYY	-0.00065	0.00000	0.00000	0.00000	0.00000
172	C10	DZZ	-0.00050	0.00000	0.00000	0.00000	0.00000
173	C10	DXY	0.00832	0.00000	0.00000	0.00000	0.00000
174	C10	DXZ	0.00000	0.00195	-0.00214	0.00255	-0.00001
175	C10	DYZ	0.00000	0.00488	-0.01979	0.00073	-0.00224
176	H16	S	-0.01950	0.00000	0.00000	0.00000	0.00000
177	H16	S	-0.01731	0.00000	0.00000	0.00000	0.00000
178	H16	PX	-0.00014	0.00000	0.00000	0.00000	0.00000
179	H16	PY	-0.00024	0.00000	0.00000	0.00000	0.00000
180	H16	PZ	0.00000	0.00165	-0.00720	0.00077	0.00862
181	H18	S	0.02449	0.00000	0.00000	0.00000	0.00000
182	H18	S	0.06222	0.00000	0.00000	0.00000	0.00000
183	H18	PX	0.00012	0.00000	0.00000	0.00000	0.00000
184	H18	PY	0.00119	0.00000	0.00000	0.00000	0.00000
185	H18	PZ	0.00000	0.00109	-0.00684	-0.00007	0.00838

MO:	36	37	38	39	40
Eigenvalues:	0.17203	0.19622	0.24449	0.26350	0.28437
(ev):	4.68115	5.33948	6.65287	7.17009	7.73808

		A	A	A	A	A	
1	H1	S	0.00000	0.00000	-0.03010	0.00068	0.00000
2	H1	S	0.00000	0.00000	-0.94876	-0.58727	0.00000
3	H1	PX	0.00000	0.00000	0.00101	0.00327	0.00000
4	H1	PY	0.00000	0.00000	0.00147	0.00243	0.00000
5	H1	PZ	0.01169	0.00436	0.00000	0.00000	0.00356
6	C1	S	0.00000	0.00000	-0.04148	-0.01226	0.00000
7	C1	S	0.00000	0.00000	0.05493	-0.00284	0.00000
8	C1	PX	0.00000	0.00000	0.12054	0.08192	0.00000
9	C1	PY	0.00000	0.00000	0.01037	0.02457	0.00000
10	C1	PZ	0.26841	0.10644	0.00000	0.00000	0.05096
11	C1	S	0.00000	0.00000	0.65003	0.44337	0.00000
12	C1	PX	0.00000	0.00000	0.44568	0.37706	0.00000
13	C1	PY	0.00000	0.00000	-0.09971	-0.04016	0.00000
14	C1	PZ	0.51787	0.20165	0.00000	0.00000	0.20857
15	C1	DXX	0.00000	0.00000	-0.01538	-0.00116	0.00000
16	C1	DYY	0.00000	0.00000	0.00981	0.00426	0.00000
17	C1	DZZ	0.00000	0.00000	0.00026	-0.00341	0.00000
18	C1	DXY	0.00000	0.00000	0.00283	0.00034	0.00000
19	C1	DXZ	0.01067	0.00249	0.00000	0.00000	0.00846
20	C1	DYZ	0.00181	-0.03054	0.00000	0.00000	0.00404
21	C2	S	0.00000	0.00000	-0.03163	0.01228	0.00000
22	C2	S	0.00000	0.00000	0.04481	-0.01915	0.00000
23	C2	PX	0.00000	0.00000	-0.09046	0.02996	0.00000
24	C2	PY	0.00000	0.00000	0.01086	0.01322	0.00000
25	C2	PZ	0.26196	-0.11263	0.00000	0.00000	0.04203
26	C2	S	0.00000	0.00000	0.42495	-0.16914	0.00000
27	C2	PX	0.00000	0.00000	-0.34087	0.25974	0.00000
28	C2	PY	0.00000	0.00000	-0.23129	0.18440	0.00000
29	C2	PZ	0.48937	-0.22077	0.00000	0.00000	0.14706
30	C2	DXX	0.00000	0.00000	-0.01616	0.00724	0.00000
31	C2	DYY	0.00000	0.00000	0.01062	-0.00524	0.00000
32	C2	DZZ	0.00000	0.00000	0.00094	0.00010	0.00000
33	C2	DXY	0.00000	0.00000	-0.00546	-0.00402	0.00000

34	C2	DXZ	-0.00993	0.00000	0.00000	0.00000	-0.00783
35	C2	DYZ	0.00264	0.03060	0.00000	0.00000	0.00435
36	C3	S	0.00000	0.00000	-0.01492	0.01377	0.00000
37	C3	S	0.00000	0.00000	0.03500	-0.04435	0.00000
38	C3	PX	0.00000	0.00000	0.00058	0.03641	0.00000
39	C3	PY	0.00000	0.00000	-0.00421	0.04455	0.00000
40	C3	PZ	-0.17069	0.21221	0.00000	0.00000	-0.10214
41	C3	S	0.00000	0.00000	0.04757	0.33499	0.00000
42	C3	PX	0.00000	0.00000	-0.04112	-0.39441	0.00000
43	C3	PY	0.00000	0.00000	-0.03003	-0.10454	0.00000
44	C3	PZ	-0.30203	0.41076	0.00000	0.00000	-0.33004
45	C3	DXX	0.00000	0.00000	0.00639	0.01384	0.00000
46	C3	DYY	0.00000	0.00000	-0.01053	-0.00845	0.00000
47	C3	DZZ	0.00000	0.00000	0.00254	-0.00073	0.00000
48	C3	DXY	0.00000	0.00000	0.01319	-0.00908	0.00000
49	C3	DXZ	0.02012	0.01384	0.00000	0.00000	0.02455
50	C3	DYZ	0.00996	0.01399	0.00000	0.00000	-0.01056
51	C4	S	0.00000	0.00000	-0.04527	-0.00636	0.00000
52	C4	S	0.00000	0.00000	0.04531	-0.00040	0.00000
53	C4	PX	0.00000	0.00000	0.06267	0.02210	0.00000
54	C4	PY	0.00000	0.00000	0.15492	0.04076	0.00000
55	C4	PZ	-0.14126	-0.26377	0.00000	0.00000	-0.00683
56	C4	S	0.00000	0.00000	0.93033	0.25155	0.00000
57	C4	PX	0.00000	0.00000	0.21689	0.00240	0.00000
58	C4	PY	0.00000	0.00000	0.45521	0.08515	0.00000
59	C4	PZ	-0.30732	-0.53076	0.00000	0.00000	-0.09599
60	C4	DXX	0.00000	0.00000	0.00698	0.00395	0.00000
61	C4	DYY	0.00000	0.00000	-0.00913	-0.00362	0.00000
62	C4	DZZ	0.00000	0.00000	-0.00199	-0.00099	0.00000
63	C4	DXY	0.00000	0.00000	-0.01537	-0.00052	0.00000
64	C4	DXZ	0.02152	-0.01403	0.00000	0.00000	0.00431
65	C4	DYZ	-0.01436	-0.00503	0.00000	0.00000	-0.00041
66	C5	S	0.00000	0.00000	-0.04611	0.00334	0.00000
67	C5	S	0.00000	0.00000	0.04953	-0.00155	0.00000
68	C5	PX	0.00000	0.00000	-0.07073	0.02378	0.00000
69	C5	PY	0.00000	0.00000	0.14039	0.00743	0.00000
70	C5	PZ	-0.12642	0.27287	0.00000	0.00000	0.01416
71	C5	S	0.00000	0.00000	0.93920	-0.25890	0.00000
72	C5	PX	0.00000	0.00000	-0.34876	0.03922	0.00000
73	C5	PY	0.00000	0.00000	0.36817	0.02304	0.00000
74	C5	PZ	-0.27144	0.54337	0.00000	0.00000	-0.03630
75	C5	DXX	0.00000	0.00000	0.00330	-0.00258	0.00000
76	C5	DYY	0.00000	0.00000	-0.00560	-0.00029	0.00000
77	C5	DZZ	0.00000	0.00000	-0.00190	0.00011	0.00000
78	C5	DXY	0.00000	0.00000	0.01758	0.00089	0.00000
79	C5	DXZ	-0.02119	-0.01351	0.00000	0.00000	-0.00523
80	C5	DYZ	-0.01618	0.00424	0.00000	0.00000	-0.00048
81	C6	S	0.00000	0.00000	-0.01711	-0.00981	0.00000
82	C6	S	0.00000	0.00000	0.04079	0.03398	0.00000
83	C6	PX	0.00000	0.00000	0.00547	0.06968	0.00000
84	C6	PY	0.00000	0.00000	0.00365	0.03766	0.00000
85	C6	PZ	-0.17964	-0.22291	0.00000	0.00000	-0.08669
86	C6	S	0.00000	0.00000	-0.06201	-0.14026	0.00000
87	C6	PX	0.00000	0.00000	0.16129	-0.17398	0.00000

88	C6	PY	0.00000	0.00000	0.05871	0.01192	0.00000
89	C6	PZ	-0.28144	-0.39166	0.00000	0.00000	-0.24812
90	C6	DXX	0.00000	0.00000	0.00658	-0.01428	0.00000
91	C6	DYY	0.00000	0.00000	-0.01692	0.00876	0.00000
92	C6	DZZ	0.00000	0.00000	0.00419	0.00329	0.00000
93	C6	DXY	0.00000	0.00000	-0.01278	0.00722	0.00000
94	C6	DXZ	-0.02003	0.01134	0.00000	0.00000	-0.02534
95	C6	DYZ	0.00715	-0.01579	0.00000	0.00000	-0.01478
96	C7	S	0.00000	0.00000	0.00748	-0.05180	0.00000
97	C7	S	0.00000	0.00000	-0.03081	0.07741	0.00000
98	C7	PX	0.00000	0.00000	0.00183	0.17642	0.00000
99	C7	PY	0.00000	0.00000	-0.04414	-0.06416	0.00000
100	C7	PZ	0.05473	-0.16151	0.00000	0.00000	0.22002
101	C7	S	0.00000	0.00000	0.07783	0.75253	0.00000
102	C7	PX	0.00000	0.00000	-0.09838	1.16302	0.00000
103	C7	PY	0.00000	0.00000	-0.16560	-0.24931	0.00000
104	C7	PZ	0.13353	-0.33716	0.00000	0.00000	0.64657
105	C7	DXX	0.00000	0.00000	0.00003	-0.00194	0.00000
106	C7	DYY	0.00000	0.00000	0.00517	-0.00149	0.00000
107	C7	DZZ	0.00000	0.00000	-0.00257	0.00011	0.00000
108	C7	DXY	0.00000	0.00000	-0.00268	0.00528	0.00000
109	C7	DXZ	-0.00123	0.00065	0.00000	0.00000	0.02833
110	C7	DYZ	-0.01543	0.01618	0.00000	0.00000	0.00822
111	H3	S	0.00000	0.00000	-0.03340	-0.00752	0.00000
112	H3	S	0.00000	0.00000	-1.16585	-0.25400	0.00000
113	H3	PX	0.00000	0.00000	0.00046	0.00087	0.00000
114	H3	PY	0.00000	0.00000	0.00213	0.00035	0.00000
115	H3	PZ	-0.00584	-0.01161	0.00000	0.00000	0.00001
116	H4	S	0.00000	0.00000	-0.03575	-0.00049	0.00000
117	H4	S	0.00000	0.00000	-1.14216	0.07585	0.00000
118	H4	PX	0.00000	0.00000	0.00049	0.00091	0.00000
119	H4	PY	0.00000	0.00000	0.00259	-0.00103	0.00000
120	H4	PZ	-0.00527	0.01185	0.00000	0.00000	0.00094
121	N1	S	0.00000	0.00000	0.00525	-0.01629	0.00000
122	N1	S	0.00000	0.00000	-0.03111	0.06533	0.00000
123	N1	PX	0.00000	0.00000	-0.01240	0.03128	0.00000
124	N1	PY	0.00000	0.00000	-0.04365	-0.03131	0.00000
125	N1	PZ	0.04739	0.18189	0.00000	0.00000	0.24716
126	N1	S	0.00000	0.00000	0.10210	-0.11950	0.00000
127	N1	PX	0.00000	0.00000	0.01666	-0.00917	0.00000
128	N1	PY	0.00000	0.00000	0.01878	-0.01871	0.00000
129	N1	PZ	0.08609	0.28939	0.00000	0.00000	0.50240
130	N1	DXX	0.00000	0.00000	-0.00530	0.00422	0.00000
131	N1	DYY	0.00000	0.00000	0.00475	-0.00454	0.00000
132	N1	DZZ	0.00000	0.00000	-0.00459	0.00914	0.00000
133	N1	DXY	0.00000	0.00000	0.00216	0.00450	0.00000
134	N1	DXZ	0.00346	0.00820	0.00000	0.00000	-0.00880
135	N1	DYZ	-0.01225	-0.01202	0.00000	0.00000	0.01465
136	H6	S	0.00000	0.00000	-0.03185	0.02282	0.00000
137	H6	S	0.00000	0.00000	-0.72120	0.37490	0.00000
138	H6	PX	0.00000	0.00000	-0.00014	0.00083	0.00000
139	H6	PY	0.00000	0.00000	0.00232	0.00021	0.00000
140	H6	PZ	0.01111	-0.00459	0.00000	0.00000	0.00290
141	C8	S	0.00000	0.00000	0.00592	0.00830	0.00000

142	C8	S	0.00000	0.00000	-0.00159	-0.03694	0.00000
143	C8	PX	0.00000	0.00000	-0.01060	0.03977	0.00000
144	C8	PY	0.00000	0.00000	-0.01295	-0.00567	0.00000
145	C8	PZ	0.18415	0.00596	0.00000	0.00000	-0.39716
146	C8	S	0.00000	0.00000	-0.19966	0.46109	0.00000
147	C8	PX	0.00000	0.00000	-0.10987	-0.03690	0.00000
148	C8	PY	0.00000	0.00000	-0.10665	0.33345	0.00000
149	C8	PZ	0.25589	0.02083	0.00000	0.00000	-0.88173
150	C8	DXX	0.00000	0.00000	0.00254	0.00938	0.00000
151	C8	DYY	0.00000	0.00000	-0.00583	0.00012	0.00000
152	C8	DZZ	0.00000	0.00000	0.00068	-0.00168	0.00000
153	C8	DXY	0.00000	0.00000	-0.00040	-0.01096	0.00000
154	C8	DXZ	0.00157	-0.02191	0.00000	0.00000	-0.00327
155	C8	DYZ	0.00926	0.00114	0.00000	0.00000	-0.00096
156	H8	S	0.00000	0.00000	0.00909	0.00182	0.00000
157	H8	S	0.00000	0.00000	0.02025	-1.66394	0.00000
158	H8	PX	0.00000	0.00000	-0.00019	0.00712	0.00000
159	H8	PY	0.00000	0.00000	-0.00338	0.00046	0.00000
160	H8	PZ	0.00271	-0.00762	0.00000	0.00000	0.01494
161	C10	S	0.00000	0.00000	0.01620	-0.07055	0.00000
162	C10	S	0.00000	0.00000	-0.02342	0.07396	0.00000
163	C10	PX	0.00000	0.00000	-0.01004	0.09134	0.00000
164	C10	PY	0.00000	0.00000	0.01628	-0.13550	0.00000
165	C10	PZ	-0.17567	0.00443	0.00000	0.00000	0.15246
166	C10	S	0.00000	0.00000	-0.27800	1.35203	0.00000
167	C10	PX	0.00000	0.00000	0.00490	0.37851	0.00000
168	C10	PY	0.00000	0.00000	0.09909	-0.53963	0.00000
169	C10	PZ	-0.32249	-0.00444	0.00000	0.00000	0.60364
170	C10	DXX	0.00000	0.00000	0.00117	-0.00188	0.00000
171	C10	DYY	0.00000	0.00000	0.00065	-0.00058	0.00000
172	C10	DZZ	0.00000	0.00000	0.00006	-0.00553	0.00000
173	C10	DXY	0.00000	0.00000	0.00030	0.00264	0.00000
174	C10	DXZ	0.00066	-0.00511	0.00000	0.00000	-0.00091
175	C10	DYZ	0.01287	0.00050	0.00000	0.00000	-0.03100
176	H16	S	0.00000	0.00000	0.00255	-0.01071	0.00000
177	H16	S	0.00000	0.00000	0.21027	-1.38758	0.00000
178	H16	PX	0.00000	0.00000	0.00002	0.00046	0.00000
179	H16	PY	0.00000	0.00000	0.00088	-0.00607	0.00000
180	H16	PZ	-0.00779	-0.00071	0.00000	0.00000	0.01053
181	H18	S	0.00000	0.00000	0.00466	-0.01850	0.00000
182	H18	S	0.00000	0.00000	0.15677	-0.48527	0.00000
183	H18	PX	0.00000	0.00000	0.00010	-0.00008	0.00000
184	H18	PY	0.00000	0.00000	0.00078	-0.00263	0.00000
185	H18	PZ	-0.00750	0.00111	0.00000	0.00000	0.00927

MO:	41	42	43	44	45
Eigenvalues:	0.28500	0.30257	0.30727	0.32265	0.33518
(ev):	7.75532	8.23342	8.36138	8.77967	9.12063

		A	A	A	A	A	
1	H1	S	0.00799	0.00866	-0.03099	-0.00037	-0.03005
2	H1	S	1.17798	0.99575	0.44056	1.23137	-0.56069
3	H1	PX	-0.00475	-0.00306	-0.00441	-0.00508	-0.00169
4	H1	PY	0.00154	0.00169	-0.00192	0.00305	0.00326

5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.03540	0.04276	0.02824	0.06147	-0.02673
7	C1	S	-0.02874	-0.05267	-0.05562	-0.09565	0.04213
8	C1	PX	-0.15265	-0.10217	-0.01008	-0.08987	0.03722
9	C1	PY	-0.00557	0.03632	0.00883	0.01148	0.02527
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.83763	-0.78626	-0.40716	-0.96621	0.02162
12	C1	PX	-0.67752	-0.59581	-0.29920	-0.69891	0.40215
13	C1	PY	-0.14190	0.13193	-0.53840	-0.32873	0.31442
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00191	0.00073	-0.01292	-0.00805	-0.00867
16	C1	DYY	-0.00217	0.00213	0.01092	0.01001	-0.00079
17	C1	DZZ	0.00305	-0.00021	-0.00076	-0.00160	-0.00152
18	C1	DXY	0.00477	0.00129	-0.00450	0.00460	0.00741
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02702	-0.02619	0.01725	0.06256	0.05613
22	C2	S	0.02331	0.02096	0.00198	-0.09402	-0.08054
23	C2	PX	-0.12607	-0.10579	0.08517	0.08277	0.11007
24	C2	PY	-0.00589	-0.01663	-0.00227	0.03404	-0.03648
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.57893	0.61987	-0.59769	-1.06597	-0.58610
27	C2	PX	-0.56078	-0.49113	0.20803	0.76586	0.98185
28	C2	PY	-0.26313	-0.05574	0.01595	0.01985	-0.40606
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00960	0.00008	0.00016	-0.00615	0.00092
31	C2	DYY	0.00828	-0.00009	-0.00411	0.00632	0.00597
32	C2	DZZ	-0.00183	-0.00133	0.00287	-0.00156	0.00173
33	C2	DXY	-0.00068	-0.00252	-0.00574	-0.00821	0.00778
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00572	-0.00822	0.00809	-0.00236	-0.00847
37	C3	S	0.04237	0.02915	0.02856	-0.01607	-0.00717
38	C3	PX	-0.08107	0.03135	0.04570	0.04318	0.02018
39	C3	PY	0.04875	0.02880	-0.00942	0.09957	-0.00697
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.61084	0.01899	-1.10983	0.00024	0.57414
42	C3	PX	-0.00101	0.41837	0.16011	-0.18569	0.11586
43	C3	PY	0.19964	-0.12814	0.16273	-0.06444	0.02935
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.01179	-0.00156	0.00749	0.00372	0.00033
46	C3	DYY	0.00421	-0.00356	-0.02218	-0.00976	0.00840
47	C3	DZZ	0.00387	0.00342	0.00268	0.00055	-0.00273
48	C3	DXY	0.00299	-0.01321	-0.00085	-0.01833	0.00029
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00381	0.00864	-0.06001	-0.04267	0.07438
52	C4	S	0.00790	0.01060	0.06702	0.03234	-0.10474
53	C4	PX	-0.02800	-0.02206	0.06570	0.05630	0.04867
54	C4	PY	-0.02871	-0.05888	0.07736	0.08485	-0.06997
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.20762	-0.52045	1.23326	0.99372	-0.96099
57	C4	PX	0.24482	0.14788	0.51336	0.52878	-0.08331
58	C4	PY	-0.12100	-0.20440	0.56097	0.38507	-0.80207

59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.00675	-0.00293	-0.00086	0.00173	0.01666
61	C4	DYY	0.00584	-0.00079	0.00337	0.00272	-0.00847
62	C4	DZZ	0.00114	0.00191	-0.00270	-0.00459	-0.00068
63	C4	DXY	-0.00292	-0.00232	0.00303	0.00815	-0.00435
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02905	-0.01341	0.02101	-0.02621	-0.09455
67	C5	S	0.01073	-0.00638	-0.04052	0.01494	0.12020
68	C5	PX	-0.08554	-0.02802	-0.01063	-0.06617	-0.00075
69	C5	PY	0.09442	0.07861	-0.01870	0.06119	0.10652
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.99007	0.55696	-0.08919	0.58773	1.39400
72	C5	PX	-0.14185	0.08983	-0.06111	-0.46232	-0.45414
73	C5	PY	0.36353	0.28858	-0.30672	0.24852	0.96058
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00866	0.00584	0.00278	0.00537	-0.01570
76	C5	DYY	-0.00259	-0.00238	0.00274	-0.00149	0.00884
77	C5	DZZ	-0.00360	-0.00259	-0.00190	-0.00431	-0.00175
78	C5	DXY	0.00007	-0.00271	-0.00048	-0.00661	-0.01199
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01593	-0.00646	-0.00535	-0.02255	0.00531
82	C6	S	-0.04478	-0.00393	-0.01803	0.04251	0.00166
83	C6	PX	-0.05883	0.01224	0.05113	-0.04062	-0.00273
84	C6	PY	0.01084	-0.01095	0.06075	0.05811	0.02304
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.13143	0.30601	0.37854	0.07653	-0.48738
87	C6	PX	0.18084	0.41041	0.16578	-0.27909	-0.00303
88	C6	PY	0.06595	0.11015	0.04905	-0.09925	-0.21228
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01588	-0.00060	-0.00206	-0.00675	-0.00336
91	C6	DYY	-0.01606	0.00218	0.01189	-0.00106	-0.00474
92	C6	DZZ	-0.00240	-0.00065	-0.00281	0.00211	0.00070
93	C6	DXY	-0.00118	0.00036	-0.00181	0.02064	0.00127
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00662	-0.01502	0.06742	-0.02984	0.02931
97	C7	S	-0.01287	-0.00308	-0.13624	0.05226	-0.01206
98	C7	PX	-0.06339	0.13039	-0.07280	0.06043	-0.02195
99	C7	PY	0.00581	0.00930	0.07957	-0.04375	0.05133
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.00441	0.44058	-0.61198	0.22009	-0.56690
102	C7	PX	-0.35485	0.41643	-0.63964	0.63772	-0.11907
103	C7	PY	0.45472	-0.37298	0.78114	0.10672	-0.09171
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.01218	-0.01266	0.00060	-0.01069	0.00311
106	C7	DYY	-0.00859	0.00986	0.01334	-0.00433	-0.00112
107	C7	DZZ	-0.00039	-0.00200	-0.00854	0.00543	0.00293
108	C7	DXY	-0.00494	0.00956	0.01318	0.00958	0.00246
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00291	-0.00956	-0.00162	0.00970	0.00622
112	H3	S	0.16063	0.35112	-1.25032	-1.01261	1.19815

113	H3	PX	-0.00235	-0.00126	0.00162	0.00450	0.00363
114	H3	PY	0.00068	-0.00216	0.00599	0.00365	-0.00644
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00441	0.00390	0.01311	0.00802	0.00534
117	H4	S	-0.88499	-0.49922	0.34001	-0.73197	-1.67065
118	H4	PX	-0.00385	-0.00266	-0.00187	-0.00558	0.00041
119	H4	PY	0.00294	0.00145	-0.00113	0.00069	0.00780
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00135	-0.01409	-0.01249	0.01606	0.00685
122	N1	S	-0.02004	0.05348	0.02271	-0.02194	-0.00947
123	N1	PX	-0.06232	0.08820	-0.00123	0.00796	0.02576
124	N1	PY	-0.00006	-0.04900	-0.02375	0.05074	-0.00605
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.15635	-0.00162	0.14231	-0.22057	-0.20549
127	N1	PX	-0.02834	-0.00065	-0.02460	-0.01737	-0.10678
128	N1	PY	0.10153	0.05758	-0.05282	-0.03908	0.08615
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.00091	-0.00105	0.00745	-0.00223	0.00115
131	N1	DYY	0.00289	0.00049	-0.01987	0.00669	-0.00377
132	N1	DZZ	-0.00383	0.00632	0.00223	0.00334	-0.00007
133	N1	DXY	-0.00977	0.00977	-0.00069	-0.00848	-0.00024
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.02758	0.00489	-0.00228	0.00144	0.02101
137	H6	S	-0.96317	-0.80302	0.54869	1.26812	1.37537
138	H6	PX	-0.00251	-0.00313	0.00244	0.00587	0.00360
139	H6	PY	-0.00009	0.00057	0.00263	0.00304	-0.00384
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01209	0.00670	-0.02425	-0.02611	-0.00886
142	C8	S	0.01755	-0.01756	0.02883	0.02386	0.01377
143	C8	PX	-0.01920	0.07574	0.13763	-0.04581	0.00792
144	C8	PY	0.06287	-0.05238	0.06167	0.00187	0.03177
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.30986	0.00530	0.36638	0.69856	0.08620
147	C8	PX	0.06976	-0.36001	0.16273	0.31456	-0.16297
148	C8	PY	-0.17749	0.00909	-0.24374	0.01348	0.21827
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00786	0.01267	-0.00934	0.00629	-0.00191
151	C8	DYY	0.00411	-0.00456	0.00685	-0.00680	0.00463
152	C8	DZZ	0.00194	-0.00337	-0.00032	0.00018	0.00038
153	C8	DXY	0.01172	-0.03070	-0.01973	0.01503	-0.01037
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.03048	-0.04162	-0.00957	-0.04395	0.01847
157	H8	S	0.57578	-0.87748	1.32511	-0.80256	0.42538
158	H8	PX	0.00101	0.00151	-0.00121	-0.00228	0.00107
159	H8	PY	0.00344	0.00346	0.00582	0.00044	0.00229
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.07105	0.05218	-0.01587	0.03459	-0.00596
162	C10	S	0.08612	-0.06157	0.02311	-0.03009	0.00047
163	C10	PX	-0.03499	0.20167	0.17336	-0.11671	0.07068
164	C10	PY	-0.12007	0.05928	-0.04792	0.03334	-0.01196
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.98993	-0.83964	0.00876	-0.62913	0.21559

167	C10	PX	-0.24665	1.09187	0.80702	-0.71069	0.41381
168	C10	PY	-0.57969	0.19726	-0.29199	-0.01223	0.02498
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.00739	0.00642	-0.00323	-0.00118	-0.00054
171	C10	DYY	-0.00199	-0.00060	-0.00495	0.00335	-0.00138
172	C10	DZZ	-0.00247	0.00148	0.00100	0.00308	0.00001
173	C10	DXY	-0.00519	0.01185	0.01227	-0.00803	0.00400
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.00265	-0.01034	-0.03875	0.02515	-0.01248
177	H16	S	-0.68886	-0.50302	-1.12812	0.99122	-0.46176
178	H16	PX	-0.00261	0.00458	0.00156	-0.00217	0.00127
179	H16	PY	-0.00261	0.00039	0.00123	-0.00114	0.00047
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.03261	0.03781	0.02639	-0.01463	0.00813
182	H18	S	-1.10230	1.68880	0.72991	-0.41110	0.36028
183	H18	PX	-0.00006	0.00258	0.00467	-0.00247	0.00155
184	H18	PY	-0.00217	0.00199	-0.00086	-0.00014	-0.00087
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	46	47	48	49	50
Eigenvalues:	0.37743	0.40578	0.43114	0.44063	0.47847
(ev):	10.27040	11.04189	11.73184	11.99020	13.01975

		A	A	A	A	A	
1	H1	S	0.00000	0.02203	-0.06158	-0.07220	0.07146
2	H1	S	0.00000	0.71283	-0.28327	0.08502	-0.05349
3	H1	PX	0.00000	-0.00276	-0.00416	-0.00524	0.00551
4	H1	PY	0.00000	0.00835	0.01169	-0.00034	0.01018
5	H1	PZ	-0.01428	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.02755	0.03317	0.04028	-0.02248
7	C1	S	0.00000	0.00717	-0.07451	-0.00932	0.01741
8	C1	PX	0.00000	-0.02354	0.08946	0.01815	-0.01263
9	C1	PY	0.00000	-0.01216	0.10950	0.05654	0.11001
10	C1	PZ	-0.19480	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.55673	-0.69026	-1.35810	1.10520
12	C1	PX	0.00000	-0.64941	0.33061	0.27918	-0.27466
13	C1	PY	0.00000	1.38673	0.22291	-0.11647	1.32139
14	C1	PZ	-0.63665	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	-0.00162	-0.02128	-0.02449	0.02217
16	C1	DYY	0.00000	0.00582	0.02345	0.01821	-0.00825
17	C1	DZZ	0.00000	0.00436	-0.00798	0.00272	-0.00162
18	C1	DXY	0.00000	0.02001	0.01645	-0.00689	0.02129
19	C1	DXZ	-0.01838	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00658	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	-0.02244	-0.02253	-0.02212	-0.00468
22	C2	S	0.00000	0.03669	0.00982	0.03383	0.02920
23	C2	PX	0.00000	0.08397	-0.04145	0.00715	0.04118
24	C2	PY	0.00000	-0.06694	-0.01439	-0.04287	0.09384
25	C2	PZ	0.21091	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	0.21522	0.71437	0.59938	0.13116
27	C2	PX	0.00000	0.21485	-0.62489	-0.03552	0.20370
28	C2	PY	0.00000	-0.67785	-0.80795	0.83916	1.32769
29	C2	PZ	0.65261	0.00000	0.00000	0.00000	0.00000

30	C2	DXX	0.00000	0.00025	0.02378	0.02850	0.00840
31	C2	DYY	0.00000	-0.00394	-0.01949	-0.02359	0.01221
32	C2	DZZ	0.00000	0.00175	-0.00008	0.00102	-0.00447
33	C2	DXY	0.00000	0.01831	0.01511	-0.00962	-0.02068
34	C2	DXZ	-0.01981	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00604	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.08716	-0.03537	-0.00414	-0.03263
37	C3	S	0.00000	0.12396	0.06332	0.00244	0.07049
38	C3	PX	0.00000	0.00108	0.01474	0.21186	0.00868
39	C3	PY	0.00000	0.03647	0.15579	-0.03466	0.03092
40	C3	PZ	0.31189	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	2.05302	-0.47711	0.33672	0.45070
42	C3	PX	0.00000	0.74814	-0.02999	0.99098	-0.00143
43	C3	PY	0.00000	0.37227	0.97884	-0.23654	0.25237
44	C3	PZ	0.74677	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.02446	0.01186	0.02544	-0.01446
46	C3	DYY	0.00000	0.03159	-0.03087	-0.01488	0.02660
47	C3	DZZ	0.00000	0.00499	0.00686	-0.00464	0.00045
48	C3	DXY	0.00000	0.00614	-0.00585	-0.00418	-0.02286
49	C3	DXZ	0.01175	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00786	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.02604	0.04491	-0.00329	0.02402
52	C4	S	0.00000	-0.02176	-0.02289	-0.00148	-0.03130
53	C4	PX	0.00000	0.08967	0.14794	0.07073	-0.09141
54	C4	PY	0.00000	0.14687	0.01491	-0.07605	0.09528
55	C4	PZ	0.19442	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-1.18641	-1.06207	0.06705	-1.08840
57	C4	PX	0.00000	0.35845	1.25299	0.55265	-1.10802
58	C4	PY	0.00000	1.02308	0.12663	-0.85952	0.69293
59	C4	PZ	0.56991	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00569	0.01884	0.01331	-0.00590
61	C4	DYY	0.00000	-0.01382	-0.02080	-0.01262	-0.00060
62	C4	DZZ	0.00000	-0.00167	0.00030	-0.00331	-0.00132
63	C4	DXY	0.00000	0.00988	0.00194	-0.00993	-0.01684
64	C4	DXZ	0.00304	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.01146	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.02520	-0.04724	0.00527	0.04578
67	C5	S	0.00000	0.02597	0.01553	0.00157	-0.02041
68	C5	PX	0.00000	0.09352	0.16933	0.10098	-0.01391
69	C5	PY	0.00000	-0.06434	-0.05679	0.10564	0.08705
70	C5	PZ	-0.19384	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.70895	1.65080	-0.29851	-1.69517
72	C5	PX	0.00000	0.48677	1.17023	0.61760	0.06408
73	C5	PY	0.00000	-0.50147	-0.53671	0.85357	0.72094
74	C5	PZ	-0.58077	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	-0.01171	-0.01063	-0.00672	-0.00248
76	C5	DYY	0.00000	0.01582	0.01797	0.00674	-0.00424
77	C5	DZZ	0.00000	0.00183	-0.00113	0.00284	0.00076
78	C5	DXY	0.00000	0.00413	-0.00099	-0.00901	0.01585
79	C5	DXZ	0.00251	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.01221	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	0.07146	0.03782	-0.02752	0.00459
82	C6	S	0.00000	-0.08511	-0.08813	0.07879	0.03061
83	C6	PX	0.00000	-0.10231	0.10608	0.17000	-0.16029

84	C6	PY	0.00000	-0.10702	-0.04346	0.03679	0.15100
85	C6	PZ	-0.33580	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.96912	-0.72554	0.66524	-0.42126
87	C6	PX	0.00000	0.10435	0.72150	0.40233	-0.33823
88	C6	PY	0.00000	-0.46621	-0.38791	0.86069	1.26540
89	C6	PZ	-0.75535	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.00945	0.00395	-0.01867	0.00208
91	C6	DYY	0.00000	0.00358	-0.00597	0.02760	0.00352
92	C6	DZZ	0.00000	-0.00689	-0.00750	0.00328	-0.00634
93	C6	DXY	0.00000	-0.00347	0.01566	-0.00283	0.01525
94	C6	DXZ	0.00347	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00282	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	-0.01208	0.03305	0.02804	-0.01872
97	C7	S	0.00000	0.01324	-0.07798	-0.02182	0.07032
98	C7	PX	0.00000	-0.03399	0.09746	-0.03045	-0.02235
99	C7	PY	0.00000	-0.01820	-0.01245	-0.03860	0.10874
100	C7	PZ	-0.06172	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	0.33061	0.21031	-1.14062	0.46981
102	C7	PX	0.00000	-0.78184	0.11618	-0.19394	-1.14574
103	C7	PY	0.00000	-1.36436	1.15215	-0.29771	0.30450
104	C7	PZ	-0.40299	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00615	0.00499	-0.02960	0.00405
106	C7	DYY	0.00000	0.00418	0.00128	0.02700	0.00649
107	C7	DZZ	0.00000	0.00185	-0.00308	-0.00388	0.00260
108	C7	DXY	0.00000	-0.01964	0.01486	0.02532	-0.00110
109	C7	DXZ	-0.00480	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.02932	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	-0.01380	-0.03819	-0.04047	-0.04644
112	H3	S	0.00000	-0.92326	-0.29414	0.40242	-0.01999
113	H3	PX	0.00000	0.00913	0.00821	0.00007	-0.00955
114	H3	PY	0.00000	-0.00472	-0.00476	-0.00546	-0.00057
115	H3	PZ	0.01209	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00000	0.01978	0.03208	0.02212	-0.06799
117	H4	S	0.00000	0.50977	0.63525	-0.34260	-0.28106
118	H4	PX	0.00000	0.00766	0.00663	-0.00248	0.00561
119	H4	PY	0.00000	0.00456	0.00587	0.00197	-0.00149
120	H4	PZ	-0.01205	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00000	-0.01083	-0.00927	-0.08647	-0.06256
122	N1	S	0.00000	0.05722	-0.00298	0.08401	0.06655
123	N1	PX	0.00000	0.10929	-0.05041	0.05750	-0.00731
124	N1	PY	0.00000	0.00178	0.06922	-0.07029	0.05344
125	N1	PZ	0.14631	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00000	-0.18353	0.36997	1.96341	1.73138
127	N1	PX	0.00000	0.05469	-0.07568	0.68926	0.76048
128	N1	PY	0.00000	0.11875	0.35593	-0.36110	0.51483
129	N1	PZ	0.37853	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00000	0.00634	0.00333	-0.00525	0.00241
131	N1	DYY	0.00000	0.01162	-0.00926	-0.01474	0.01063
132	N1	DZZ	0.00000	-0.00058	-0.00355	-0.02216	-0.02015
133	N1	DXY	0.00000	-0.00044	-0.00459	0.01317	-0.00325
134	N1	DXZ	-0.00018	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	-0.02202	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.00000	0.00345	0.05863	0.08373	0.01486
137	H6	S	0.00000	0.20774	-0.71393	-0.09938	0.23437

138	H6	PX	0.00000	0.00049	-0.00741	-0.00638	-0.00276
139	H6	PY	0.00000	-0.00774	-0.00806	0.00503	0.01346
140	H6	PZ	0.01474	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00000	0.07175	-0.08607	0.05805	-0.02680
142	C8	S	0.00000	-0.03215	0.08894	-0.03719	0.10276
143	C8	PX	0.00000	-0.11134	0.08893	0.21469	-0.02264
144	C8	PY	0.00000	-0.00053	-0.01737	-0.02860	-0.12113
145	C8	PZ	0.00037	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.00000	-2.26608	2.66384	-1.88145	0.95554
147	C8	PX	0.00000	-0.95066	0.52156	1.40078	-0.03361
148	C8	PY	0.00000	0.40665	-1.23174	0.04214	-2.18970
149	C8	PZ	0.00046	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00000	0.00642	-0.00860	0.01361	-0.00508
151	C8	DYY	0.00000	-0.00882	0.01897	-0.02485	0.01774
152	C8	DZZ	0.00000	0.00274	0.00200	-0.00566	-0.00058
153	C8	DXY	0.00000	-0.01927	0.00050	-0.00828	0.00060
154	C8	DXZ	-0.02167	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00101	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00000	0.02641	0.00819	-0.12296	0.01984
157	H8	S	0.00000	0.13141	0.15173	0.32785	0.83967
158	H8	PX	0.00000	-0.00180	0.00114	-0.01034	-0.00450
159	H8	PY	0.00000	-0.00776	0.00571	-0.00068	-0.00177
160	H8	PZ	-0.00753	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00000	-0.03805	0.05039	-0.03273	0.03781
162	C10	S	0.00000	-0.00852	0.02820	-0.01110	0.07093
163	C10	PX	0.00000	-0.00349	-0.03411	-0.14969	0.00009
164	C10	PY	0.00000	-0.02790	0.03254	-0.04840	0.05233
165	C10	PZ	0.00891	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00000	1.26674	-2.04767	0.98608	-2.15973
167	C10	PX	0.00000	0.58155	-0.51526	-1.01902	-0.06662
168	C10	PY	0.00000	0.72319	-1.39967	0.71693	-1.65225
169	C10	PZ	0.00407	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00000	0.01068	-0.01586	0.01456	-0.00945
171	C10	DYY	0.00000	-0.00219	0.00148	-0.00083	0.00795
172	C10	DZZ	0.00000	-0.00887	0.01357	-0.01194	0.01007
173	C10	DXY	0.00000	0.00272	0.00872	0.03546	0.01052
174	C10	DXZ	-0.00752	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00015	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00000	-0.00506	-0.04310	-0.07049	-0.06946
177	H16	S	0.00000	-0.48389	0.37918	0.72256	-0.17885
178	H16	PX	0.00000	0.00495	-0.00517	0.00019	-0.00105
179	H16	PY	0.00000	0.00311	-0.00365	0.01382	-0.00085
180	H16	PZ	-0.00095	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00000	0.03554	-0.02216	0.10737	-0.01146
182	H18	S	0.00000	0.19138	-0.28790	-0.95919	-0.07605
183	H18	PX	0.00000	0.00076	0.00086	-0.00240	0.00198
184	H18	PY	0.00000	0.00329	-0.00699	-0.00747	-0.00941
185	H18	PZ	0.00186	0.00000	0.00000	0.00000	0.00000

MO:	51	52	53	54	55
Eigenvalues:	0.49030	0.51970	0.54355	0.60485	0.67678
(ev):	13.34168	14.14184	14.79076	16.45886	18.41607

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1	H1	S	-0.01427	-0.03883	0.10299	0.07621	0.02263
2	H1	S	0.65913	-0.05137	-0.80123	-0.26307	-0.04286
3	H1	PX	-0.00179	-0.00407	0.01031	0.00894	0.00074
4	H1	PY	-0.00558	0.00803	0.00619	-0.00094	-0.01485
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.07350	0.00307	0.01004	0.01635	0.03748
7	C1	S	0.06177	0.00404	-0.01098	-0.04092	-0.08733
8	C1	PX	-0.16840	-0.00023	0.08290	0.02372	0.09263
9	C1	PY	0.02254	0.13338	-0.07018	0.23132	0.18922
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	2.05776	-0.24854	-0.50426	0.66036	-0.57445
12	C1	PX	-1.32308	-0.00977	1.07669	0.30135	0.25775
13	C1	PY	-0.79341	1.64943	-0.63109	1.01084	-1.61620
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00152	-0.01221	0.04103	0.01635	-0.00344
16	C1	DYY	0.00678	0.00834	-0.04132	-0.00345	0.01212
17	C1	DZZ	-0.00122	-0.00082	-0.00103	-0.00645	-0.01430
18	C1	DXY	-0.01019	0.01337	0.02318	-0.00557	-0.01669
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08744	0.00462	0.01663	-0.01740	-0.01295
22	C2	S	0.06910	-0.02408	0.04397	-0.01017	0.08527
23	C2	PX	0.15913	-0.04462	-0.04015	0.02475	0.03178
24	C2	PY	0.02454	0.17089	-0.14162	0.04600	0.13851
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	2.64763	0.41942	-1.44982	0.17842	0.70070
27	C2	PX	1.45754	-0.12867	-0.95832	0.77557	-0.07870
28	C2	PY	-0.33865	1.67089	-0.64312	-1.25593	0.52442
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01871	0.00102	0.03321	-0.03486	0.04801
31	C2	DYY	-0.00943	-0.00977	-0.02164	0.02839	0.01322
32	C2	DZZ	0.00020	0.00190	-0.00322	-0.00354	-0.01474
33	C2	DXY	0.01303	-0.01263	-0.00428	0.00735	0.00139
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.07192	0.00974	0.02860	-0.07749	-0.04116
37	C3	S	-0.04278	-0.07145	0.04352	0.04383	0.01215
38	C3	PX	-0.08835	0.09417	-0.17921	-0.06520	-0.10106
39	C3	PY	-0.05524	0.19523	0.07037	-0.02752	-0.04573
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-2.04248	0.52213	-1.10102	2.83680	0.67669
42	C3	PX	-0.73525	0.78577	-1.26728	-0.28726	0.12447
43	C3	PY	-0.79744	1.39096	0.94945	-0.39230	-1.66383
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00101	-0.00962	-0.00219	0.01796	-0.00089
46	C3	DYY	0.00540	-0.00609	0.03732	-0.01097	-0.03627
47	C3	DZZ	-0.00852	0.00394	-0.00900	0.00685	0.01582
48	C3	DXY	0.00477	-0.01692	-0.01580	-0.03217	-0.03211
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.03699	0.03841	-0.00942	-0.02968	-0.02648
52	C4	S	-0.03443	-0.00534	-0.10014	0.04084	0.04666
53	C4	PX	0.15936	-0.02083	-0.03148	-0.08066	0.20663
54	C4	PY	0.03200	0.04984	0.10790	-0.04604	-0.13551

55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.95524	-1.76945	1.43224	0.64331	0.96979
57	C4	PX	0.10820	-0.21702	0.21880	-2.06549	0.60266
58	C4	PY	0.92814	0.53582	-0.56872	0.29822	-1.01452
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.02993	0.00792	-0.00590	-0.00754	0.00150
61	C4	DYY	0.02134	-0.01929	0.02224	0.00372	0.00417
62	C4	DZZ	-0.00134	0.00276	-0.01317	0.00393	-0.00059
63	C4	DXY	-0.01811	-0.02396	0.02648	-0.01712	-0.01180
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02283	0.01208	-0.00672	0.03083	0.02533
67	C5	S	-0.02948	-0.01600	-0.05464	0.02177	0.03205
68	C5	PX	-0.07994	0.08867	-0.01180	-0.19944	-0.03773
69	C5	PY	0.04274	0.05465	0.06313	-0.09646	-0.00320
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.69363	-1.07104	1.14021	-1.10059	-0.51836
72	C5	PX	0.64673	1.09997	-0.68945	-1.71537	0.65675
73	C5	PY	1.22667	0.44228	-0.65265	-0.13441	1.10596
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.03924	0.00157	-0.00335	0.00191	-0.01926
76	C5	DYY	0.03056	-0.01353	0.01800	-0.00871	0.03146
77	C5	DZZ	-0.00051	0.00003	-0.00741	0.00073	-0.00420
78	C5	DXY	0.00947	0.02829	-0.03124	0.01952	-0.01177
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.05328	-0.03661	0.08129	0.05694	0.03769
82	C6	S	-0.01967	-0.04885	0.05381	-0.07916	0.09048
83	C6	PX	0.18764	-0.04425	-0.03057	0.05270	-0.03807
84	C6	PY	-0.11615	0.07881	0.07772	0.07334	0.09536
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-1.58038	2.35462	-2.60046	-1.96479	-1.81687
87	C6	PX	0.63566	-0.61256	0.06268	-0.35854	0.62264
88	C6	PY	-1.04955	-0.16344	2.01068	-0.72264	1.98262
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.01463	-0.01739	0.02101	0.01006	0.03554
91	C6	DYY	0.02560	0.01688	0.02265	-0.03002	-0.01824
92	C6	DZZ	-0.00669	0.00692	-0.01887	-0.00525	-0.01479
93	C6	DXY	-0.00171	0.02894	0.00864	0.00756	0.03761
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.01824	0.00890	-0.04585	0.08715	0.00232
97	C7	S	0.07761	-0.04465	0.09997	-0.13183	-0.23520
98	C7	PX	-0.01396	0.05493	-0.02860	0.23037	-0.03001
99	C7	PY	0.03250	0.09474	0.15516	0.15263	-0.08748
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.07545	-0.08110	1.19192	-2.39016	-0.06388
102	C7	PX	0.76496	0.41173	0.00752	1.76302	0.04354
103	C7	PY	0.61259	0.44255	1.29911	-0.43818	-1.63376
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.02123	0.00157	0.03569	-0.01865	-0.04456
106	C7	DYY	-0.01126	-0.02055	-0.00698	-0.00053	-0.01454
107	C7	DZZ	0.00088	0.00455	-0.00472	-0.01230	-0.00298
108	C7	DXY	-0.01101	0.02891	0.00265	0.01457	0.00110

109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00711	-0.10122	0.11400	-0.03964	-0.00977
112	H3	S	-0.50993	-0.03714	-0.06424	0.34488	0.32379
113	H3	PX	-0.01818	-0.00403	0.00786	-0.01217	-0.00901
114	H3	PY	0.01037	-0.00687	0.00387	0.00195	0.00038
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.02602	-0.09449	0.10061	-0.04628	0.06360
117	H4	S	-0.44439	0.24494	-0.15707	-0.20638	-0.34633
118	H4	PX	0.01891	0.00824	-0.01045	0.00430	0.00587
119	H4	PY	0.01362	-0.00674	0.00305	0.00022	0.01481
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.02228	0.06133	-0.08276	-0.01170	0.00584
122	N1	S	0.04651	-0.02315	0.04549	0.00476	-0.01860
123	N1	PX	-0.00062	-0.07276	0.01197	0.07515	-0.14493
124	N1	PY	0.04381	0.12835	0.14395	-0.06739	0.28232
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.14259	-2.01169	2.67197	0.13945	0.58854
127	N1	PX	-0.18583	-0.73939	0.66788	-0.05580	-0.29675
128	N1	PY	-0.01099	-0.38253	0.78200	-0.00207	1.81568
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00476	-0.00067	0.00653	0.01356	-0.00056
131	N1	DYY	-0.01821	-0.01137	0.00387	-0.02093	0.04100
132	N1	DZZ	-0.00238	0.03768	-0.04988	-0.00321	-0.01273
133	N1	DXY	0.01781	-0.00948	-0.00661	-0.02618	-0.01922
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.04367	0.00382	0.07110	-0.12393	0.11181
137	H6	S	0.59411	-0.17236	-0.52972	0.39123	-0.17694
138	H6	PX	-0.00128	-0.00041	-0.00757	0.01284	-0.01239
139	H6	PY	-0.00813	0.00467	0.00335	-0.00799	0.00495
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.02609	-0.02933	0.02608	-0.04696	-0.04975
142	C8	S	-0.04201	-0.02565	0.12892	0.05560	-0.06999
143	C8	PX	0.08527	0.06016	0.02942	0.09293	-0.35871
144	C8	PY	-0.01766	0.23805	0.13554	0.15765	0.16002
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.20217	-0.87336	-1.81052	0.64377	0.68897
147	C8	PX	0.55610	-0.13349	0.76425	1.41909	-2.01277
148	C8	PY	0.13151	2.87915	0.98822	1.28746	0.28063
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.00495	-0.02009	-0.00486	-0.00558	-0.02052
151	C8	DYY	0.03447	-0.03555	0.02023	-0.01773	-0.05226
152	C8	DZZ	-0.00802	0.01797	0.00051	0.01688	0.02682
153	C8	DXY	0.00745	0.00436	0.01138	-0.04858	0.01696
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.02982	0.00081	0.02173	-0.01617	-0.10895
157	H8	S	-0.43863	-0.08131	0.02113	-0.76945	-0.34375
158	H8	PX	0.00627	0.00537	0.00725	0.00138	-0.00821
159	H8	PY	0.00107	0.01832	0.00665	0.00194	-0.01240
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.00872	-0.03329	-0.03234	-0.00186	0.00353
162	C10	S	0.06738	-0.10696	0.05772	-0.09036	-0.18689

163	C10	PX	0.01291	0.02814	0.02298	-0.13784	-0.08461
164	C10	PY	0.10221	-0.07966	0.09318	-0.09325	-0.16797
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.09196	2.55093	1.12400	0.93862	0.18108
167	C10	PX	-0.34665	0.23721	-0.21923	-0.54354	1.13862
168	C10	PY	0.22986	2.06353	1.52188	0.74524	0.07089
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00556	0.00709	0.02336	0.00673	-0.03029
171	C10	DYY	-0.00882	-0.00140	-0.00240	-0.00973	-0.01333
172	C10	DZZ	0.00532	-0.00772	-0.00388	-0.00467	0.00089
173	C10	DXY	0.00052	-0.01686	0.00238	0.06286	-0.03737
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.01826	0.11310	0.06227	-0.14365	0.02553
177	H16	S	0.40690	0.18864	0.56184	0.59776	-0.71765
178	H16	PX	-0.00078	0.00080	0.00418	0.00315	0.00502
179	H16	PY	0.00265	-0.00269	0.00703	0.01687	-0.00467
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.00361	0.01194	0.07839	0.19555	-0.04932
182	H18	S	-0.05706	0.32387	0.25862	-0.44740	0.65254
183	H18	PX	-0.00321	-0.00304	-0.00510	0.00127	0.01650
184	H18	PY	0.00184	0.01122	-0.00218	-0.01648	0.00925
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

M0:	56	57	58	59	60
Eigenvalues:	0.69523	0.71512	0.73307	0.74791	0.76776
(ev):	18.91831	19.45933	19.94784	20.35166	20.89194

			A	A	A	A	A
1	H1	S	0.06892	0.05056	0.00000	0.14966	0.00000
2	H1	S	0.29864	-0.17617	0.00000	0.08336	0.00000
3	H1	PX	-0.00441	-0.00809	0.00000	0.01080	0.00000
4	H1	PY	-0.00333	-0.00225	0.00000	-0.00042	0.00000
5	H1	PZ	0.00000	0.00000	-0.00573	0.00000	0.00050
6	C1	S	-0.01403	-0.02018	0.00000	0.00099	0.00000
7	C1	S	-0.04470	-0.37082	0.00000	0.32524	0.00000
8	C1	PX	0.07418	0.14509	0.00000	-0.04744	0.00000
9	C1	PY	-0.28108	0.25823	0.00000	0.01106	0.00000
10	C1	PZ	0.00000	0.00000	-0.44924	0.00000	-0.14109
11	C1	S	0.02882	1.04424	0.00000	-0.29038	0.00000
12	C1	PX	-0.66667	-0.29101	0.00000	-0.21613	0.00000
13	C1	PY	1.41642	-0.24273	0.00000	1.16566	0.00000
14	C1	PZ	0.00000	0.00000	0.35965	0.00000	0.11240
15	C1	DXX	0.01206	-0.01105	0.00000	0.06760	0.00000
16	C1	DYY	-0.03354	-0.06484	0.00000	0.03000	0.00000
17	C1	DZZ	0.00899	-0.00591	0.00000	-0.00817	0.00000
18	C1	DXY	-0.01461	0.00522	0.00000	-0.00759	0.00000
19	C1	DXZ	0.00000	0.00000	0.02022	0.00000	0.01220
20	C1	DYZ	0.00000	0.00000	-0.01264	0.00000	-0.01092
21	C2	S	-0.03210	0.02347	0.00000	0.07388	0.00000
22	C2	S	-0.15177	-0.36041	0.00000	0.15407	0.00000
23	C2	PX	-0.05113	-0.22547	0.00000	-0.12185	0.00000
24	C2	PY	-0.09471	0.12163	0.00000	0.32697	0.00000
25	C2	PZ	0.00000	0.00000	-0.32660	0.00000	-0.30425

26	C2	S	0.65352	-0.07583	0.00000	-1.41985	0.00000
27	C2	PX	0.07358	0.02490	0.00000	-1.00155	0.00000
28	C2	PY	-1.03628	-0.14639	0.00000	-2.08684	0.00000
29	C2	PZ	0.00000	0.00000	0.23266	0.00000	0.26924
30	C2	DXX	0.01293	-0.02333	0.00000	0.07699	0.00000
31	C2	DYY	-0.07004	-0.03746	0.00000	0.05271	0.00000
32	C2	DZZ	0.00862	-0.00710	0.00000	-0.04883	0.00000
33	C2	DXY	-0.02542	0.02100	0.00000	-0.00095	0.00000
34	C2	DXZ	0.00000	0.00000	-0.01851	0.00000	-0.01468
35	C2	DYZ	0.00000	0.00000	-0.00779	0.00000	-0.02025
36	C3	S	0.05490	-0.00482	0.00000	0.06761	0.00000
37	C3	S	-0.14849	-0.45192	0.00000	0.21847	0.00000
38	C3	PX	0.32751	-0.04370	0.00000	0.17688	0.00000
39	C3	PY	-0.17304	-0.03228	0.00000	0.02240	0.00000
40	C3	PZ	0.00000	0.00000	-0.34603	0.00000	-0.04261
41	C3	S	-0.07984	-0.65097	0.00000	-2.41115	0.00000
42	C3	PX	1.95298	-0.47332	0.00000	1.43583	0.00000
43	C3	PY	0.08630	0.68031	0.00000	1.69180	0.00000
44	C3	PZ	0.00000	0.00000	0.15968	0.00000	0.05153
45	C3	DXX	-0.00797	-0.09252	0.00000	0.06114	0.00000
46	C3	DYY	0.04051	-0.07811	0.00000	0.03308	0.00000
47	C3	DZZ	-0.02855	0.01924	0.00000	-0.03093	0.00000
48	C3	DXY	-0.01516	-0.06829	0.00000	-0.03322	0.00000
49	C3	DXZ	0.00000	0.00000	-0.00453	0.00000	0.01001
50	C3	DYZ	0.00000	0.00000	0.01808	0.00000	-0.02396
51	C4	S	-0.01808	0.02570	0.00000	0.01678	0.00000
52	C4	S	-0.13015	-0.30800	0.00000	0.23331	0.00000
53	C4	PX	-0.10496	0.17869	0.00000	0.00895	0.00000
54	C4	PY	0.13259	0.09501	0.00000	-0.02082	0.00000
55	C4	PZ	0.00000	0.00000	-0.36051	0.00000	-0.32562
56	C4	S	-0.24751	-0.26206	0.00000	-0.97401	0.00000
57	C4	PX	-0.73060	-0.05359	0.00000	-0.74892	0.00000
58	C4	PY	0.29531	0.54445	0.00000	0.88838	0.00000
59	C4	PZ	0.00000	0.00000	0.24528	0.00000	0.24418
60	C4	DXX	-0.04454	-0.05579	0.00000	-0.00217	0.00000
61	C4	DYY	-0.01114	0.00241	0.00000	0.05601	0.00000
62	C4	DZZ	0.00818	-0.00683	0.00000	-0.00964	0.00000
63	C4	DXY	0.03905	0.01344	0.00000	0.02137	0.00000
64	C4	DXZ	0.00000	0.00000	-0.00517	0.00000	0.00839
65	C4	DYZ	0.00000	0.00000	0.02606	0.00000	0.01110
66	C5	S	0.02214	-0.02895	0.00000	-0.01305	0.00000
67	C5	S	-0.27542	-0.24873	0.00000	0.34811	0.00000
68	C5	PX	-0.04278	-0.15727	0.00000	-0.22806	0.00000
69	C5	PY	0.21112	0.00165	0.00000	-0.22001	0.00000
70	C5	PZ	0.00000	0.00000	-0.36154	0.00000	-0.34296
71	C5	S	0.35755	0.68699	0.00000	1.22494	0.00000
72	C5	PX	-0.87559	0.33335	0.00000	-0.49337	0.00000
73	C5	PY	-0.50887	-0.37321	0.00000	-1.24425	0.00000
74	C5	PZ	0.00000	0.00000	0.24772	0.00000	0.26389
75	C5	DXX	-0.01464	-0.06171	0.00000	0.05145	0.00000
76	C5	DYY	0.00199	-0.02451	0.00000	0.06159	0.00000
77	C5	DZZ	-0.01909	0.00915	0.00000	-0.01277	0.00000
78	C5	DXY	-0.02784	-0.01906	0.00000	-0.00284	0.00000
79	C5	DXZ	0.00000	0.00000	0.00112	0.00000	-0.00556

80	C5	DYZ	0.00000	0.00000	0.01626	0.00000	0.02354
81	C6	S	-0.00545	-0.02806	0.00000	-0.07742	0.00000
82	C6	S	-0.25122	-0.37212	0.00000	0.41437	0.00000
83	C6	PX	0.23921	-0.19009	0.00000	0.13340	0.00000
84	C6	PY	-0.00234	-0.16428	0.00000	0.09667	0.00000
85	C6	PZ	0.00000	0.00000	-0.37678	0.00000	-0.02906
86	C6	S	0.64720	1.16243	0.00000	0.38987	0.00000
87	C6	PX	2.14425	-0.47071	0.00000	1.84528	0.00000
88	C6	PY	-0.40261	-0.56908	0.00000	0.08168	0.00000
89	C6	PZ	0.00000	0.00000	0.26801	0.00000	-0.03171
90	C6	DXX	-0.08061	-0.06455	0.00000	0.01949	0.00000
91	C6	DYY	0.02771	-0.05692	0.00000	-0.01811	0.00000
92	C6	DZZ	-0.00226	0.01152	0.00000	0.03604	0.00000
93	C6	DXY	0.00708	0.05822	0.00000	0.03933	0.00000
94	C6	DXZ	0.00000	0.00000	0.00362	0.00000	-0.00944
95	C6	DYZ	0.00000	0.00000	0.00235	0.00000	-0.00790
96	C7	S	0.02385	-0.04428	0.00000	-0.03626	0.00000
97	C7	S	-0.02775	-0.19028	0.00000	0.13394	0.00000
98	C7	PX	0.19257	-0.11429	0.00000	0.01039	0.00000
99	C7	PY	0.35878	-0.01965	0.00000	0.22222	0.00000
100	C7	PZ	0.00000	0.00000	-0.38102	0.00000	0.44797
101	C7	S	-0.25804	1.31888	0.00000	1.96468	0.00000
102	C7	PX	-0.42660	-0.47791	0.00000	-1.66957	0.00000
103	C7	PY	-1.53831	0.83158	0.00000	0.46757	0.00000
104	C7	PZ	0.00000	0.00000	0.32958	0.00000	-0.36572
105	C7	DXX	-0.00045	-0.09515	0.00000	-0.00560	0.00000
106	C7	DYY	-0.00598	-0.00290	0.00000	0.03864	0.00000
107	C7	DZZ	-0.00078	0.02886	0.00000	0.00185	0.00000
108	C7	DXY	0.00448	0.02512	0.00000	0.04831	0.00000
109	C7	DXZ	0.00000	0.00000	0.02057	0.00000	-0.00896
110	C7	DYZ	0.00000	0.00000	-0.02121	0.00000	0.00369
111	H3	S	0.06727	0.08680	0.00000	0.12979	0.00000
112	H3	S	-0.09535	-0.37471	0.00000	-0.23099	0.00000
113	H3	PX	0.00731	-0.00969	0.00000	-0.00126	0.00000
114	H3	PY	-0.00761	0.00602	0.00000	0.01429	0.00000
115	H3	PZ	0.00000	0.00000	-0.00284	0.00000	-0.00423
116	H4	S	0.13939	0.00026	0.00000	0.13184	0.00000
117	H4	S	-0.23477	0.09087	0.00000	0.38212	0.00000
118	H4	PX	-0.00457	0.01121	0.00000	0.00336	0.00000
119	H4	PY	-0.00095	-0.00452	0.00000	0.01497	0.00000
120	H4	PZ	0.00000	0.00000	-0.00549	0.00000	-0.00087
121	N1	S	0.02136	0.00883	0.00000	0.00057	0.00000
122	N1	S	-0.01846	0.02293	0.00000	-0.09993	0.00000
123	N1	PX	-0.04600	0.14551	0.00000	0.03780	0.00000
124	N1	PY	0.15291	-0.08275	0.00000	-0.05563	0.00000
125	N1	PZ	0.00000	0.00000	-0.07137	0.00000	0.09813
126	N1	S	-1.13260	-0.24592	0.00000	0.78941	0.00000
127	N1	PX	-0.99834	0.28230	0.00000	0.07155	0.00000
128	N1	PY	0.91179	-0.83174	0.00000	0.35523	0.00000
129	N1	PZ	0.00000	0.00000	-0.00110	0.00000	0.01559
130	N1	DXX	-0.00846	-0.01597	0.00000	-0.03430	0.00000
131	N1	DYY	-0.05156	0.02652	0.00000	0.01989	0.00000
132	N1	DZZ	0.03709	0.02474	0.00000	-0.03030	0.00000
133	N1	DXY	0.02937	-0.01309	0.00000	-0.00167	0.00000

134	N1	DXZ	0.00000	0.00000	-0.01499	0.00000	0.00211
135	N1	DYZ	0.00000	0.00000	-0.02203	0.00000	0.00198
136	H6	S	0.05115	0.05757	0.00000	0.25880	0.00000
137	H6	S	-0.23537	-0.09977	0.00000	-0.51264	0.00000
138	H6	PX	0.00344	0.00853	0.00000	-0.02297	0.00000
139	H6	PY	0.00654	-0.00862	0.00000	-0.00749	0.00000
140	H6	PZ	0.00000	0.00000	-0.00306	0.00000	-0.00292
141	C8	S	-0.04494	0.02663	0.00000	-0.00946	0.00000
142	C8	S	-0.23694	-0.16566	0.00000	0.01794	0.00000
143	C8	PX	0.02283	-0.03799	0.00000	0.05385	0.00000
144	C8	PY	-0.00383	-0.07629	0.00000	0.06709	0.00000
145	C8	PZ	0.00000	0.00000	-0.20391	0.00000	0.34340
146	C8	S	1.28181	-0.27566	0.00000	-0.64381	0.00000
147	C8	PX	-1.73367	0.53535	0.00000	-0.62412	0.00000
148	C8	PY	0.47013	-1.16125	0.00000	-1.29958	0.00000
149	C8	PZ	0.00000	0.00000	0.07960	0.00000	-0.24746
150	C8	DXX	-0.07507	0.01844	0.00000	0.01227	0.00000
151	C8	DYY	-0.01102	-0.05602	0.00000	-0.05302	0.00000
152	C8	DZZ	0.02481	-0.00964	0.00000	0.01249	0.00000
153	C8	DXY	-0.04193	-0.00375	0.00000	-0.00765	0.00000
154	C8	DXZ	0.00000	0.00000	-0.00908	0.00000	0.00687
155	C8	DYZ	0.00000	0.00000	0.01088	0.00000	-0.03428
156	H8	S	0.05962	-0.27197	0.00000	-0.12523	0.00000
157	H8	S	-0.05290	0.46387	0.00000	0.88067	0.00000
158	H8	PX	0.00253	-0.01863	0.00000	-0.00710	0.00000
159	H8	PY	0.00156	0.00543	0.00000	0.01025	0.00000
160	H8	PZ	0.00000	0.00000	-0.00396	0.00000	0.00900
161	C10	S	0.00420	0.00110	0.00000	0.00193	0.00000
162	C10	S	-0.18237	-0.05450	0.00000	-0.12835	0.00000
163	C10	PX	-0.12790	-0.00977	0.00000	-0.00636	0.00000
164	C10	PY	-0.03164	-0.10597	0.00000	-0.19341	0.00000
165	C10	PZ	0.00000	0.00000	-0.27598	0.00000	0.68377
166	C10	S	0.23300	-0.59333	0.00000	-0.57581	0.00000
167	C10	PX	0.75928	-0.16293	0.00000	0.15531	0.00000
168	C10	PY	-0.46811	-0.28653	0.00000	-0.15194	0.00000
169	C10	PZ	0.00000	0.00000	0.25610	0.00000	-0.61444
170	C10	DXX	-0.04765	-0.00388	0.00000	-0.01726	0.00000
171	C10	DYY	-0.01909	-0.00160	0.00000	-0.00979	0.00000
172	C10	DZZ	0.01287	-0.00524	0.00000	-0.00546	0.00000
173	C10	DXY	0.02128	0.00131	0.00000	-0.00196	0.00000
174	C10	DXZ	0.00000	0.00000	0.00207	0.00000	-0.00237
175	C10	DYZ	0.00000	0.00000	-0.01807	0.00000	0.03120
176	H16	S	-0.15906	-0.02875	0.00000	0.00884	0.00000
177	H16	S	-0.44672	-0.00905	0.00000	-0.12542	0.00000
178	H16	PX	-0.00208	-0.00307	0.00000	-0.00782	0.00000
179	H16	PY	-0.00531	0.00737	0.00000	0.00230	0.00000
180	H16	PZ	0.00000	0.00000	-0.00309	0.00000	0.00971
181	H18	S	-0.04325	0.00760	0.00000	-0.01869	0.00000
182	H18	S	0.10096	-0.15283	0.00000	0.03448	0.00000
183	H18	PX	0.01341	0.00378	0.00000	0.00668	0.00000
184	H18	PY	0.00313	0.00415	0.00000	0.00689	0.00000
185	H18	PZ	0.00000	0.00000	-0.00523	0.00000	0.01258

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Eigenvalues:	0.76851	0.78593	0.79889	0.80783	0.82464
(ev):	20.91219	21.38635	21.73883	21.98228	22.43952

		A	A	A	A	A	
1	H1	S	0.05991	-0.11608	0.29890	0.00000	0.01014
2	H1	S	-0.12974	0.02067	0.14356	0.00000	0.10166
3	H1	PX	0.00120	-0.01357	0.02172	0.00000	0.00253
4	H1	PY	0.00949	-0.00180	-0.00779	0.00000	0.00281
5	H1	PZ	0.00000	0.00000	0.00000	-0.00107	0.00000
6	C1	S	0.03518	0.01230	0.05679	0.00000	0.00030
7	C1	S	-0.21685	-0.34114	0.33078	0.00000	0.24981
8	C1	PX	0.15041	0.12373	0.07385	0.00000	-0.07491
9	C1	PY	0.26805	-0.18307	0.21346	0.00000	0.18075
10	C1	PZ	0.00000	0.00000	0.00000	-0.58788	0.00000
11	C1	S	0.67258	-0.09028	-0.64051	0.00000	-0.05614
12	C1	PX	-0.17656	0.02005	-0.04877	0.00000	-0.11725
13	C1	PY	2.03758	0.24443	-0.41225	0.00000	0.69911
14	C1	PZ	0.00000	0.00000	0.00000	0.59310	0.00000
15	C1	DXX	-0.00156	-0.06352	0.09283	0.00000	0.02034
16	C1	DYY	0.01995	-0.01416	0.09836	0.00000	0.03849
17	C1	DZZ	-0.03213	0.00360	-0.04732	0.00000	-0.00515
18	C1	DXY	0.00483	-0.03832	-0.01021	0.00000	0.01545
19	C1	DXZ	0.00000	0.00000	0.00000	0.03802	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.00590	0.00000
21	C2	S	-0.02432	0.01250	-0.01235	0.00000	0.00038
22	C2	S	0.23309	-0.13136	-0.44045	0.00000	-0.00872
23	C2	PX	0.14915	-0.08899	-0.14426	0.00000	0.02245
24	C2	PY	-0.20283	0.37291	-0.04284	0.00000	0.11482
25	C2	PZ	0.00000	0.00000	0.00000	0.52192	0.00000
26	C2	S	-0.95006	0.51333	0.51529	0.00000	-0.50906
27	C2	PX	-0.26676	0.06782	0.15930	0.00000	-0.53367
28	C2	PY	-2.09369	-0.56957	0.25999	0.00000	-0.70642
29	C2	PZ	0.00000	0.00000	0.00000	-0.45809	0.00000
30	C2	DXX	0.01495	0.00506	-0.05273	0.00000	0.00287
31	C2	DYY	-0.01207	0.00797	-0.07586	0.00000	-0.03393
32	C2	DZZ	0.02464	-0.02008	0.00905	0.00000	0.00424
33	C2	DXY	0.00348	-0.01290	0.00779	0.00000	-0.03250
34	C2	DXZ	0.00000	0.00000	0.00000	0.03776	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.01545	0.00000
36	C3	S	-0.04843	0.00073	-0.02539	0.00000	0.02110
37	C3	S	0.02213	-0.11342	0.30004	0.00000	-0.34889
38	C3	PX	0.15506	0.22695	0.32955	0.00000	0.16207
39	C3	PY	0.21968	-0.13916	-0.00934	0.00000	0.26772
40	C3	PZ	0.00000	0.00000	0.00000	-0.17567	0.00000
41	C3	S	-0.13548	0.83370	0.37374	0.00000	-0.37391
42	C3	PX	2.01321	0.46891	-0.22206	0.00000	0.79824
43	C3	PY	0.65258	-0.32778	-0.28075	0.00000	0.51970
44	C3	PZ	0.00000	0.00000	0.00000	0.05192	0.00000
45	C3	DXX	-0.01428	0.03113	0.04425	0.00000	-0.03397
46	C3	DYY	-0.06752	-0.02452	0.00152	0.00000	-0.03018
47	C3	DZZ	0.03503	-0.01532	0.00423	0.00000	-0.00536
48	C3	DXY	-0.00181	0.00882	-0.02496	0.00000	-0.00983
49	C3	DXZ	0.00000	0.00000	0.00000	-0.00633	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.00382	0.00000

51	C4	S	-0.03276	-0.06260	0.02417	0.00000	0.03767
52	C4	S	0.14778	-0.21561	0.16713	0.00000	0.36071
53	C4	PX	-0.17058	-0.10221	0.47489	0.00000	-0.05910
54	C4	PY	-0.06217	-0.05891	-0.15641	0.00000	0.00090
55	C4	PZ	0.00000	0.00000	0.00000	-0.13304	0.00000
56	C4	S	-0.23467	0.48432	-0.01888	0.00000	-0.94272
57	C4	PX	-2.25359	0.10827	-0.43034	0.00000	-0.53566
58	C4	PY	0.87726	-0.26304	0.08399	0.00000	0.56644
59	C4	PZ	0.00000	0.00000	0.00000	0.15664	0.00000
60	C4	DXX	-0.00410	-0.09848	0.05014	0.00000	0.08308
61	C4	DYY	-0.01067	-0.08195	0.03831	0.00000	0.06555
62	C4	DZZ	0.02544	0.05163	-0.03002	0.00000	-0.02827
63	C4	DXY	-0.00859	-0.00233	0.02950	0.00000	-0.01393
64	C4	DXZ	0.00000	0.00000	0.00000	-0.02396	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.04343	0.00000
66	C5	S	0.03643	0.03050	-0.03962	0.00000	0.00419
67	C5	S	-0.11399	-0.20239	-0.17951	0.00000	0.21878
68	C5	PX	-0.18873	-0.35786	0.19478	0.00000	0.18830
69	C5	PY	0.03706	-0.07840	0.09287	0.00000	0.09043
70	C5	PZ	0.00000	0.00000	0.00000	0.34910	0.00000
71	C5	S	0.31822	0.18796	0.00758	0.00000	0.20500
72	C5	PX	-2.17471	0.26392	-0.09872	0.00000	-0.58656
73	C5	PY	-1.09997	0.38681	-0.10993	0.00000	-0.82696
74	C5	PZ	0.00000	0.00000	0.00000	-0.36986	0.00000
75	C5	DXX	0.01048	0.01401	-0.08805	0.00000	0.04865
76	C5	DYY	0.02344	-0.01159	-0.03673	0.00000	0.04422
77	C5	DZZ	-0.02968	-0.02197	0.03535	0.00000	-0.01261
78	C5	DXY	-0.01620	0.01461	-0.01332	0.00000	0.02549
79	C5	DXZ	0.00000	0.00000	0.00000	-0.00789	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.04401	0.00000
81	C6	S	0.04094	-0.03681	-0.01770	0.00000	-0.01616
82	C6	S	0.02709	-0.07084	-0.21298	0.00000	-0.31150
83	C6	PX	0.10103	0.16601	0.08935	0.00000	0.21875
84	C6	PY	-0.23438	0.17793	-0.06928	0.00000	0.27008
85	C6	PZ	0.00000	0.00000	0.00000	0.19291	0.00000
86	C6	S	-0.35749	-0.21110	0.39940	0.00000	0.56985
87	C6	PX	2.16678	0.35271	-0.29014	0.00000	0.75836
88	C6	PY	0.06968	0.05423	-0.06311	0.00000	0.00004
89	C6	PZ	0.00000	0.00000	0.00000	-0.16094	0.00000
90	C6	DXX	0.00014	-0.04478	-0.04952	0.00000	-0.07967
91	C6	DYY	0.06388	-0.03907	-0.02456	0.00000	-0.00960
92	C6	DZZ	-0.02595	0.02545	0.00944	0.00000	0.01055
93	C6	DXY	-0.00708	0.03447	0.01812	0.00000	0.00545
94	C6	DXZ	0.00000	0.00000	0.00000	-0.01418	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00633	0.00000
96	C7	S	-0.00847	0.02062	0.04291	0.00000	-0.07327
97	C7	S	-0.02395	0.32289	0.31458	0.00000	-0.21496
98	C7	PX	-0.08102	-0.12998	-0.00519	0.00000	-0.09502
99	C7	PY	-0.37477	-0.16599	-0.03836	0.00000	-0.09360
100	C7	PZ	0.00000	0.00000	0.00000	-0.37253	0.00000
101	C7	S	0.45781	-0.96314	-0.93216	0.00000	1.37585
102	C7	PX	-1.12290	0.09062	0.17322	0.00000	-0.83369
103	C7	PY	-0.05217	-0.66754	-0.44091	0.00000	-0.02639
104	C7	PZ	0.00000	0.00000	0.00000	0.45915	0.00000

105	C7	DXX	-0.01951	0.06174	0.06971	0.00000	-0.08984
106	C7	DYY	0.01966	0.04396	0.06946	0.00000	-0.07757
107	C7	DZZ	0.01182	-0.00930	-0.02655	0.00000	0.05414
108	C7	DXY	0.02986	-0.01744	-0.00031	0.00000	-0.00523
109	C7	DXZ	0.00000	0.00000	0.00000	0.02397	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.00462	0.00000
111	H3	S	-0.07233	-0.26365	0.20688	0.00000	0.12707
112	H3	S	0.28680	0.10060	0.01279	0.00000	0.01806
113	H3	PX	-0.01079	-0.01072	0.00341	0.00000	0.00650
114	H3	PY	0.00062	-0.01843	0.01285	0.00000	0.01273
115	H3	PZ	0.00000	0.00000	0.00000	0.00736	0.00000
116	H4	S	0.10487	0.03775	-0.10384	0.00000	0.02256
117	H4	S	-0.29569	-0.12719	-0.01740	0.00000	0.26542
118	H4	PX	-0.01109	0.00634	0.01296	0.00000	-0.00227
119	H4	PY	0.00297	0.00551	-0.00784	0.00000	0.00004
120	H4	PZ	0.00000	0.00000	0.00000	-0.00496	0.00000
121	N1	S	-0.00680	-0.00637	0.00814	0.00000	-0.01573
122	N1	S	0.03420	-0.01260	-0.03536	0.00000	0.06548
123	N1	PX	0.11476	0.00270	0.00582	0.00000	0.04804
124	N1	PY	0.17776	-0.07229	0.02057	0.00000	-0.08110
125	N1	PZ	0.00000	0.00000	0.00000	0.13991	0.00000
126	N1	S	0.25704	0.28200	-0.24964	0.00000	-0.12299
127	N1	PX	-0.42401	-0.01856	-0.04361	0.00000	-0.27302
128	N1	PY	0.45209	0.36673	-0.13182	0.00000	0.57814
129	N1	PZ	0.00000	0.00000	0.00000	-0.04811	0.00000
130	N1	DXX	-0.01365	0.01799	-0.00087	0.00000	0.03370
131	N1	DYY	-0.00675	-0.00684	-0.01325	0.00000	-0.05185
132	N1	DZZ	-0.00883	-0.01702	-0.00446	0.00000	0.03299
133	N1	DXY	0.04645	-0.02843	-0.00342	0.00000	-0.01304
134	N1	DXZ	0.00000	0.00000	0.00000	0.02228	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.01015	0.00000
136	H6	S	-0.01219	0.04159	-0.05781	0.00000	-0.03581
137	H6	S	-0.00984	-0.08132	-0.11236	0.00000	-0.32330
138	H6	PX	-0.00139	-0.00239	0.01533	0.00000	0.00079
139	H6	PY	-0.00615	-0.00417	0.00364	0.00000	0.00101
140	H6	PZ	0.00000	0.00000	0.00000	0.00086	0.00000
141	C8	S	0.02530	0.03682	0.00070	0.00000	0.06703
142	C8	S	-0.05389	0.50258	0.34689	0.00000	-0.13366
143	C8	PX	0.15586	-0.12928	0.09555	0.00000	-0.36102
144	C8	PY	-0.05744	0.04710	0.04662	0.00000	-0.08220
145	C8	PZ	0.00000	0.00000	0.00000	0.16039	0.00000
146	C8	S	-0.18596	-1.02517	-0.47459	0.00000	-0.51090
147	C8	PX	-1.09166	-0.19790	-0.10899	0.00000	-0.66399
148	C8	PY	-0.34133	0.33978	0.26550	0.00000	0.13407
149	C8	PZ	0.00000	0.00000	0.00000	-0.22468	0.00000
150	C8	DXX	0.02613	0.06572	0.03360	0.00000	-0.01821
151	C8	DYY	0.01399	0.09046	0.03951	0.00000	0.06569
152	C8	DZZ	-0.01855	-0.01671	0.00292	0.00000	-0.03456
153	C8	DXY	0.01417	0.02237	0.00703	0.00000	-0.00203
154	C8	DXZ	0.00000	0.00000	0.00000	-0.02153	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	-0.03083	0.00000
156	H8	S	-0.03991	0.14197	0.21492	0.00000	-0.23416
157	H8	S	0.67699	-0.08312	-0.08339	0.00000	0.36346
158	H8	PX	-0.00998	0.00958	0.01275	0.00000	-0.02520

159	H8	PY	0.00609	-0.01824	-0.01772	0.00000	0.00061
160	H8	PZ	0.00000	0.00000	0.00000	-0.00007	0.00000
161	C10	S	-0.00641	0.00398	0.00904	0.00000	-0.02119
162	C10	S	0.04377	0.39121	0.17676	0.00000	0.27140
163	C10	PX	0.13453	0.00494	0.04535	0.00000	-0.16104
164	C10	PY	0.02747	0.19926	0.02907	0.00000	0.37758
165	C10	PZ	0.00000	0.00000	0.00000	0.34115	0.00000
166	C10	S	-0.24455	-0.17521	-0.04456	0.00000	-0.05458
167	C10	PX	-0.03174	0.17312	-0.08448	0.00000	0.83573
168	C10	PY	-0.20942	0.17637	0.15154	0.00000	-0.30384
169	C10	PZ	0.00000	0.00000	0.00000	-0.30962	0.00000
170	C10	DXX	-0.01142	0.06902	0.03575	0.00000	0.01958
171	C10	DYY	0.00155	0.03582	0.02595	0.00000	-0.00213
172	C10	DZZ	0.00465	-0.00774	-0.00954	0.00000	0.02194
173	C10	DXY	-0.05385	-0.01824	-0.01393	0.00000	-0.00442
174	C10	DXZ	0.00000	0.00000	0.00000	0.00760	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.01940	0.00000
176	H16	S	0.16347	0.14141	0.12804	0.00000	-0.11169
177	H16	S	-0.15679	-0.03245	0.04932	0.00000	-0.38744
178	H16	PX	-0.01158	0.01554	0.00217	0.00000	0.02350
179	H16	PY	-0.01642	-0.00629	-0.00842	0.00000	-0.00004
180	H16	PZ	0.00000	0.00000	0.00000	0.00567	0.00000
181	H18	S	-0.21554	0.10435	0.02761	0.00000	0.05325
182	H18	S	0.08728	0.25657	0.03090	0.00000	0.42769
183	H18	PX	-0.00379	-0.01009	-0.00833	0.00000	0.00776
184	H18	PY	0.01935	-0.00598	0.00054	0.00000	-0.00079
185	H18	PZ	0.00000	0.00000	0.00000	0.00229	0.00000

MO:	66	67	68	69	70
Eigenvalues:	0.83599	0.83701	0.87468	0.88089	0.89452
(ev):	22.74835	22.77633	23.80135	23.97035	24.34108

		A	A	A	A	A	
1	H1	S	0.00000	0.20055	0.00000	0.14232	0.00000
2	H1	S	0.00000	-0.11086	0.00000	-0.14291	0.00000
3	H1	PX	0.00000	0.00531	0.00000	0.01066	0.00000
4	H1	PY	0.00000	0.00166	0.00000	-0.00683	0.00000
5	H1	PZ	-0.00546	0.00000	0.00406	0.00000	-0.00071
6	C1	S	0.00000	0.02281	0.00000	0.05224	0.00000
7	C1	S	0.00000	-0.10687	0.00000	-0.02612	0.00000
8	C1	PX	0.00000	0.15149	0.00000	0.11407	0.00000
9	C1	PY	0.00000	0.07182	0.00000	-0.09651	0.00000
10	C1	PZ	0.16669	0.00000	-0.01395	0.00000	0.52113
11	C1	S	0.00000	-0.28064	0.00000	-0.50442	0.00000
12	C1	PX	0.00000	-0.00263	0.00000	0.27558	0.00000
13	C1	PY	0.00000	-0.99505	0.00000	-0.31963	0.00000
14	C1	PZ	-0.15049	0.00000	-0.07650	0.00000	-0.73907
15	C1	DXX	0.00000	0.03634	0.00000	0.03473	0.00000
16	C1	DYY	0.00000	-0.02185	0.00000	0.06406	0.00000
17	C1	DZZ	0.00000	-0.02489	0.00000	-0.04050	0.00000
18	C1	DXY	0.00000	0.01447	0.00000	-0.01660	0.00000
19	C1	DXZ	-0.02963	0.00000	0.01591	0.00000	-0.01003
20	C1	DYZ	0.03202	0.00000	0.00543	0.00000	-0.01361
21	C2	S	0.00000	-0.00282	0.00000	0.05035	0.00000

22	C2	S	0.00000	0.32734	0.00000	0.04501	0.00000
23	C2	PX	0.00000	-0.02360	0.00000	-0.09239	0.00000
24	C2	PY	0.00000	0.20807	0.00000	-0.10213	0.00000
25	C2	PZ	-0.27576	0.00000	0.17101	0.00000	0.55619
26	C2	S	0.00000	0.54544	0.00000	-0.33323	0.00000
27	C2	PX	0.00000	0.83284	0.00000	-0.17832	0.00000
28	C2	PY	0.00000	1.53212	0.00000	0.20514	0.00000
29	C2	PZ	0.26295	0.00000	-0.27645	0.00000	-0.80710
30	C2	DXX	0.00000	0.06294	0.00000	0.03290	0.00000
31	C2	DYY	0.00000	0.03194	0.00000	0.08164	0.00000
32	C2	DZZ	0.00000	-0.00554	0.00000	-0.03814	0.00000
33	C2	DXY	0.00000	-0.01728	0.00000	0.01187	0.00000
34	C2	DXZ	-0.01613	0.00000	0.03340	0.00000	0.00266
35	C2	DYZ	0.02251	0.00000	0.03468	0.00000	-0.01284
36	C3	S	0.00000	-0.06709	0.00000	-0.01104	0.00000
37	C3	S	0.00000	-0.15839	0.00000	0.09521	0.00000
38	C3	PX	0.00000	0.11752	0.00000	0.06427	0.00000
39	C3	PY	0.00000	-0.04420	0.00000	0.21209	0.00000
40	C3	PZ	-0.30209	0.00000	-0.12239	0.00000	-0.07142
41	C3	S	0.00000	1.54306	0.00000	0.02160	0.00000
42	C3	PX	0.00000	-1.32054	0.00000	-0.34329	0.00000
43	C3	PY	0.00000	-0.84248	0.00000	-0.17328	0.00000
44	C3	PZ	0.26232	0.00000	0.09488	0.00000	0.16903
45	C3	DXX	0.00000	-0.09110	0.00000	-0.00772	0.00000
46	C3	DYY	0.00000	-0.04627	0.00000	0.02279	0.00000
47	C3	DZZ	0.00000	0.04646	0.00000	0.00729	0.00000
48	C3	DXY	0.00000	-0.00364	0.00000	-0.00348	0.00000
49	C3	DXZ	0.01060	0.00000	0.00603	0.00000	-0.00662
50	C3	DYZ	0.02013	0.00000	-0.04260	0.00000	0.02935
51	C4	S	0.00000	-0.00608	0.00000	-0.04227	0.00000
52	C4	S	0.00000	0.38371	0.00000	-0.11712	0.00000
53	C4	PX	0.00000	-0.16223	0.00000	0.26490	0.00000
54	C4	PY	0.00000	0.02338	0.00000	-0.19198	0.00000
55	C4	PZ	0.57755	0.00000	-0.32873	0.00000	-0.33756
56	C4	S	0.00000	-0.36671	0.00000	0.61047	0.00000
57	C4	PX	0.00000	1.00015	0.00000	0.07520	0.00000
58	C4	PY	0.00000	-0.86988	0.00000	-0.19017	0.00000
59	C4	PZ	-0.61064	0.00000	0.52083	0.00000	0.42013
60	C4	DXX	0.00000	0.02924	0.00000	-0.05101	0.00000
61	C4	DYY	0.00000	0.07328	0.00000	-0.07426	0.00000
62	C4	DZZ	0.00000	0.00036	0.00000	0.03522	0.00000
63	C4	DXY	0.00000	0.03448	0.00000	0.01735	0.00000
64	C4	DXZ	-0.01772	0.00000	-0.01448	0.00000	0.04242
65	C4	DYZ	-0.03650	0.00000	-0.00259	0.00000	-0.00950
66	C5	S	0.00000	0.06061	0.00000	-0.03861	0.00000
67	C5	S	0.00000	0.37205	0.00000	-0.11149	0.00000
68	C5	PX	0.00000	-0.07039	0.00000	-0.24202	0.00000
69	C5	PY	0.00000	0.10652	0.00000	-0.19766	0.00000
70	C5	PZ	0.18310	0.00000	0.53025	0.00000	-0.49041
71	C5	S	0.00000	-1.70309	0.00000	0.43218	0.00000
72	C5	PX	0.00000	1.29060	0.00000	0.40601	0.00000
73	C5	PY	0.00000	1.01284	0.00000	0.14072	0.00000
74	C5	PZ	-0.12685	0.00000	-0.67911	0.00000	0.65708

75	C5	DXX	0.00000	0.09289	0.00000	-0.04702	0.00000
76	C5	DYY	0.00000	0.10681	0.00000	-0.07467	0.00000
77	C5	DZZ	0.00000	-0.05648	0.00000	0.03144	0.00000
78	C5	DXY	0.00000	-0.04313	0.00000	-0.01582	0.00000
79	C5	DXZ	0.03430	0.00000	0.00367	0.00000	-0.04153
80	C5	DYZ	0.00457	0.00000	-0.03828	0.00000	-0.01207
81	C6	S	0.00000	-0.00495	0.00000	0.00123	0.00000
82	C6	S	0.00000	-0.35410	0.00000	0.02761	0.00000
83	C6	PX	0.00000	-0.43917	0.00000	-0.19788	0.00000
84	C6	PY	0.00000	0.01311	0.00000	0.24924	0.00000
85	C6	PZ	-0.39316	0.00000	-0.56031	0.00000	-0.04509
86	C6	S	0.00000	0.71989	0.00000	0.00188	0.00000
87	C6	PX	0.00000	-1.30302	0.00000	0.00726	0.00000
88	C6	PY	0.00000	-0.41065	0.00000	-0.08424	0.00000
89	C6	PZ	0.33809	0.00000	0.79605	0.00000	0.17120
90	C6	DXX	0.00000	-0.07410	0.00000	0.00325	0.00000
91	C6	DYY	0.00000	-0.03062	0.00000	0.02403	0.00000
92	C6	DZZ	0.00000	0.00703	0.00000	-0.00430	0.00000
93	C6	DXY	0.00000	0.00666	0.00000	-0.00514	0.00000
94	C6	DXZ	-0.00328	0.00000	-0.00138	0.00000	0.00345
95	C6	DYZ	-0.02061	0.00000	0.02021	0.00000	0.00633
96	C7	S	0.00000	0.05248	0.00000	-0.00212	0.00000
97	C7	S	0.00000	-0.05708	0.00000	-0.00320	0.00000
98	C7	PX	0.00000	0.06606	0.00000	-0.04018	0.00000
99	C7	PY	0.00000	-0.04466	0.00000	0.01517	0.00000
100	C7	PZ	-0.36241	0.00000	0.52867	0.00000	-0.21095
101	C7	S	0.00000	-1.42772	0.00000	-0.01715	0.00000
102	C7	PX	0.00000	1.13778	0.00000	0.27458	0.00000
103	C7	PY	0.00000	-0.19293	0.00000	-0.00754	0.00000
104	C7	PZ	0.33142	0.00000	-0.79236	0.00000	0.07472
105	C7	DXX	0.00000	0.02924	0.00000	0.03616	0.00000
106	C7	DYY	0.00000	0.00599	0.00000	-0.04151	0.00000
107	C7	DZZ	0.00000	-0.01575	0.00000	0.00180	0.00000
108	C7	DXY	0.00000	-0.02913	0.00000	-0.01761	0.00000
109	C7	DXZ	0.01769	0.00000	-0.03219	0.00000	0.00798
110	C7	DYZ	-0.00664	0.00000	0.00908	0.00000	-0.00156
111	H3	S	0.00000	0.19336	0.00000	-0.17011	0.00000
112	H3	S	0.00000	0.19096	0.00000	0.05687	0.00000
113	H3	PX	0.00000	0.00694	0.00000	-0.00434	0.00000
114	H3	PY	0.00000	0.00892	0.00000	-0.01328	0.00000
115	H3	PZ	-0.00246	0.00000	-0.00398	0.00000	-0.00016
116	H4	S	0.00000	0.40178	0.00000	-0.16205	0.00000
117	H4	S	0.00000	-0.08079	0.00000	0.04049	0.00000
118	H4	PX	0.00000	-0.00888	0.00000	0.00756	0.00000
119	H4	PY	0.00000	0.02242	0.00000	-0.01093	0.00000
120	H4	PZ	0.00048	0.00000	-0.00492	0.00000	-0.00082
121	N1	S	0.00000	0.00915	0.00000	-0.01488	0.00000
122	N1	S	0.00000	0.00693	0.00000	0.04598	0.00000
123	N1	PX	0.00000	-0.00587	0.00000	0.07943	0.00000
124	N1	PY	0.00000	-0.04256	0.00000	-0.07013	0.00000
125	N1	PZ	-0.06538	0.00000	-0.18773	0.00000	0.06906
126	N1	S	0.00000	-0.86845	0.00000	-0.15173	0.00000
127	N1	PX	0.00000	0.00823	0.00000	-0.08686	0.00000
128	N1	PY	0.00000	-0.74596	0.00000	0.06801	0.00000

129	N1	PZ	-0.01559	0.00000	-0.06651	0.00000	-0.21476
130	N1	DXX	0.00000	-0.02254	0.00000	0.00381	0.00000
131	N1	DYY	0.00000	-0.01756	0.00000	-0.04320	0.00000
132	N1	DZZ	0.00000	0.03827	0.00000	0.02264	0.00000
133	N1	DXY	0.00000	0.01318	0.00000	0.01978	0.00000
134	N1	DXZ	-0.01319	0.00000	-0.03617	0.00000	0.00032
135	N1	DYZ	-0.00618	0.00000	-0.02831	0.00000	0.00497
136	H6	S	0.00000	0.19945	0.00000	0.13078	0.00000
137	H6	S	0.00000	0.43021	0.00000	-0.07836	0.00000
138	H6	PX	0.00000	-0.00596	0.00000	-0.00886	0.00000
139	H6	PY	0.00000	0.00543	0.00000	-0.00277	0.00000
140	H6	PZ	-0.00085	0.00000	-0.00928	0.00000	0.00251
141	C8	S	0.00000	-0.00031	0.00000	0.05529	0.00000
142	C8	S	0.00000	-0.01722	0.00000	-0.44679	0.00000
143	C8	PX	0.00000	0.22020	0.00000	0.13866	0.00000
144	C8	PY	0.00000	-0.07494	0.00000	0.22849	0.00000
145	C8	PZ	-0.11181	0.00000	-0.35690	0.00000	-0.44388
146	C8	S	0.00000	0.35443	0.00000	0.26802	0.00000
147	C8	PX	0.00000	0.62351	0.00000	-0.09761	0.00000
148	C8	PY	0.00000	0.81283	0.00000	0.24928	0.00000
149	C8	PZ	0.11319	0.00000	0.59988	0.00000	0.65560
150	C8	DXX	0.00000	-0.01768	0.00000	-0.06711	0.00000
151	C8	DYY	0.00000	0.01161	0.00000	0.08250	0.00000
152	C8	DZZ	0.00000	0.00022	0.00000	-0.03830	0.00000
153	C8	DXY	0.00000	-0.01543	0.00000	-0.01328	0.00000
154	C8	DXZ	-0.00999	0.00000	0.02066	0.00000	-0.00872
155	C8	DYZ	-0.04163	0.00000	0.01911	0.00000	-0.01519
156	H8	S	0.00000	0.24636	0.00000	0.10738	0.00000
157	H8	S	0.00000	-0.59047	0.00000	-0.25350	0.00000
158	H8	PX	0.00000	0.01609	0.00000	0.01113	0.00000
159	H8	PY	0.00000	-0.00899	0.00000	-0.00444	0.00000
160	H8	PZ	-0.00262	0.00000	-0.00824	0.00000	-0.00383
161	C10	S	0.00000	0.00397	0.00000	-0.07419	0.00000
162	C10	S	0.00000	0.08857	0.00000	-0.27981	0.00000
163	C10	PX	0.00000	0.06888	0.00000	0.03772	0.00000
164	C10	PY	0.00000	0.08145	0.00000	0.43199	0.00000
165	C10	PZ	0.56387	0.00000	0.08735	0.00000	0.34323
166	C10	S	0.00000	0.34978	0.00000	1.25121	0.00000
167	C10	PX	0.00000	-0.43675	0.00000	-0.06015	0.00000
168	C10	PY	0.00000	0.13665	0.00000	-0.37254	0.00000
169	C10	PZ	-0.60810	0.00000	-0.20054	0.00000	-0.52027
170	C10	DXX	0.00000	0.02057	0.00000	-0.09628	0.00000
171	C10	DYY	0.00000	0.01595	0.00000	-0.13795	0.00000
172	C10	DZZ	0.00000	-0.00171	0.00000	0.07351	0.00000
173	C10	DXY	0.00000	0.02671	0.00000	0.02246	0.00000
174	C10	DXZ	0.00511	0.00000	-0.01296	0.00000	0.00410
175	C10	DYZ	0.00615	0.00000	-0.02530	0.00000	-0.01495
176	H16	S	0.00000	0.00356	0.00000	-0.39026	0.00000
177	H16	S	0.00000	0.29143	0.00000	-0.03889	0.00000
178	H16	PX	0.00000	-0.00251	0.00000	-0.00818	0.00000
179	H16	PY	0.00000	0.00043	0.00000	0.01575	0.00000
180	H16	PZ	0.00959	0.00000	0.00064	0.00000	0.00519
181	H18	S	0.00000	0.04317	0.00000	-0.31767	0.00000
182	H18	S	0.00000	-0.27906	0.00000	-0.22393	0.00000

183	H18	PX	0.00000	-0.01317	0.00000	0.00337	0.00000
184	H18	PY	0.00000	-0.00511	0.00000	0.01219	0.00000
185	H18	PZ	0.00749	0.00000	0.00713	0.00000	0.00333

MO:		71	72	73	74	75
Eigenvalues:		0.90242	0.91918	0.94821	0.98293	0.98712
(ev):		24.55622	25.01221	25.80209	26.74691	26.86081

		A	A	A	A	A	
1	H1	S	0.10876	-0.32127	0.00000	0.00000	-0.04656
2	H1	S	-0.28532	0.23389	0.00000	0.00000	-0.02970
3	H1	PX	0.00962	-0.02198	0.00000	0.00000	-0.00526
4	H1	PY	-0.00034	0.00576	0.00000	0.00000	-0.01844
5	H1	PZ	0.00000	0.00000	0.00500	-0.01694	0.00000
6	C1	S	0.02685	-0.07254	0.00000	0.00000	-0.00510
7	C1	S	0.04034	-0.14989	0.00000	0.00000	-0.01351
8	C1	PX	0.06391	-0.15448	0.00000	0.00000	-0.00016
9	C1	PY	-0.09683	0.34820	0.00000	0.00000	0.04053
10	C1	PZ	0.00000	0.00000	0.26789	0.47586	0.00000
11	C1	S	-0.61499	0.97571	0.00000	0.00000	-0.48385
12	C1	PX	0.34426	-0.20229	0.00000	0.00000	0.21290
13	C1	PY	-1.27150	0.25796	0.00000	0.00000	-0.59206
14	C1	PZ	0.00000	0.00000	-0.35703	-0.93196	0.00000
15	C1	DXX	0.05916	-0.11926	0.00000	0.00000	-0.01577
16	C1	DYY	0.00392	-0.08383	0.00000	0.00000	-0.02170
17	C1	DZZ	-0.03984	0.07316	0.00000	0.00000	0.01120
18	C1	DXY	0.01299	0.01594	0.00000	0.00000	-0.01380
19	C1	DXZ	0.00000	0.00000	0.01649	-0.02479	0.00000
20	C1	DYZ	0.00000	0.00000	-0.03827	-0.01701	0.00000
21	C2	S	-0.07530	0.00593	0.00000	0.00000	0.02445
22	C2	S	-0.13280	-0.15014	0.00000	0.00000	0.17521
23	C2	PX	0.12504	-0.07795	0.00000	0.00000	0.00212
24	C2	PY	0.41878	0.09689	0.00000	0.00000	0.02661
25	C2	PZ	0.00000	0.00000	-0.41350	0.13724	0.00000
26	C2	S	0.99729	0.33617	0.00000	0.00000	-0.38110
27	C2	PX	0.17678	0.16989	0.00000	0.00000	-0.43104
28	C2	PY	0.78658	-0.98130	0.00000	0.00000	0.19883
29	C2	PZ	0.00000	0.00000	0.74379	-0.22262	0.00000
30	C2	DXX	-0.11837	0.02052	0.00000	0.00000	0.04397
31	C2	DYY	-0.08868	-0.02198	0.00000	0.00000	0.03057
32	C2	DZZ	0.07305	-0.02951	0.00000	0.00000	-0.02539
33	C2	DXY	-0.02516	-0.02191	0.00000	0.00000	-0.04152
34	C2	DXZ	0.00000	0.00000	-0.01556	0.02452	0.00000
35	C2	DYZ	0.00000	0.00000	0.01489	0.00025	0.00000
36	C3	S	0.01512	-0.01762	0.00000	0.00000	0.00224
37	C3	S	0.28245	-0.09035	0.00000	0.00000	0.16469
38	C3	PX	-0.11123	0.01728	0.00000	0.00000	-0.16227
39	C3	PY	0.14009	-0.43986	0.00000	0.00000	-0.15604
40	C3	PZ	0.00000	0.00000	0.56025	-0.43775	0.00000
41	C3	S	-0.19674	0.39895	0.00000	0.00000	-0.00414
42	C3	PX	-1.20394	0.43716	0.00000	0.00000	-0.11136
43	C3	PY	-0.53668	0.20398	0.00000	0.00000	0.41881
44	C3	PZ	0.00000	0.00000	-0.81917	0.70397	0.00000
45	C3	DXX	0.05673	-0.00966	0.00000	0.00000	-0.00774

46	C3	DYY	0.06572	-0.04906	0.00000	0.00000	0.02983
47	C3	DZZ	-0.02209	0.00401	0.00000	0.00000	0.00131
48	C3	DXY	-0.03233	-0.00198	0.00000	0.00000	-0.05777
49	C3	DXZ	0.00000	0.00000	-0.00520	0.03007	0.00000
50	C3	DYZ	0.00000	0.00000	0.04364	0.04918	0.00000
51	C4	S	-0.02588	0.06250	0.00000	0.00000	0.00060
52	C4	S	0.30672	-0.13451	0.00000	0.00000	-0.03888
53	C4	PX	-0.20928	-0.11462	0.00000	0.00000	0.08053
54	C4	PY	-0.06920	0.27754	0.00000	0.00000	-0.00945
55	C4	PZ	0.00000	0.00000	-0.54962	-0.25052	0.00000
56	C4	S	0.06395	-0.10772	0.00000	0.00000	0.22574
57	C4	PX	1.53652	-0.71437	0.00000	0.00000	0.51758
58	C4	PY	-0.85746	0.34225	0.00000	0.00000	-0.14771
59	C4	PZ	0.00000	0.00000	0.96411	0.57750	0.00000
60	C4	DXX	0.01262	0.06173	0.00000	0.00000	0.00302
61	C4	DYY	0.00886	0.05909	0.00000	0.00000	-0.02407
62	C4	DZZ	0.02673	-0.06353	0.00000	0.00000	0.00289
63	C4	DXY	-0.01612	-0.04124	0.00000	0.00000	-0.03349
64	C4	DXZ	0.00000	0.00000	0.01263	-0.00172	0.00000
65	C4	DYZ	0.00000	0.00000	0.01893	-0.02192	0.00000
66	C5	S	0.06101	-0.00271	0.00000	0.00000	-0.02373
67	C5	S	-0.20009	0.28110	0.00000	0.00000	0.06868
68	C5	PX	0.03816	0.26816	0.00000	0.00000	-0.01188
69	C5	PY	0.29835	0.01844	0.00000	0.00000	0.10344
70	C5	PZ	0.00000	0.00000	0.44202	0.11930	0.00000
71	C5	S	-0.16770	-0.34542	0.00000	0.00000	0.35500
72	C5	PX	1.18343	-1.06551	0.00000	0.00000	0.50113
73	C5	PY	0.71700	-0.44402	0.00000	0.00000	-0.43942
74	C5	PZ	0.00000	0.00000	-0.90052	-0.23238	0.00000
75	C5	DXX	0.05139	0.02704	0.00000	0.00000	0.00478
76	C5	DYY	0.04365	0.03569	0.00000	0.00000	-0.03185
77	C5	DZZ	-0.06117	0.01035	0.00000	0.00000	0.01357
78	C5	DXY	0.06183	0.01568	0.00000	0.00000	0.04977
79	C5	DXZ	0.00000	0.00000	-0.00787	0.00596	0.00000
80	C5	DYZ	0.00000	0.00000	0.02149	-0.01645	0.00000
81	C6	S	0.00840	-0.00476	0.00000	0.00000	0.05463
82	C6	S	-0.18320	0.07920	0.00000	0.00000	-0.08835
83	C6	PX	0.19225	0.01231	0.00000	0.00000	0.02517
84	C6	PY	-0.22361	0.13923	0.00000	0.00000	0.48162
85	C6	PZ	0.00000	0.00000	0.03324	-0.30240	0.00000
86	C6	S	-0.06381	-0.64071	0.00000	0.00000	0.32353
87	C6	PX	-1.36787	0.75741	0.00000	0.00000	-0.20264
88	C6	PY	0.45952	-0.55305	0.00000	0.00000	-0.55792
89	C6	PZ	0.00000	0.00000	-0.07166	0.35246	0.00000
90	C6	DXX	-0.02636	0.01159	0.00000	0.00000	-0.02266
91	C6	DYY	-0.00654	0.00916	0.00000	0.00000	0.15849
92	C6	DZZ	-0.01113	0.00224	0.00000	0.00000	-0.05903
93	C6	DXY	0.03932	0.01856	0.00000	0.00000	0.06370
94	C6	DXZ	0.00000	0.00000	0.01467	-0.03138	0.00000
95	C6	DYZ	0.00000	0.00000	-0.02461	0.01161	0.00000
96	C7	S	-0.01634	0.05513	0.00000	0.00000	-0.00059
97	C7	S	0.31477	0.21456	0.00000	0.00000	0.08812
98	C7	PX	-0.18936	-0.11211	0.00000	0.00000	-0.12482
99	C7	PY	0.08389	-0.14982	0.00000	0.00000	0.10342

100	C7	PZ	0.00000	0.00000	-0.48330	-0.09699	0.00000
101	C7	S	-0.65194	-0.42519	0.00000	0.00000	0.09534
102	C7	PX	0.76867	0.30553	0.00000	0.00000	0.49429
103	C7	PY	0.42592	-0.45872	0.00000	0.00000	-0.51400
104	C7	PZ	0.00000	0.00000	0.82834	0.24976	0.00000
105	C7	DXX	0.00153	0.09548	0.00000	0.00000	-0.04978
106	C7	DYY	0.01528	0.09186	0.00000	0.00000	0.04103
107	C7	DZZ	0.01912	-0.06404	0.00000	0.00000	0.00785
108	C7	DXY	0.02422	-0.02579	0.00000	0.00000	-0.01177
109	C7	DXZ	0.00000	0.00000	0.01569	-0.00171	0.00000
110	C7	DYZ	0.00000	0.00000	0.00983	-0.03151	0.00000
111	H3	S	-0.09476	0.19325	0.00000	0.00000	-0.05742
112	H3	S	0.22203	-0.07424	0.00000	0.00000	0.00563
113	H3	PX	0.00867	-0.00491	0.00000	0.00000	0.00521
114	H3	PY	-0.00722	0.01400	0.00000	0.00000	-0.01027
115	H3	PZ	0.00000	0.00000	0.01013	0.00047	0.00000
116	H4	S	0.13370	-0.00784	0.00000	0.00000	-0.18100
117	H4	S	-0.02701	0.09486	0.00000	0.00000	0.50607
118	H4	PX	0.01020	-0.00592	0.00000	0.00000	0.01753
119	H4	PY	0.00835	0.00330	0.00000	0.00000	-0.02376
120	H4	PZ	0.00000	0.00000	0.00089	-0.00639	0.00000
121	N1	S	-0.00097	-0.00443	0.00000	0.00000	-0.02681
122	N1	S	-0.04128	0.01058	0.00000	0.00000	0.04286
123	N1	PX	0.22851	0.08362	0.00000	0.00000	0.66019
124	N1	PY	0.01241	0.04346	0.00000	0.00000	0.21896
125	N1	PZ	0.00000	0.00000	-0.05079	0.12473	0.00000
126	N1	S	0.34193	0.10500	0.00000	0.00000	-1.12902
127	N1	PX	0.21058	-0.11400	0.00000	0.00000	-0.91734
128	N1	PY	-0.42210	0.26459	0.00000	0.00000	0.10142
129	N1	PZ	0.00000	0.00000	0.09342	0.03610	0.00000
130	N1	DXX	-0.01695	0.01643	0.00000	0.00000	-0.09168
131	N1	DYY	-0.00195	-0.00648	0.00000	0.00000	-0.18552
132	N1	DZZ	-0.02445	-0.02003	0.00000	0.00000	0.05889
133	N1	DXY	-0.01086	-0.01825	0.00000	0.00000	0.00280
134	N1	DXZ	0.00000	0.00000	-0.01540	0.03098	0.00000
135	N1	DYZ	0.00000	0.00000	0.01779	-0.03103	0.00000
136	H6	S	-0.35328	0.03459	0.00000	0.00000	0.02741
137	H6	S	0.20375	-0.12044	0.00000	0.00000	-0.27696
138	H6	PX	0.02639	-0.00343	0.00000	0.00000	-0.00210
139	H6	PY	0.00272	0.00770	0.00000	0.00000	0.00221
140	H6	PZ	0.00000	0.00000	0.00707	-0.00849	0.00000
141	C8	S	0.01811	0.02930	0.00000	0.00000	0.00747
142	C8	S	-0.14889	0.12998	0.00000	0.00000	-0.25959
143	C8	PX	-0.01884	0.11789	0.00000	0.00000	0.26527
144	C8	PY	0.14152	0.39160	0.00000	0.00000	-0.39673
145	C8	PZ	0.00000	0.00000	0.01280	0.75053	0.00000
146	C8	S	0.29980	-0.28144	0.00000	0.00000	1.07337
147	C8	PX	0.87934	-0.31771	0.00000	0.00000	-0.86084
148	C8	PY	-0.10697	-0.37678	0.00000	0.00000	1.10883
149	C8	PZ	0.00000	0.00000	-0.14284	-1.30499	0.00000
150	C8	DXX	0.03114	0.02333	0.00000	0.00000	0.03093
151	C8	DYY	0.00887	0.08287	0.00000	0.00000	-0.00947
152	C8	DZZ	-0.02792	-0.02111	0.00000	0.00000	-0.02704
153	C8	DXY	0.00873	0.00676	0.00000	0.00000	-0.09493

154	C8	DXZ	0.00000	0.00000	-0.00081	-0.00825	0.00000
155	C8	DYZ	0.00000	0.00000	-0.04355	0.04624	0.00000
156	H8	S	-0.13030	0.19321	0.00000	0.00000	-0.03565
157	H8	S	-0.07093	-0.37859	0.00000	0.00000	-0.28333
158	H8	PX	0.00216	0.02285	0.00000	0.00000	0.00664
159	H8	PY	0.00321	-0.02446	0.00000	0.00000	-0.01140
160	H8	PZ	0.00000	0.00000	0.00994	0.00877	0.00000
161	C10	S	-0.03410	-0.04966	0.00000	0.00000	0.02875
162	C10	S	-0.32541	-0.23891	0.00000	0.00000	0.19323
163	C10	PX	0.09463	0.03345	0.00000	0.00000	-0.01351
164	C10	PY	0.01622	0.18530	0.00000	0.00000	-0.11536
165	C10	PZ	0.00000	0.00000	0.14498	-0.28426	0.00000
166	C10	S	0.74055	0.66318	0.00000	0.00000	-0.13044
167	C10	PX	-0.51956	-0.05211	0.00000	0.00000	0.13273
168	C10	PY	-0.04689	-0.20170	0.00000	0.00000	0.08102
169	C10	PZ	0.00000	0.00000	-0.16222	0.68871	0.00000
170	C10	DXX	-0.07177	-0.06723	0.00000	0.00000	0.02556
171	C10	DYY	-0.07487	-0.11138	0.00000	0.00000	0.07436
172	C10	DZZ	0.02591	0.04635	0.00000	0.00000	-0.02854
173	C10	DXY	-0.00591	-0.01468	0.00000	0.00000	0.00824
174	C10	DXZ	0.00000	0.00000	0.01515	0.00298	0.00000
175	C10	DYZ	0.00000	0.00000	0.01647	0.00050	0.00000
176	H16	S	-0.18744	-0.18747	0.00000	0.00000	0.13453
177	H16	S	0.13517	-0.08214	0.00000	0.00000	0.01928
178	H16	PX	-0.01526	-0.00799	0.00000	0.00000	-0.00931
179	H16	PY	0.01347	0.00554	0.00000	0.00000	-0.02469
180	H16	PZ	0.00000	0.00000	0.00164	0.00890	0.00000
181	H18	S	-0.22753	-0.28233	0.00000	0.00000	0.05411
182	H18	S	-0.30220	-0.08322	0.00000	0.00000	0.02499
183	H18	PX	0.00450	0.00525	0.00000	0.00000	0.00110
184	H18	PY	0.00309	0.01662	0.00000	0.00000	0.00837
185	H18	PZ	0.00000	0.00000	-0.00564	0.00552	0.00000

MO:	76	77	78	79	80
Eigenvalues:	1.04060	1.04963	1.05374	1.07556	1.08597
(ev):	28.31629	28.56182	28.67377	29.26760	29.55087

		A	A	A	A	A	
1	H1	S	0.00000	-0.00292	0.15600	-0.30413	0.13931
2	H1	S	0.00000	-0.41857	-0.87875	1.12984	-1.35907
3	H1	PX	0.00000	0.01999	0.05019	-0.07865	0.07335
4	H1	PY	0.00000	0.00757	0.01953	-0.01905	0.00279
5	H1	PZ	-0.02346	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.00543	0.01659	-0.01993	0.01890
7	C1	S	0.00000	0.04194	-0.15595	0.25187	-0.12598
8	C1	PX	0.00000	-0.17775	-0.27197	0.41358	-0.49004
9	C1	PY	0.00000	0.00103	0.07902	0.03971	-0.03986
10	C1	PZ	0.22148	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.05828	0.39462	-0.59413	-0.13261
12	C1	PX	0.00000	0.64702	1.03340	-1.02902	2.12878
13	C1	PY	0.00000	0.16296	0.00997	-0.05122	0.29149
14	C1	PZ	-0.86851	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.02417	0.05959	-0.13673	0.02891
16	C1	DYY	0.00000	-0.00668	-0.03426	0.08672	-0.02578

17	C1	DZZ	0.00000	-0.00968	-0.04410	0.05072	-0.02431
18	C1	DXY	0.00000	-0.01236	0.05243	0.03485	0.02720
19	C1	DXZ	-0.01280	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00761	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.00363	-0.00079	0.01019	0.02132
22	C2	S	0.00000	-0.21087	0.13334	-0.18399	-0.27640
23	C2	PX	0.00000	0.08826	-0.09186	0.14129	0.42885
24	C2	PY	0.00000	0.01332	-0.08303	0.05888	0.10374
25	C2	PZ	-0.36201	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.32410	0.00976	0.59425	-0.02360
27	C2	PX	0.00000	-0.55732	0.48233	-0.10193	-1.61724
28	C2	PY	0.00000	-0.05588	-0.05342	-0.26611	-0.62472
29	C2	PZ	1.06059	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.01994	-0.00147	0.07489	0.09449
31	C2	DYY	0.00000	-0.02400	0.01734	-0.04759	-0.08746
32	C2	DZZ	0.00000	0.00891	0.00637	-0.02981	-0.04093
33	C2	DXY	0.00000	0.00884	0.00754	0.04927	-0.00718
34	C2	DXZ	-0.01199	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02713	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.00338	0.01577	0.01986	0.00218
37	C3	S	0.00000	0.11493	0.15901	0.17243	-0.09792
38	C3	PX	0.00000	0.02665	0.06770	-0.14665	0.18548
39	C3	PY	0.00000	-0.12569	0.12425	0.19534	-0.03448
40	C3	PZ	-0.67347	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	0.08420	1.05724	-0.48209	1.01177
42	C3	PX	0.00000	-0.38081	-0.46521	0.96597	-0.57250
43	C3	PY	0.00000	0.71516	-0.58062	-1.16437	0.26419
44	C3	PZ	1.66304	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.01881	-0.01210	-0.00823	-0.03483
46	C3	DYY	0.00000	0.00919	0.11848	0.03341	0.05837
47	C3	DZZ	0.00000	0.00272	-0.03184	0.00029	-0.01050
48	C3	DXY	0.00000	0.03562	-0.00803	-0.01703	0.03391
49	C3	DXZ	-0.00579	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00238	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00659	-0.00381	-0.03161	-0.01620
52	C4	S	0.00000	0.08223	-0.05131	0.24131	0.13485
53	C4	PX	0.00000	-0.11422	-0.00500	0.24575	0.21497
54	C4	PY	0.00000	-0.08485	0.15762	0.47874	0.33304
55	C4	PZ	-0.20681	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.18554	0.45395	0.00572	0.51882
57	C4	PX	0.00000	0.20723	-0.38304	-1.16762	-1.11907
58	C4	PY	0.00000	0.36863	-0.59825	-1.58387	-1.35344
59	C4	PZ	0.67088	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	-0.01775	-0.00803	0.08179	0.00269
61	C4	DYY	0.00000	0.03849	0.01386	-0.12242	-0.00868
62	C4	DZZ	0.00000	-0.00358	-0.00701	0.05256	0.01997
63	C4	DXY	0.00000	-0.00626	-0.02245	-0.07318	-0.08021
64	C4	DXZ	-0.00732	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.01247	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.00609	-0.00493	0.03089	-0.00226
67	C5	S	0.00000	0.02494	-0.00585	-0.12044	-0.04054
68	C5	PX	0.00000	-0.15534	-0.06666	0.28921	0.00443
69	C5	PY	0.00000	0.03821	0.03329	-0.43447	0.03574
70	C5	PZ	0.28920	0.00000	0.00000	0.00000	0.00000

71	C5	S	0.00000	0.35622	-0.40394	-0.26468	0.24348
72	C5	PX	0.00000	0.36488	-0.16407	-1.44039	-0.52317
73	C5	PY	0.00000	-0.51410	0.00240	1.56288	-0.41099
74	C5	PZ	-0.81008	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.01898	-0.01374	-0.03520	-0.04995
76	C5	DYY	0.00000	-0.01167	-0.02147	0.07843	0.04517
77	C5	DZZ	0.00000	0.00641	0.00797	-0.04114	-0.00109
78	C5	DXY	0.00000	0.01851	0.01052	-0.06472	0.04273
79	C5	DXZ	0.00040	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00108	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00158	-0.01207	-0.01499	-0.00987
82	C6	S	0.00000	-0.46520	0.19854	-0.29100	0.01396
83	C6	PX	0.00000	0.21487	-0.13046	-0.04744	-0.02449
84	C6	PY	0.00000	0.26060	-0.24335	-0.04298	-0.04573
85	C6	PZ	0.60710	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.37785	-0.04720	0.78329	-0.53699
87	C6	PX	0.00000	-0.50055	0.17336	0.70101	0.30592
88	C6	PY	0.00000	0.53555	-0.43840	0.56820	0.77449
89	C6	PZ	-1.50926	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.04827	0.00183	-0.00045	-0.05102
91	C6	DYY	0.00000	-0.09797	0.02840	-0.03807	0.02269
92	C6	DZZ	0.00000	0.01257	0.00551	-0.00600	0.01207
93	C6	DXY	0.00000	0.02404	-0.01848	0.03192	-0.00866
94	C6	DXZ	0.00988	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.04068	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.01705	0.03073	-0.00116	0.00434
97	C7	S	0.00000	-0.04724	-0.17405	0.23066	-0.22457
98	C7	PX	0.00000	-0.26351	-0.69643	-0.05664	-0.21872
99	C7	PY	0.00000	-0.13748	0.23162	0.15994	0.02934
100	C7	PZ	0.17540	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	1.01338	-0.27457	-0.87469	-0.33183
102	C7	PX	0.00000	0.37399	2.99524	0.17570	1.12445
103	C7	PY	0.00000	0.31218	-1.07381	-0.82528	-0.01212
104	C7	PZ	-0.76773	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.02933	0.06232	0.03632	-0.00665
106	C7	DYY	0.00000	0.03443	-0.04882	-0.02131	-0.04802
107	C7	DZZ	0.00000	-0.02477	-0.05588	0.01289	-0.00492
108	C7	DXY	0.00000	-0.02746	-0.01497	0.01574	-0.06104
109	C7	DXZ	0.01379	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.01014	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.00000	-0.00050	-0.02529	-0.34993	-0.21613
112	H3	S	0.00000	-0.25523	0.35238	1.60489	1.15311
113	H3	PX	0.00000	0.00155	-0.00906	-0.05828	-0.02771
114	H3	PY	0.00000	0.01406	-0.01411	-0.08045	-0.06042
115	H3	PZ	0.00835	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.00000	-0.06388	-0.01063	0.28597	-0.03449
117	H4	S	0.00000	0.37141	0.06907	-1.50467	0.04550
118	H4	PX	0.00000	0.00248	0.00109	-0.05996	-0.00658
119	H4	PY	0.00000	-0.02094	-0.01023	0.06721	-0.01084
120	H4	PZ	-0.01437	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.00000	-0.05899	0.02618	-0.00756	0.00128
122	N1	S	0.00000	0.19496	-0.03495	-0.01027	-0.09316
123	N1	PX	0.00000	-0.33052	0.04979	0.01787	-0.02739
124	N1	PY	0.00000	-0.09679	-0.01945	-0.07736	0.01329

125	N1	PZ	0.15618	0.00000	0.00000	0.00000	0.00000
126	N1	S	0.00000	0.04733	-1.15100	-0.09080	0.96336
127	N1	PX	0.00000	1.10857	-0.65455	-0.06290	0.07650
128	N1	PY	0.00000	0.86752	-0.31978	0.35801	0.06942
129	N1	PZ	-0.02934	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00000	-0.06451	-0.01592	-0.04778	-0.01471
131	N1	DYY	0.00000	0.01589	0.01844	-0.00534	0.03521
132	N1	DZZ	0.00000	0.14205	-0.02863	0.03045	-0.03703
133	N1	DXY	0.00000	0.00885	0.03511	0.01310	-0.01560
134	N1	DXZ	0.02978	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.02788	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.00000	-0.01992	0.04772	0.13148	0.25655
137	H6	S	0.00000	-0.26884	0.29450	-0.39754	-1.33941
138	H6	PX	0.00000	-0.01315	0.01173	-0.03384	-0.07898
139	H6	PY	0.00000	-0.02703	0.00139	0.00221	-0.00365
140	H6	PZ	0.02368	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00000	-0.01605	0.00991	0.00287	-0.00979
142	C8	S	0.00000	-0.62849	0.18592	-0.09794	-0.08721
143	C8	PX	0.00000	0.36073	-0.01674	0.16841	-0.21767
144	C8	PY	0.00000	-0.22155	-0.06427	-0.08656	-0.11087
145	C8	PZ	-0.33331	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.00000	1.03465	0.70384	0.29666	0.34647
147	C8	PX	0.00000	-1.01452	-0.44399	-0.83294	1.32921
148	C8	PY	0.00000	-0.23962	1.79620	0.25406	0.77057
149	C8	PZ	0.73537	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00000	-0.01407	0.05448	0.00692	-0.01785
151	C8	DYY	0.00000	-0.13345	0.06652	-0.01231	-0.00584
152	C8	DZZ	0.00000	0.00677	-0.03101	-0.00619	0.00314
153	C8	DXY	0.00000	0.04833	0.07996	0.00806	-0.02037
154	C8	DXZ	-0.01745	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00666	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.00000	0.14922	0.10201	0.01647	0.12393
157	H8	S	0.00000	-0.38804	-2.04629	-0.15472	-0.73552
158	H8	PX	0.00000	0.03901	0.09678	0.00880	0.03029
159	H8	PY	0.00000	-0.00882	-0.02662	0.01268	-0.02855
160	H8	PZ	-0.01768	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00000	0.01261	0.00604	0.00592	0.00442
162	C10	S	0.00000	-0.33528	-0.02067	-0.00126	-0.09432
163	C10	PX	0.00000	-0.14997	-0.56117	-0.17838	0.61225
164	C10	PY	0.00000	-0.04869	0.09502	0.01281	-0.07303
165	C10	PZ	0.01851	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.00000	-0.10202	1.16414	0.02233	0.62218
167	C10	PX	0.00000	0.64467	1.67132	0.70579	-1.92821
168	C10	PY	0.00000	-0.02942	0.10134	-0.08733	0.37926
169	C10	PZ	-0.21116	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.00000	0.00524	0.00146	0.00558	0.00590
171	C10	DYY	0.00000	-0.01758	0.02641	0.00979	0.00635
172	C10	DZZ	0.00000	-0.01209	-0.03074	-0.00737	-0.01408
173	C10	DXY	0.00000	-0.04492	-0.07147	-0.01219	0.09604
174	C10	DXZ	-0.01628	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	-0.00334	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.00000	0.26803	0.08931	0.05859	-0.15123
177	H16	S	0.00000	-0.49691	-1.08310	-0.41878	1.15281
178	H16	PX	0.00000	0.02865	0.05419	0.01728	-0.05284

179	H16	PY	0.00000	-0.02415	-0.04465	-0.01403	0.04434
180	H16	PZ	-0.00891	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.00000	0.00147	-0.07430	-0.00213	0.17075
182	H18	S	0.00000	0.37281	0.85007	0.34030	-1.16968
183	H18	PX	0.00000	-0.00871	0.05060	0.01294	-0.06077
184	H18	PY	0.00000	0.02763	0.01497	0.01047	-0.05048
185	H18	PZ	0.00048	0.00000	0.00000	0.00000	0.00000

MO:	81	82	83	84	85
Eigenvalues:	1.10437	1.12072	1.12717	1.13890	1.16081
(ev):	30.05141	30.49639	30.67181	30.99115	31.58731

		A	A	A	A	A	
1	H1	S	0.17054	-0.06642	0.00000	-0.26320	0.05922
2	H1	S	-0.74859	-0.20358	0.00000	1.56623	-0.39589
3	H1	PX	0.04873	0.01274	0.00000	-0.10272	0.00736
4	H1	PY	-0.01804	-0.02592	0.00000	0.00110	0.01658
5	H1	PZ	0.00000	0.00000	0.00361	0.00000	0.00000
6	C1	S	0.01103	-0.00156	0.00000	0.00048	0.00237
7	C1	S	-0.22353	-0.24102	0.00000	0.76989	0.09874
8	C1	PX	-0.24835	-0.04153	0.00000	0.52089	-0.07924
9	C1	PY	-0.02225	0.06288	0.00000	0.03885	-0.00664
10	C1	PZ	0.00000	0.00000	-0.05861	0.00000	0.00000
11	C1	S	-0.27150	0.54082	0.00000	-1.66412	-0.59511
12	C1	PX	0.95466	0.35591	0.00000	-1.66545	0.64059
13	C1	PY	-0.09910	-0.26463	0.00000	0.22595	0.29425
14	C1	PZ	0.00000	0.00000	0.23216	0.00000	0.00000
15	C1	DXX	0.04140	-0.04731	0.00000	-0.03676	0.02138
16	C1	DYY	-0.06643	-0.01103	0.00000	0.08879	-0.00015
17	C1	DZZ	-0.00940	0.00429	0.00000	0.05198	-0.01072
18	C1	DXY	-0.00658	0.01855	0.00000	-0.02110	0.03078
19	C1	DXZ	0.00000	0.00000	-0.01507	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.01475	0.00000	0.00000
21	C2	S	0.01744	-0.00974	0.00000	-0.00053	0.01863
22	C2	S	-0.19955	0.37680	0.00000	-0.50007	0.28768
23	C2	PX	0.61669	-0.41299	0.00000	0.29509	-0.11117
24	C2	PY	0.03052	-0.09357	0.00000	-0.08586	-0.35667
25	C2	PZ	0.00000	0.00000	-0.07457	0.00000	0.00000
26	C2	S	-0.24573	-0.80353	0.00000	1.44286	-0.40700
27	C2	PX	-2.62724	1.28102	0.00000	-1.01842	0.54528
28	C2	PY	0.26037	0.30025	0.00000	-0.36456	2.15583
29	C2	PZ	0.00000	0.00000	-0.11507	0.00000	0.00000
30	C2	DXX	0.04660	-0.09229	0.00000	-0.00239	0.04515
31	C2	DYY	-0.05839	0.07137	0.00000	-0.03967	0.02490
32	C2	DZZ	-0.02718	0.05375	0.00000	-0.03092	-0.00417
33	C2	DXY	0.00263	0.01523	0.00000	-0.02829	0.05090
34	C2	DXZ	0.00000	0.00000	0.02125	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.02027	0.00000	0.00000
36	C3	S	-0.01159	0.01287	0.00000	-0.00169	0.00883
37	C3	S	-0.13696	-0.24890	0.00000	0.12116	0.49063
38	C3	PX	-0.09697	-0.04589	0.00000	-0.08666	0.05638
39	C3	PY	-0.05431	0.19556	0.00000	-0.08325	-0.21550
40	C3	PZ	0.00000	0.00000	0.17743	0.00000	0.00000
41	C3	S	-0.85795	1.38983	0.00000	-1.16502	-0.68981

42	C3	PX	0.60926	0.09813	0.00000	0.84679	-0.57817
43	C3	PY	0.80799	-1.12068	0.00000	0.64242	1.16653
44	C3	PZ	0.00000	0.00000	-0.50215	0.00000	0.00000
45	C3	DXX	-0.03794	-0.00208	0.00000	-0.01382	0.03525
46	C3	DYY	-0.03821	0.03121	0.00000	-0.00701	0.01420
47	C3	DZZ	0.01945	-0.02614	0.00000	0.01010	0.00326
48	C3	DXY	-0.00990	-0.07622	0.00000	0.03715	0.05070
49	C3	DXZ	0.00000	0.00000	-0.03186	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.01463	0.00000	0.00000
51	C4	S	-0.00956	-0.01251	0.00000	0.00004	0.00111
52	C4	S	0.07598	0.40280	0.00000	0.21763	0.12736
53	C4	PX	0.12961	0.25064	0.00000	-0.19605	0.03407
54	C4	PY	0.07370	0.40080	0.00000	-0.02031	0.28412
55	C4	PZ	0.00000	0.00000	0.05565	0.00000	0.00000
56	C4	S	-0.25789	-0.52527	0.00000	-1.40315	-0.67559
57	C4	PX	0.15831	-0.73135	0.00000	0.92884	-0.07601
58	C4	PY	-0.43667	-1.07665	0.00000	0.85378	-0.83388
59	C4	PZ	0.00000	0.00000	-0.14579	0.00000	0.00000
60	C4	DXX	-0.02195	0.06281	0.00000	-0.01076	-0.02057
61	C4	DYY	0.00202	-0.07214	0.00000	-0.01269	0.01305
62	C4	DZZ	0.02112	0.05569	0.00000	0.01629	0.01415
63	C4	DXY	-0.04709	-0.09860	0.00000	-0.04468	-0.01680
64	C4	DXZ	0.00000	0.00000	-0.00406	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	-0.01977	0.00000	0.00000
66	C5	S	-0.00416	-0.01300	0.00000	-0.01236	-0.00470
67	C5	S	0.16433	0.61231	0.00000	0.21094	0.13825
68	C5	PX	-0.13295	-0.21572	0.00000	-0.45296	-0.24431
69	C5	PY	0.21547	0.31920	0.00000	0.41744	-0.01744
70	C5	PZ	0.00000	0.00000	0.05784	0.00000	0.00000
71	C5	S	0.43439	-1.96403	0.00000	0.25378	-1.52653
72	C5	PX	0.98076	0.14931	0.00000	1.44675	1.12850
73	C5	PY	-0.94135	-0.38798	0.00000	-1.51772	0.54397
74	C5	PZ	0.00000	0.00000	-0.03199	0.00000	0.00000
75	C5	DXX	-0.02186	0.04033	0.00000	0.04771	-0.00633
76	C5	DYY	0.04931	-0.07688	0.00000	-0.06809	-0.01810
77	C5	DZZ	0.00758	0.07605	0.00000	0.04842	0.01176
78	C5	DXY	0.05699	0.10955	0.00000	0.06139	-0.04465
79	C5	DXZ	0.00000	0.00000	0.01574	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	-0.02391	0.00000	0.00000
81	C6	S	-0.00697	0.00329	0.00000	0.01269	-0.00080
82	C6	S	-0.10397	-0.13040	0.00000	-0.01895	-0.41561
83	C6	PX	-0.10133	0.13253	0.00000	-0.20139	0.12261
84	C6	PY	-0.15027	-0.02744	0.00000	-0.02467	-0.04514
85	C6	PZ	0.00000	0.00000	-0.31306	0.00000	0.00000
86	C6	S	1.30742	0.11707	0.00000	1.22989	2.34602
87	C6	PX	0.49481	-0.77553	0.00000	1.08428	-1.61357
88	C6	PY	1.18253	-0.28445	0.00000	-1.30990	-0.51188
89	C6	PZ	0.00000	0.00000	0.96836	0.00000	0.00000
90	C6	DXX	-0.00501	0.00055	0.00000	0.01156	-0.01197
91	C6	DYY	0.01980	-0.01976	0.00000	0.04950	0.00856
92	C6	DZZ	-0.00707	-0.00085	0.00000	-0.01783	-0.02507
93	C6	DXY	-0.04410	0.03585	0.00000	0.03060	-0.03464
94	C6	DXZ	0.00000	0.00000	0.01148	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	-0.07510	0.00000	0.00000

96	C7	S	-0.00777	-0.00621	0.00000	0.01015	0.02339
97	C7	S	0.16953	0.20728	0.00000	-0.21837	0.76796
98	C7	PX	0.52263	0.12899	0.00000	-0.18729	-0.02504
99	C7	PY	-0.03350	0.26366	0.00000	-0.01214	-0.53624
100	C7	PZ	0.00000	0.00000	0.04454	0.00000	0.00000
101	C7	S	1.12712	-0.91158	0.00000	0.64794	-2.21606
102	C7	PX	-2.45689	-0.40255	0.00000	0.45995	0.86971
103	C7	PY	0.27356	-1.12461	0.00000	0.26469	2.17836
104	C7	PZ	0.00000	0.00000	-0.10557	0.00000	0.00000
105	C7	DXX	0.00214	0.03500	0.00000	0.03295	-0.03810
106	C7	DYY	0.05993	-0.04556	0.00000	-0.02340	0.14226
107	C7	DZZ	-0.00084	0.02233	0.00000	-0.03005	0.01067
108	C7	DXY	0.06603	0.05030	0.00000	-0.05488	-0.04904
109	C7	DXZ	0.00000	0.00000	-0.03184	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	-0.03660	0.00000	0.00000
111	H3	S	-0.09521	-0.30212	0.00000	-0.04840	-0.04673
112	H3	S	0.34364	1.28929	0.00000	-0.35559	0.57514
113	H3	PX	0.00035	-0.02612	0.00000	-0.01033	-0.02775
114	H3	PY	-0.02993	-0.08537	0.00000	0.00767	-0.03135
115	H3	PZ	0.00000	0.00000	-0.00950	0.00000	0.00000
116	H4	S	-0.12130	-0.31945	0.00000	-0.27894	0.06184
117	H4	S	0.78610	1.06050	0.00000	1.53118	0.17635
118	H4	PX	0.02252	0.03778	0.00000	0.02882	-0.00348
119	H4	PY	-0.03700	-0.07828	0.00000	-0.09209	-0.02060
120	H4	PZ	0.00000	0.00000	-0.00880	0.00000	0.00000
121	N1	S	0.00606	-0.00277	0.00000	0.01710	0.00780
122	N1	S	-0.02725	0.06148	0.00000	0.07680	-0.13461
123	N1	PX	0.05354	-0.21793	0.00000	-0.03580	0.01674
124	N1	PY	-0.12702	0.09998	0.00000	0.10893	0.05458
125	N1	PZ	0.00000	0.00000	0.94786	0.00000	0.00000
126	N1	S	0.27273	-0.22168	0.00000	-0.65558	-0.69961
127	N1	PX	-0.07039	0.49795	0.00000	-0.25869	-0.12042
128	N1	PY	0.32673	-0.36452	0.00000	-0.69708	-0.92731
129	N1	PZ	0.00000	0.00000	-1.51403	0.00000	0.00000
130	N1	DXX	0.02060	0.03103	0.00000	0.02813	-0.04825
131	N1	DYY	-0.00718	-0.00603	0.00000	0.03648	-0.06161
132	N1	DZZ	-0.01784	0.02609	0.00000	-0.00904	0.02173
133	N1	DXY	0.02780	0.00702	0.00000	-0.03907	-0.04660
134	N1	DXZ	0.00000	0.00000	0.04814	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.01921	0.00000	0.00000
136	H6	S	0.14534	-0.23023	0.00000	0.17851	0.13615
137	H6	S	-1.69128	1.23714	0.00000	-0.95466	0.37991
138	H6	PX	-0.08929	0.07584	0.00000	-0.06576	0.01048
139	H6	PY	-0.00209	-0.02689	0.00000	-0.01525	0.00183
140	H6	PZ	0.00000	0.00000	-0.01159	0.00000	0.00000
141	C8	S	0.00664	0.00054	0.00000	0.00278	-0.01994
142	C8	S	0.20223	0.17648	0.00000	0.14697	-0.27329
143	C8	PX	0.24871	0.09104	0.00000	-0.15870	-0.46762
144	C8	PY	0.11548	0.06466	0.00000	0.06945	-0.15561
145	C8	PZ	0.00000	0.00000	-0.17311	0.00000	0.00000
146	C8	S	-1.14689	-0.82305	0.00000	-0.13973	1.20743
147	C8	PX	-1.51533	-0.25296	0.00000	0.61968	2.24809
148	C8	PY	-0.87249	-0.61949	0.00000	-0.21094	1.39999
149	C8	PZ	0.00000	0.00000	0.65172	0.00000	0.00000

150	C8	DXX	0.00693	-0.04576	0.00000	0.00092	0.06237
151	C8	DYY	0.01364	0.02035	0.00000	0.02505	-0.08530
152	C8	DZZ	0.00576	0.01873	0.00000	0.00000	-0.00939
153	C8	DXY	-0.01691	0.02242	0.00000	0.01910	0.04331
154	C8	DXZ	0.00000	0.00000	0.02388	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.04817	0.00000	0.00000
156	H8	S	-0.07820	-0.02704	0.00000	0.10042	-0.12421
157	H8	S	1.41266	0.19734	0.00000	-0.55942	0.54773
158	H8	PX	-0.05885	-0.01592	0.00000	0.03632	-0.04408
159	H8	PY	0.03062	-0.00421	0.00000	-0.00304	0.02535
160	H8	PZ	0.00000	0.00000	-0.00961	0.00000	0.00000
161	C10	S	-0.01086	0.00475	0.00000	0.00313	-0.01620
162	C10	S	0.15292	0.11517	0.00000	-0.06240	-0.07303
163	C10	PX	-0.53911	0.12922	0.00000	0.00792	-0.10317
164	C10	PY	0.02316	0.01869	0.00000	0.00615	-0.22663
165	C10	PZ	0.00000	0.00000	-0.05425	0.00000	0.00000
166	C10	S	-0.61062	-0.41966	0.00000	0.06110	0.72734
167	C10	PX	1.76168	-0.30700	0.00000	-0.15516	-0.01185
168	C10	PY	-0.20853	-0.25237	0.00000	-0.08945	0.91707
169	C10	PZ	0.00000	0.00000	-0.08302	0.00000	0.00000
170	C10	DXX	-0.02818	0.01462	0.00000	0.01487	-0.08763
171	C10	DYY	0.00385	0.01055	0.00000	-0.00947	0.01405
172	C10	DZZ	0.02680	-0.00346	0.00000	-0.01576	0.04924
173	C10	DXY	-0.07116	0.00044	0.00000	0.01269	0.00423
174	C10	DXZ	0.00000	0.00000	0.04584	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	-0.01389	0.00000	0.00000
176	H16	S	0.06006	0.01312	0.00000	-0.03790	-0.28706
177	H16	S	-0.90755	0.07101	0.00000	0.03554	0.44720
178	H16	PX	0.03399	-0.01343	0.00000	0.00581	-0.00686
179	H16	PY	-0.03953	0.00762	0.00000	0.00704	0.02563
180	H16	PZ	0.00000	0.00000	0.00919	0.00000	0.00000
181	H18	S	-0.20992	-0.02972	0.00000	0.07859	-0.02687
182	H18	S	1.13908	-0.17302	0.00000	-0.20210	0.35309
183	H18	PX	0.06440	-0.01160	0.00000	-0.00488	0.04027
184	H18	PY	0.04515	-0.00043	0.00000	-0.01018	-0.02164
185	H18	PZ	0.00000	0.00000	-0.01369	0.00000	0.00000

MO:	86	87	88	89	90
Eigenvalues:	1.17402	1.20020	1.20276	1.21434	1.26398
(ev):	31.94659	32.65918	32.72891	33.04385	34.39462

		A	A	A	A	A	
1	H1	S	0.02982	0.15425	-0.02512	-0.00349	0.17840
2	H1	S	-0.01642	-0.18456	-0.13090	-0.06578	0.63368
3	H1	PX	-0.00079	0.01526	0.00471	-0.00137	-0.02843
4	H1	PY	-0.00075	0.01216	-0.00375	-0.00353	0.02074
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00043	-0.00549	-0.00708	-0.00081	-0.00759
7	C1	S	-0.06755	0.34765	-0.27529	0.12050	0.00406
8	C1	PX	0.04921	-0.18605	-0.02605	-0.08978	0.30258
9	C1	PY	-0.02900	-0.11016	0.23567	0.66862	0.25385
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.05709	-1.55995	0.23819	-1.29299	-0.83817
12	C1	PX	0.03460	0.23998	0.03533	0.40369	-0.76290

13	C1	PY	0.13812	0.23158	-0.96220	-3.81727	-2.51393
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.01506	0.09285	-0.00417	0.02323	-0.01546
16	C1	DYY	0.00244	-0.05461	-0.05176	-0.03558	-0.03666
17	C1	DZZ	0.00448	-0.00586	-0.00328	0.01214	0.04332
18	C1	DXY	-0.00012	-0.00791	0.02814	0.13399	0.07887
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00378	0.00391	0.00514	-0.00095	0.00602
22	C2	S	0.22732	-0.36090	-0.14346	-0.01731	0.15227
23	C2	PX	-0.01359	-0.14057	0.23699	-0.00288	0.22004
24	C2	PY	0.02847	-0.17489	-0.44312	0.12019	-0.18691
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.62406	1.88838	0.72687	0.35458	0.57820
27	C2	PX	-0.08463	0.34407	-0.24005	-0.05462	-0.79441
28	C2	PY	0.21044	1.32691	2.62770	-1.22201	3.18247
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01515	-0.07404	0.04534	-0.03311	0.00484
31	C2	DYY	0.01010	0.04205	-0.02651	0.02238	0.06641
32	C2	DZZ	0.00189	-0.00075	-0.02789	0.01855	-0.03776
33	C2	DXY	-0.01155	0.02994	0.10390	-0.03178	0.03956
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00064	-0.01691	0.01196	0.01546	-0.00012
37	C3	S	0.09304	-0.25381	0.17235	0.39603	0.12115
38	C3	PX	0.07569	-0.16453	-0.15801	0.28299	0.39109
39	C3	PY	-0.09202	-0.22271	0.22287	0.27148	-0.01952
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.41952	1.51557	0.24854	-3.02710	0.41529
42	C3	PX	-0.22632	0.57515	0.01236	-1.22808	-2.81676
43	C3	PY	0.40820	-0.02519	-0.48145	-0.92170	-1.37299
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.01984	-0.00689	0.02157	-0.02161	0.10048
46	C3	DYY	-0.02341	-0.01259	0.05255	0.03138	-0.04985
47	C3	DZZ	0.00830	-0.00794	-0.02493	0.01637	-0.00246
48	C3	DXY	0.01598	0.00546	-0.09004	-0.09059	-0.00497
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00389	0.03589	-0.00719	0.00592	-0.00346
52	C4	S	-0.06130	0.95229	-0.29495	-0.29042	-0.43402
53	C4	PX	0.15713	-0.24603	-0.21065	-0.53497	-0.02683
54	C4	PY	0.10127	0.38069	-0.18968	0.17592	0.37645
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.09990	-3.68930	0.69608	2.17466	0.62021
57	C4	PX	-0.47829	1.91673	0.96408	3.17756	1.96570
58	C4	PY	-0.19932	-1.62233	0.09430	-1.30887	-1.90869
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00332	-0.02465	-0.03117	-0.02011	-0.04903
61	C4	DYY	-0.03247	0.15276	0.02758	0.03902	-0.01408
62	C4	DZZ	0.01167	0.01379	-0.02476	-0.02185	0.00498
63	C4	DXY	-0.00875	0.01329	0.02124	-0.13067	-0.01064
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00506	-0.03562	0.00534	-0.02091	0.01112

67	C5	S	0.12064	-0.71041	0.37952	-0.64821	0.28367
68	C5	PX	0.04192	-0.34590	-0.19971	-0.08425	-0.15529
69	C5	PY	0.13953	-0.40662	-0.21747	-0.10079	-0.01835
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.56635	2.04909	-1.85001	3.38599	-1.49108
72	C5	PX	-0.13249	2.54989	1.52706	0.57690	2.54843
73	C5	PY	-0.26009	2.02415	0.81927	0.46335	1.50861
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.01340	0.01516	0.01666	0.00844	-0.00670
76	C5	DYY	0.02403	-0.13713	0.02368	-0.09960	0.02490
77	C5	DZZ	0.00180	-0.00064	0.00325	0.00221	0.00326
78	C5	DXY	0.01664	-0.02790	-0.09909	0.08860	-0.01449
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00362	0.01127	-0.01671	-0.00441	0.00683
82	C6	S	0.22548	0.00731	-0.71668	0.21291	0.47793
83	C6	PX	0.01189	0.00726	0.28164	-0.22466	0.45889
84	C6	PY	-0.12125	0.13837	-0.03506	-0.00409	-0.07566
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.05713	0.38652	3.58425	-1.43611	-1.33693
87	C6	PX	-0.31697	-0.33185	-1.75955	1.19538	-3.22320
88	C6	PY	0.17908	-0.09473	-0.31675	-0.05305	1.58787
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01593	0.02789	-0.01338	-0.02724	0.04086
91	C6	DYY	0.03097	0.01510	0.02129	0.00037	0.03170
92	C6	DZZ	-0.00401	-0.01444	-0.03711	0.02904	-0.00852
93	C6	DXY	-0.03440	-0.00245	0.03290	0.01251	-0.10589
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00345	0.00828	-0.01009	-0.00074	-0.01602
97	C7	S	0.08350	-0.27386	0.27957	0.43891	-0.57739
98	C7	PX	0.11993	0.13093	-0.04332	0.18815	-0.08773
99	C7	PY	-0.15456	-0.06913	0.38695	0.09112	-0.01390
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.15908	-0.01967	-0.24102	-0.49171	0.91196
102	C7	PX	-0.47843	-0.15750	0.06766	-0.50881	1.00507
103	C7	PY	0.72599	-0.58314	-1.04769	0.25107	0.03226
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.04215	-0.04086	0.03900	0.00997	-0.07766
106	C7	DYY	0.04307	0.00038	-0.01082	0.03111	0.00811
107	C7	DZZ	0.00897	-0.00496	-0.00030	0.01406	-0.01006
108	C7	DXY	-0.00554	0.03024	0.05358	-0.01270	0.01595
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.04781	0.15901	0.13852	-0.06487	0.12199
112	H3	S	0.28303	0.81409	-0.63899	-0.21501	0.35505
113	H3	PX	-0.00370	-0.02095	0.00474	0.00375	0.00010
114	H3	PY	-0.01988	-0.04504	0.04639	0.02075	-0.01778
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.00839	-0.07042	0.17849	-0.22074	0.01434
117	H4	S	0.19953	-0.62980	0.05735	-0.24348	0.18890
118	H4	PX	0.01387	-0.01809	-0.01617	-0.01871	0.02825
119	H4	PY	-0.00895	0.03032	-0.00574	0.00930	-0.00002
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

121	N1	S	0.01386	-0.00735	-0.00269	0.00488	0.00297
122	N1	S	-0.05895	0.04656	-0.22175	-0.04685	-0.07672
123	N1	PX	0.13272	0.06901	-0.11266	-0.08660	-0.01055
124	N1	PY	-0.08366	0.13138	0.25103	-0.03497	-0.31504
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.01992	-0.04897	-0.38978	0.36216	0.16757
127	N1	PX	-0.31967	-0.02024	0.52236	-0.16813	0.34862
128	N1	PY	-0.05802	-0.16423	-1.28405	0.29980	0.67328
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.00473	0.03278	-0.02793	-0.01518	0.02806
131	N1	DYY	0.00108	-0.03702	-0.13240	0.01536	-0.02815
132	N1	DZZ	-0.03357	-0.00731	0.01309	-0.00058	-0.01728
133	N1	DXY	0.01098	-0.01298	-0.04327	0.03308	0.04829
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.02761	-0.07790	0.20001	-0.00233	-0.20073
137	H6	S	0.06008	0.14334	-0.41071	0.03213	-0.41419
138	H6	PX	0.00982	0.00600	-0.04339	-0.00182	-0.01086
139	H6	PY	0.01174	-0.00761	-0.01114	-0.01366	0.01810
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00514	0.00803	0.01300	-0.01142	-0.00522
142	C8	S	-0.27157	0.21871	0.36240	-0.35597	-0.20155
143	C8	PX	-0.09786	0.10837	-0.03349	-0.08860	0.11672
144	C8	PY	0.08733	0.15060	0.18001	-0.08374	0.02727
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.72681	-0.59598	-1.40413	1.01669	0.88660
147	C8	PX	0.28867	-0.14063	0.35052	-0.11025	-0.25600
148	C8	PY	0.00175	-0.15192	-0.55630	-0.45321	0.43465
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.01477	-0.00023	-0.03786	-0.06146	-0.00267
151	C8	DYY	-0.00163	0.04755	0.06814	-0.02468	0.00842
152	C8	DZZ	-0.01630	-0.00853	-0.00500	0.01393	-0.00880
153	C8	DXY	-0.01850	-0.01860	0.03514	0.00282	-0.02917
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.03794	-0.18092	-0.18951	0.10342	-0.06811
157	H8	S	0.61753	0.08502	-0.08783	0.43705	-0.65646
158	H8	PX	-0.01725	-0.01819	-0.00725	-0.03463	0.01572
159	H8	PY	0.01462	0.00080	-0.01749	-0.01368	-0.02375
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.01956	-0.00068	0.00709	0.01095	-0.00503
162	C10	S	-1.08540	-0.04953	-0.10628	0.08333	0.31377
163	C10	PX	-0.03293	0.02342	0.19243	-0.01595	0.09102
164	C10	PY	0.52524	0.18242	0.24474	-0.00558	0.01001
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	2.26069	0.35197	0.49022	-0.83420	-0.55050
167	C10	PX	0.07093	-0.26290	-0.52147	0.21881	-0.35028
168	C10	PY	-0.89295	-0.28458	-0.57391	-0.32526	0.15355
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.15461	0.03697	0.07684	0.02278	-0.01016
171	C10	DYY	-0.11933	-0.01599	-0.01465	0.00019	-0.00017
172	C10	DZZ	-0.13357	-0.02425	-0.05887	-0.00187	0.04114
173	C10	DXY	-0.02055	-0.04529	0.00171	0.02498	-0.02062
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.50713	0.19854	0.05267	-0.01495	0.04475
177	H16	S	-1.33270	-0.25463	-0.22129	-0.05092	0.39493
178	H16	PX	0.11384	0.01373	0.01124	0.00628	-0.02611
179	H16	PY	-0.02789	-0.02136	0.00888	0.01244	-0.00809
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.55364	-0.07371	0.15066	0.17433	-0.16281
182	H18	S	-1.22153	-0.27387	-0.75350	0.03319	0.15690
183	H18	PX	-0.09914	-0.01813	-0.04504	-0.00080	0.00088
184	H18	PY	-0.01555	0.01729	-0.01413	-0.01162	0.01957
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	91	92	93	94	95
Eigenvalues:	1.28550	1.29727	1.37046	1.40396	1.42126
(ev):	34.98037	35.30045	37.29226	38.20382	38.67438

			A	A	A	A	A
1	H1	S	0.08176	0.32724	0.15722	-0.30634	-0.03606
2	H1	S	-0.02695	0.38163	0.42653	-0.30806	-0.04483
3	H1	PX	0.01234	0.00127	-0.02084	-0.01848	-0.00855
4	H1	PY	0.01871	-0.01196	0.01444	-0.00484	-0.02472
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00066	0.01213	0.01388	0.02867	0.01285
7	C1	S	0.29001	0.69833	-0.10942	0.49163	0.16520
8	C1	PX	-0.14965	-0.02991	0.29158	-0.12523	0.03211
9	C1	PY	-0.02896	-0.04825	-0.03227	0.13323	-0.11749
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.12888	-2.00109	-1.35539	-2.39296	-1.03875
12	C1	PX	-0.11789	-0.19617	-0.65799	1.55221	0.31980
13	C1	PY	1.04893	-1.92623	1.63202	0.46968	0.29624
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.05804	0.08845	0.02382	0.00571	0.03950
16	C1	DYY	-0.00334	-0.00541	-0.07681	0.02875	-0.00672
17	C1	DZZ	-0.00271	0.02603	0.01414	-0.01331	-0.03332
18	C1	DXY	0.04332	0.04223	-0.04458	-0.01454	-0.06889
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.00488	0.02849	0.00422	0.01894	0.01561
22	C2	S	0.10943	0.71394	0.68584	0.38720	0.43304
23	C2	PX	-0.09137	0.04622	0.32807	-0.12236	0.03778
24	C2	PY	0.25441	0.03002	0.10944	-0.11050	-0.17597
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.85015	-2.66294	-1.04144	-2.34365	-1.60061
27	C2	PX	0.52175	0.02981	-0.17769	0.23828	-0.35260
28	C2	PY	-1.59912	-0.34802	-1.28915	1.04880	-0.08324
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.02458	0.10596	0.09063	0.08192	0.04987
31	C2	DYY	-0.04705	-0.01826	0.02015	-0.01507	0.01613
32	C2	DZZ	0.03518	0.00385	0.00305	-0.01658	-0.02109
33	C2	DXY	-0.06637	-0.00258	-0.06779	0.02503	0.06818
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.01468	-0.02188	-0.02150	-0.00165	-0.00108
37	C3	S	0.75768	-0.34630	-0.59223	-0.20060	-0.16853

38	C3	PX	-0.34584	0.24689	-0.22166	-0.21903	0.03637
39	C3	PY	-0.06371	-0.14317	0.04520	0.06427	-0.40622
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.92276	0.44397	2.72739	2.56475	-0.24545
42	C3	PX	2.14701	-2.05724	1.80153	1.20666	0.16241
43	C3	PY	-0.36205	-0.70337	0.79418	0.58811	1.61450
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.06279	-0.08470	-0.00898	0.01259	-0.03283
46	C3	DYY	0.09910	-0.02870	-0.02030	0.04790	-0.00016
47	C3	DZZ	-0.02325	0.04019	-0.01903	-0.04811	-0.01672
48	C3	DXY	0.00575	0.00763	-0.01232	0.02368	-0.00616
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.01411	-0.02515	0.00801	-0.00098	0.00729
52	C4	S	-0.48466	-0.56098	0.22895	-0.00156	0.34241
53	C4	PX	0.06291	-0.11912	0.09107	-0.10442	-0.07766
54	C4	PY	0.18599	0.05491	0.03764	-0.08651	-0.22133
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.88028	3.08138	-1.51700	0.91761	-0.00728
57	C4	PX	-1.31833	1.37951	-0.50643	-0.04630	0.43602
58	C4	PY	0.19437	-0.47262	-0.48189	-0.24234	0.64138
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.06072	-0.01445	-0.01793	-0.01309	0.06553
61	C4	DYY	-0.03733	-0.07835	0.03797	0.08045	0.02918
62	C4	DZZ	0.01574	0.01011	0.01225	-0.05523	-0.05023
63	C4	DXY	-0.04375	-0.09783	0.04114	-0.04163	-0.00685
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00082	-0.01153	-0.02313	-0.00057	-0.00013
67	C5	S	-0.32325	-0.09708	-0.70142	-0.30423	0.05905
68	C5	PX	0.08772	0.25010	0.14531	-0.17029	0.08149
69	C5	PY	0.39333	-0.07417	0.17228	0.15922	-0.13632
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.30782	1.53529	2.47264	-0.01419	0.96419
72	C5	PX	-1.28314	-1.02690	-0.74840	0.11005	-0.63324
73	C5	PY	-1.69900	0.00968	-0.15886	-0.30626	0.40362
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.08350	-0.01309	-0.07596	-0.03750	0.04544
76	C5	DYY	0.02216	0.01425	-0.03177	-0.01234	0.00866
77	C5	DZZ	0.01574	-0.00742	0.00444	-0.00675	-0.05144
78	C5	DXY	0.03588	0.08726	0.09820	-0.01128	0.02265
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.01131	-0.01195	0.00271	-0.01395	-0.02923
82	C6	S	-0.11480	-0.59621	0.20704	-0.18734	-0.34913
83	C6	PX	-0.26191	0.08022	0.12299	0.05287	-0.03888
84	C6	PY	0.14445	0.08223	0.11042	-0.34829	-0.52072
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.90232	0.77606	-0.29715	0.06570	0.49993
87	C6	PX	1.66999	-1.34615	0.42272	-0.51427	0.91178
88	C6	PY	-1.19651	-0.26400	-1.37201	2.21260	1.51123
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.08865	-0.12690	0.01935	0.01684	-0.03221
91	C6	DYY	-0.05800	0.03266	0.02509	-0.10169	-0.06317

92	C6	DZZ	-0.00934	0.00975	-0.00121	0.01960	0.01284
93	C6	DXY	0.01740	0.01748	0.00033	-0.10850	-0.05043
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01781	0.01049	0.00780	-0.01511	0.00797
97	C7	S	-0.16064	-0.21952	0.46560	0.00645	0.09638
98	C7	PX	0.13173	0.01317	-0.23737	0.06710	-0.11892
99	C7	PY	-0.10337	-0.08076	0.00901	0.22930	0.11754
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.29567	0.04003	-0.20298	-0.07480	1.04069
102	C7	PX	0.24149	0.87128	-0.21329	-0.44117	0.11201
103	C7	PY	-0.90890	0.54323	-1.16364	-1.70549	0.21837
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.04811	-0.04501	0.10678	-0.00598	-0.02124
106	C7	DYY	0.00944	0.04401	-0.00731	-0.02627	0.05857
107	C7	DZZ	-0.01769	-0.01898	-0.00852	0.01823	-0.01690
108	C7	DXY	0.03029	0.03877	0.06300	0.02121	-0.03033
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.02153	-0.35358	0.35934	0.03713	-0.19324
112	H3	S	0.14151	-0.24210	0.38368	-0.12784	-0.35953
113	H3	PX	-0.01774	0.02202	0.02805	-0.00887	0.01961
114	H3	PY	-0.00126	-0.01223	-0.00942	0.02440	-0.00494
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.18353	-0.19809	-0.33728	-0.03815	-0.30464
117	H4	S	0.40461	-0.34485	-0.30493	0.14481	-0.41194
118	H4	PX	0.00331	-0.02407	0.02287	-0.00591	-0.01451
119	H4	PY	-0.01175	0.00270	0.00630	-0.02448	-0.01057
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.00220	-0.00896	-0.00331	0.01448	0.01691
122	N1	S	-0.21259	0.09644	-0.32931	0.02551	-0.05693
123	N1	PX	-0.15482	-0.04556	-0.19598	0.14738	0.06348
124	N1	PY	-0.07960	0.21213	-0.04439	-0.56504	-0.20312
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.18370	0.43118	-0.37392	-0.36359	0.02813
127	N1	PX	0.02983	0.65977	0.29038	-0.60997	-0.49118
128	N1	PY	0.16782	-1.14489	0.24206	1.80582	1.35697
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.06661	0.06116	-0.12914	0.00278	-0.02666
131	N1	DYY	-0.05870	-0.01632	-0.05546	0.08035	0.03666
132	N1	DZZ	0.01829	0.00402	0.01874	-0.01576	-0.00077
133	N1	DXY	-0.02600	-0.06159	-0.01238	0.02902	0.06025
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.20989	0.15595	0.15235	0.33899	0.09566
137	H6	S	0.32292	0.30529	-0.03528	0.32257	0.02483
138	H6	PX	0.00097	0.00663	-0.02504	0.00758	0.00531
139	H6	PY	0.02640	-0.01923	-0.00505	0.03134	-0.01595
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.00231	0.01392	0.01506	0.02035	-0.03931
142	C8	S	-0.18717	0.61489	0.23334	0.50812	-0.93291
143	C8	PX	0.12829	-0.01745	0.13013	0.13961	0.01819
144	C8	PY	0.26971	0.10939	-0.00452	-0.35960	0.44445
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

146	C8	S	1.08124	-1.70960	-0.97578	-2.61031	5.01961
147	C8	PX	-0.38628	1.58371	-1.64355	-1.67094	-1.11321
148	C8	PY	-0.82178	-0.76463	-0.34514	3.58371	-1.67611
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.04540	0.06596	0.04613	0.09253	-0.03749
151	C8	DYY	0.04923	0.00335	-0.00123	-0.03046	0.03081
152	C8	DZZ	-0.03020	-0.00166	-0.01707	0.01237	-0.02865
153	C8	DXY	-0.00019	0.02652	0.06281	-0.09352	-0.02367
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.45381	-0.16295	-0.02720	0.00512	-0.04302
157	H8	S	-0.05111	-0.28127	-0.05851	-0.06090	-0.13454
158	H8	PX	-0.04372	-0.00453	0.01627	-0.00897	0.01128
159	H8	PY	-0.00411	0.01594	0.00625	-0.02494	-0.01819
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00400	-0.00729	0.00009	-0.02719	0.02444
162	C10	S	0.60982	-0.38589	-0.09142	-0.59623	0.96214
163	C10	PX	0.11875	-0.01897	0.04527	0.12245	0.06046
164	C10	PY	0.26909	-0.10203	-0.02381	-0.04487	0.18165
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-1.77339	0.75961	0.12338	4.24857	-4.34075
167	C10	PX	-0.39742	-0.78787	1.04415	0.02630	0.18280
168	C10	PY	-0.85700	0.21952	-0.13781	1.76899	-1.60957
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.08486	-0.02775	0.01331	-0.13557	0.13646
171	C10	DYY	-0.02228	0.00075	-0.00499	0.06026	-0.10051
172	C10	DZZ	0.01225	-0.02774	-0.02066	0.01375	0.05349
173	C10	DXY	-0.03093	-0.07979	0.09428	0.01271	0.00941
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.12906	0.16168	-0.32658	-0.00299	0.05007
177	H16	S	0.10385	0.02986	-0.31721	0.00135	0.19028
178	H16	PX	-0.01155	0.00665	-0.00145	-0.02060	-0.01462
179	H16	PY	0.00178	-0.02161	0.04309	-0.03947	0.02355
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.04625	-0.24915	0.30252	-0.18571	0.17691
182	H18	S	-0.10693	-0.30206	0.14054	-0.06206	0.27466
183	H18	PX	-0.01338	0.00056	-0.01028	-0.02758	-0.00115
184	H18	PY	0.02227	0.02082	-0.03963	-0.00168	0.01812
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	96	97	98	99	100
Eigenvalues:	1.46880	1.47855	1.48237	1.57062	1.58697
(ev):	39.96810	40.23338	40.33727	42.73883	43.18366

		A	A	A	A	A	
1	H1	S	0.35209	0.00000	0.23318	0.00000	0.00000
2	H1	S	0.35735	0.00000	0.30278	0.00000	0.00000
3	H1	PX	0.02038	0.00000	-0.00957	0.00000	0.00000
4	H1	PY	-0.00626	0.00000	-0.00076	0.00000	0.00000
5	H1	PZ	0.00000	0.04687	0.00000	0.08627	0.13416
6	C1	S	0.02858	0.00000	0.02352	0.00000	0.00000
7	C1	S	0.83761	0.00000	0.11966	0.00000	0.00000
8	C1	PX	-0.20786	0.00000	0.15425	0.00000	0.00000

9	C1	PY	0.11396	0.00000	-0.03319	0.00000	0.00000
10	C1	PZ	0.00000	-0.00086	0.00000	0.05904	0.10554
11	C1	S	-2.56910	0.00000	-2.10165	0.00000	0.00000
12	C1	PX	-0.33384	0.00000	-0.54411	0.00000	0.00000
13	C1	PY	0.02333	0.00000	1.67934	0.00000	0.00000
14	C1	PZ	0.00000	0.02684	0.00000	-0.04023	-0.07801
15	C1	DXX	0.13022	0.00000	0.10175	0.00000	0.00000
16	C1	DYY	-0.01550	0.00000	-0.06327	0.00000	0.00000
17	C1	DZZ	-0.02005	0.00000	-0.03850	0.00000	0.00000
18	C1	DXY	-0.00044	0.00000	-0.00892	0.00000	0.00000
19	C1	DXZ	0.00000	0.10179	0.00000	0.20242	0.31469
20	C1	DYZ	0.00000	0.28078	0.00000	-0.16259	0.12329
21	C2	S	-0.00312	0.00000	-0.01794	0.00000	0.00000
22	C2	S	-0.26941	0.00000	-0.27514	0.00000	0.00000
23	C2	PX	-0.17505	0.00000	0.13011	0.00000	0.00000
24	C2	PY	-0.11624	0.00000	0.04906	0.00000	0.00000
25	C2	PZ	0.00000	-0.01510	0.00000	0.08056	-0.02043
26	C2	S	-0.50902	0.00000	2.14573	0.00000	0.00000
27	C2	PX	-0.77960	0.00000	-1.28472	0.00000	0.00000
28	C2	PY	0.82483	0.00000	-1.95828	0.00000	0.00000
29	C2	PZ	0.00000	0.04217	0.00000	-0.02004	-0.04447
30	C2	DXX	-0.05654	0.00000	-0.13208	0.00000	0.00000
31	C2	DYY	-0.00653	0.00000	0.09923	0.00000	0.00000
32	C2	DZZ	0.01135	0.00000	-0.01296	0.00000	0.00000
33	C2	DXY	0.03686	0.00000	0.01120	0.00000	0.00000
34	C2	DXZ	0.00000	-0.10342	0.00000	-0.25299	0.04389
35	C2	DYZ	0.00000	0.25735	0.00000	-0.13521	-0.13824
36	C3	S	-0.02373	0.00000	0.01995	0.00000	0.00000
37	C3	S	-0.70914	0.00000	0.00682	0.00000	0.00000
38	C3	PX	-0.24486	0.00000	-0.14085	0.00000	0.00000
39	C3	PY	-0.06796	0.00000	-0.31938	0.00000	0.00000
40	C3	PZ	0.00000	-0.02475	0.00000	-0.04917	-0.05419
41	C3	S	2.74285	0.00000	0.27212	0.00000	0.00000
42	C3	PX	1.81043	0.00000	3.79255	0.00000	0.00000
43	C3	PY	-0.90454	0.00000	1.09394	0.00000	0.00000
44	C3	PZ	0.00000	-0.02445	0.00000	0.12206	0.00673
45	C3	DXX	-0.01649	0.00000	-0.04923	0.00000	0.00000
46	C3	DYY	-0.01161	0.00000	0.09565	0.00000	0.00000
47	C3	DZZ	-0.01584	0.00000	-0.06522	0.00000	0.00000
48	C3	DXY	0.00806	0.00000	-0.04340	0.00000	0.00000
49	C3	DXZ	0.00000	-0.24107	0.00000	0.17967	0.13608
50	C3	DYZ	0.00000	-0.25201	0.00000	-0.09060	-0.32590
51	C4	S	-0.01305	0.00000	-0.00744	0.00000	0.00000
52	C4	S	-0.48679	0.00000	-0.22960	0.00000	0.00000
53	C4	PX	-0.10235	0.00000	0.07744	0.00000	0.00000
54	C4	PY	0.09991	0.00000	-0.01972	0.00000	0.00000
55	C4	PZ	0.00000	-0.02140	0.00000	0.04130	0.02045
56	C4	S	1.15906	0.00000	0.34801	0.00000	0.00000
57	C4	PX	0.91413	0.00000	-0.64028	0.00000	0.00000
58	C4	PY	0.56774	0.00000	0.03957	0.00000	0.00000
59	C4	PZ	0.00000	0.01092	0.00000	-0.00419	-0.02130
60	C4	DXX	-0.04617	0.00000	0.03550	0.00000	0.00000
61	C4	DYY	-0.01891	0.00000	-0.00475	0.00000	0.00000
62	C4	DZZ	-0.01320	0.00000	-0.04808	0.00000	0.00000

63	C4	DXY	-0.08643	0.00000	0.03964	0.00000	0.00000
64	C4	DXZ	0.00000	0.26205	0.00000	-0.11781	0.08316
65	C4	DYZ	0.00000	-0.02566	0.00000	0.23723	0.16087
66	C5	S	0.00752	0.00000	0.01711	0.00000	0.00000
67	C5	S	0.26518	0.00000	0.50402	0.00000	0.00000
68	C5	PX	-0.08230	0.00000	0.08124	0.00000	0.00000
69	C5	PY	-0.03450	0.00000	-0.21202	0.00000	0.00000
70	C5	PZ	0.00000	-0.01841	0.00000	0.03776	0.02920
71	C5	S	-0.51248	0.00000	-0.16967	0.00000	0.00000
72	C5	PX	0.90215	0.00000	-0.82078	0.00000	0.00000
73	C5	PY	-0.80435	0.00000	0.36843	0.00000	0.00000
74	C5	PZ	0.00000	0.00622	0.00000	-0.01744	0.02584
75	C5	DXX	0.00715	0.00000	0.04775	0.00000	0.00000
76	C5	DYY	0.05002	0.00000	0.03697	0.00000	0.00000
77	C5	DZZ	-0.01279	0.00000	-0.03464	0.00000	0.00000
78	C5	DXY	-0.05132	0.00000	0.02029	0.00000	0.00000
79	C5	DXZ	0.00000	-0.25596	0.00000	0.08227	-0.01447
80	C5	DYZ	0.00000	-0.04628	0.00000	0.25346	0.12361
81	C6	S	0.00336	0.00000	-0.00846	0.00000	0.00000
82	C6	S	0.25616	0.00000	0.00842	0.00000	0.00000
83	C6	PX	0.10424	0.00000	-0.46359	0.00000	0.00000
84	C6	PY	-0.06757	0.00000	-0.02901	0.00000	0.00000
85	C6	PZ	0.00000	-0.00656	0.00000	-0.02943	-0.04813
86	C6	S	-0.42322	0.00000	0.24520	0.00000	0.00000
87	C6	PX	0.15126	0.00000	4.68138	0.00000	0.00000
88	C6	PY	2.23739	0.00000	0.36925	0.00000	0.00000
89	C6	PZ	0.00000	-0.02832	0.00000	-0.01305	0.22659
90	C6	DXX	0.05100	0.00000	0.02919	0.00000	0.00000
91	C6	DYY	-0.02527	0.00000	-0.08077	0.00000	0.00000
92	C6	DZZ	-0.01269	0.00000	0.01819	0.00000	0.00000
93	C6	DXY	-0.00342	0.00000	-0.06839	0.00000	0.00000
94	C6	DXZ	0.00000	0.26754	0.00000	-0.21345	-0.09119
95	C6	DYZ	0.00000	-0.20465	0.00000	-0.16717	0.08240
96	C7	S	-0.00372	0.00000	0.03741	0.00000	0.00000
97	C7	S	0.03504	0.00000	0.61443	0.00000	0.00000
98	C7	PX	-0.02993	0.00000	-0.08502	0.00000	0.00000
99	C7	PY	-0.18598	0.00000	0.08666	0.00000	0.00000
100	C7	PZ	0.00000	-0.09141	0.00000	-0.05841	-0.04640
101	C7	S	0.00293	0.00000	-2.79485	0.00000	0.00000
102	C7	PX	-1.20302	0.00000	1.74568	0.00000	0.00000
103	C7	PY	-1.77834	0.00000	-2.05526	0.00000	0.00000
104	C7	PZ	0.00000	0.11677	0.00000	-0.07420	-0.00298
105	C7	DXX	0.06880	0.00000	-0.03590	0.00000	0.00000
106	C7	DYY	-0.05533	0.00000	0.10270	0.00000	0.00000
107	C7	DZZ	0.00568	0.00000	-0.04428	0.00000	0.00000
108	C7	DXY	0.03810	0.00000	0.01162	0.00000	0.00000
109	C7	DXZ	0.00000	-0.20173	0.00000	-0.28350	0.12062
110	C7	DYZ	0.00000	0.07140	0.00000	0.03346	0.36828
111	H3	S	-0.42691	0.00000	-0.01238	0.00000	0.00000
112	H3	S	-0.49435	0.00000	-0.06675	0.00000	0.00000
113	H3	PX	-0.01519	0.00000	0.01670	0.00000	0.00000
114	H3	PY	-0.01343	0.00000	-0.00601	0.00000	0.00000
115	H3	PZ	0.00000	0.02945	0.00000	0.07090	0.06825
116	H4	S	0.39287	0.00000	-0.09257	0.00000	0.00000

117	H4	S	0.46767	0.00000	-0.24050	0.00000	0.00000
118	H4	PX	-0.02004	0.00000	0.00794	0.00000	0.00000
119	H4	PY	0.00576	0.00000	0.01490	0.00000	0.00000
120	H4	PZ	0.00000	0.02986	0.00000	0.07325	0.06004
121	N1	S	-0.00358	0.00000	-0.00023	0.00000	0.00000
122	N1	S	-0.14004	0.00000	0.02303	0.00000	0.00000
123	N1	PX	0.07524	0.00000	-0.15027	0.00000	0.00000
124	N1	PY	0.03745	0.00000	-0.13100	0.00000	0.00000
125	N1	PZ	0.00000	-0.08370	0.00000	-0.03790	0.11746
126	N1	S	0.19625	0.00000	-0.30537	0.00000	0.00000
127	N1	PX	-0.20929	0.00000	-1.16943	0.00000	0.00000
128	N1	PY	1.40402	0.00000	1.39159	0.00000	0.00000
129	N1	PZ	0.00000	0.08964	0.00000	-0.03504	-0.28934
130	N1	DXX	-0.08345	0.00000	-0.00689	0.00000	0.00000
131	N1	DYY	0.00184	0.00000	0.02265	0.00000	0.00000
132	N1	DZZ	-0.00168	0.00000	0.01057	0.00000	0.00000
133	N1	DXY	0.04268	0.00000	0.06570	0.00000	0.00000
134	N1	DXZ	0.00000	0.14574	0.00000	0.01123	0.04183
135	N1	DYZ	0.00000	0.00931	0.00000	0.20030	-0.10882
136	H6	S	-0.23095	0.00000	-0.44504	0.00000	0.00000
137	H6	S	-0.17698	0.00000	-0.70455	0.00000	0.00000
138	H6	PX	0.02866	0.00000	0.00152	0.00000	0.00000
139	H6	PY	0.01429	0.00000	-0.01798	0.00000	0.00000
140	H6	PZ	0.00000	0.03852	0.00000	0.11335	-0.02391
141	C8	S	0.00335	0.00000	0.00297	0.00000	0.00000
142	C8	S	0.02437	0.00000	0.15914	0.00000	0.00000
143	C8	PX	0.33581	0.00000	-0.06204	0.00000	0.00000
144	C8	PY	-0.00788	0.00000	-0.40484	0.00000	0.00000
145	C8	PZ	0.00000	0.09873	0.00000	0.01253	-0.02662
146	C8	S	-0.30531	0.00000	-0.68199	0.00000	0.00000
147	C8	PX	-3.57722	0.00000	-0.48597	0.00000	0.00000
148	C8	PY	0.21873	0.00000	5.04708	0.00000	0.00000
149	C8	PZ	0.00000	-0.24358	0.00000	0.05252	0.10779
150	C8	DXX	0.00931	0.00000	0.00429	0.00000	0.00000
151	C8	DYY	0.01051	0.00000	-0.00100	0.00000	0.00000
152	C8	DZZ	-0.00341	0.00000	0.01512	0.00000	0.00000
153	C8	DXY	-0.00802	0.00000	-0.00142	0.00000	0.00000
154	C8	DXZ	0.00000	0.00858	0.00000	0.23838	-0.31908
155	C8	DYZ	0.00000	0.20601	0.00000	0.15923	-0.15634
156	H8	S	0.14954	0.00000	-0.43854	0.00000	0.00000
157	H8	S	0.19932	0.00000	-0.59414	0.00000	0.00000
158	H8	PX	-0.00306	0.00000	-0.05076	0.00000	0.00000
159	H8	PY	-0.02030	0.00000	-0.02237	0.00000	0.00000
160	H8	PZ	0.00000	-0.06973	0.00000	-0.14697	-0.01716
161	C10	S	0.00261	0.00000	-0.02273	0.00000	0.00000
162	C10	S	0.06467	0.00000	-0.36424	0.00000	0.00000
163	C10	PX	-0.02956	0.00000	0.16886	0.00000	0.00000
164	C10	PY	0.04756	0.00000	0.09353	0.00000	0.00000
165	C10	PZ	0.00000	0.04396	0.00000	0.03654	-0.07658
166	C10	S	-0.03913	0.00000	4.51643	0.00000	0.00000
167	C10	PX	2.03054	0.00000	-0.29469	0.00000	0.00000
168	C10	PY	-0.24883	0.00000	1.74596	0.00000	0.00000
169	C10	PZ	0.00000	0.07836	0.00000	-0.01761	0.02753
170	C10	DXX	0.02321	0.00000	-0.12451	0.00000	0.00000

171	C10	DYY	-0.01209	0.00000	0.08516	0.00000	0.00000
172	C10	DZZ	-0.00545	0.00000	0.00617	0.00000	0.00000
173	C10	DXY	0.14377	0.00000	-0.01235	0.00000	0.00000
174	C10	DXZ	0.00000	-0.00871	0.00000	0.13069	-0.16458
175	C10	DYZ	0.00000	-0.15089	0.00000	-0.12950	0.17589
176	H16	S	-0.39299	0.00000	0.00913	0.00000	0.00000
177	H16	S	-0.62793	0.00000	0.08507	0.00000	0.00000
178	H16	PX	0.00307	0.00000	-0.02055	0.00000	0.00000
179	H16	PY	0.04130	0.00000	-0.03147	0.00000	0.00000
180	H16	PZ	0.00000	0.04569	0.00000	0.08034	-0.10348
181	H18	S	0.41741	0.00000	-0.09664	0.00000	0.00000
182	H18	S	0.51922	0.00000	-0.24699	0.00000	0.00000
183	H18	PX	-0.00320	0.00000	-0.02819	0.00000	0.00000
184	H18	PY	-0.04204	0.00000	-0.02539	0.00000	0.00000
185	H18	PZ	0.00000	0.04294	0.00000	-0.01564	0.01945

MO:	101	102	103	104	105
Eigenvalues:	1.60573	1.61528	1.62909	1.64045	1.67320
(ev):	43.69417	43.95390	44.32986	44.63889	45.53021

		A	A	A	A	A	
1	H1	S	0.23470	0.00000	0.05320	0.00000	0.64365
2	H1	S	0.43635	0.00000	-0.06868	0.00000	1.09696
3	H1	PX	0.01240	0.00000	-0.02394	0.00000	0.03991
4	H1	PY	0.01161	0.00000	0.03883	0.00000	-0.00900
5	H1	PZ	0.00000	0.06181	0.00000	-0.02292	0.00000
6	C1	S	-0.00321	0.00000	0.04221	0.00000	-0.02074
7	C1	S	-0.06720	0.00000	0.56814	0.00000	-0.60185
8	C1	PX	0.02954	0.00000	-0.01459	0.00000	0.26696
9	C1	PY	0.00961	0.00000	0.09405	0.00000	0.12267
10	C1	PZ	0.00000	0.03294	0.00000	0.00550	0.00000
11	C1	S	1.30979	0.00000	-4.60293	0.00000	1.50755
12	C1	PX	-1.47670	0.00000	1.06435	0.00000	-3.36563
13	C1	PY	0.37033	0.00000	2.44930	0.00000	0.39395
14	C1	PZ	0.00000	0.07764	0.00000	-0.04001	0.00000
15	C1	DXX	0.03508	0.00000	0.09068	0.00000	0.06796
16	C1	DYY	-0.02836	0.00000	-0.01168	0.00000	-0.10330
17	C1	DZZ	0.01968	0.00000	-0.06557	0.00000	0.02037
18	C1	DXY	0.03328	0.00000	-0.02864	0.00000	-0.03828
19	C1	DXZ	0.00000	0.08318	0.00000	-0.04438	0.00000
20	C1	DYZ	0.00000	-0.05265	0.00000	0.15297	0.00000
21	C2	S	-0.03955	0.00000	0.03774	0.00000	-0.02240
22	C2	S	-0.39828	0.00000	0.68530	0.00000	-0.58081
23	C2	PX	0.02904	0.00000	0.15409	0.00000	-0.22243
24	C2	PY	-0.25256	0.00000	0.11771	0.00000	0.03574
25	C2	PZ	0.00000	-0.03971	0.00000	-0.06354	0.00000
26	C2	S	3.96853	0.00000	-3.59111	0.00000	1.89652
27	C2	PX	1.13775	0.00000	-2.34958	0.00000	3.08026
28	C2	PY	-1.09815	0.00000	0.29035	0.00000	0.09477
29	C2	PZ	0.00000	0.13075	0.00000	0.07116	0.00000
30	C2	DXX	-0.05529	0.00000	-0.00505	0.00000	0.04023
31	C2	DYY	0.01490	0.00000	0.02005	0.00000	-0.09318
32	C2	DZZ	0.06170	0.00000	-0.02452	0.00000	0.03575
33	C2	DXY	-0.07482	0.00000	0.02012	0.00000	0.01844

34	C2	DXZ	0.00000	0.11161	0.00000	0.22930	0.00000
35	C2	DYZ	0.00000	-0.15221	0.00000	0.01240	0.00000
36	C3	S	-0.02363	0.00000	0.00302	0.00000	0.01699
37	C3	S	-0.66667	0.00000	-0.35574	0.00000	0.22284
38	C3	PX	-0.10405	0.00000	-0.43006	0.00000	-0.40360
39	C3	PY	0.34631	0.00000	-0.06764	0.00000	-0.14553
40	C3	PZ	0.00000	0.06151	0.00000	-0.00847	0.00000
41	C3	S	1.20682	0.00000	1.25758	0.00000	-1.32959
42	C3	PX	1.00935	0.00000	4.09456	0.00000	1.70346
43	C3	PY	-1.99571	0.00000	3.27783	0.00000	0.54717
44	C3	PZ	0.00000	-0.20145	0.00000	0.04106	0.00000
45	C3	DXX	-0.12205	0.00000	0.03196	0.00000	0.07715
46	C3	DYY	0.01818	0.00000	0.03822	0.00000	-0.05557
47	C3	DZZ	0.03394	0.00000	-0.09836	0.00000	0.00415
48	C3	DXY	-0.03233	0.00000	-0.01399	0.00000	-0.03982
49	C3	DXZ	0.00000	-0.06615	0.00000	0.14317	0.00000
50	C3	DYZ	0.00000	-0.02239	0.00000	-0.28288	0.00000
51	C4	S	-0.00132	0.00000	-0.00856	0.00000	0.01375
52	C4	S	0.06266	0.00000	-0.41206	0.00000	0.35643
53	C4	PX	-0.04035	0.00000	0.17537	0.00000	-0.24352
54	C4	PY	0.00240	0.00000	0.13305	0.00000	-0.05123
55	C4	PZ	0.00000	-0.01856	0.00000	-0.08921	0.00000
56	C4	S	-1.06085	0.00000	0.21046	0.00000	-1.81053
57	C4	PX	-0.03521	0.00000	-0.89652	0.00000	0.81995
58	C4	PY	0.95012	0.00000	-0.75453	0.00000	1.99137
59	C4	PZ	0.00000	-0.02418	0.00000	0.06265	0.00000
60	C4	DXX	-0.00841	0.00000	-0.08338	0.00000	0.07306
61	C4	DYY	-0.05312	0.00000	0.05946	0.00000	-0.07764
62	C4	DZZ	0.06484	0.00000	-0.03161	0.00000	0.02548
63	C4	DXY	0.00738	0.00000	-0.01505	0.00000	0.00204
64	C4	DXZ	0.00000	-0.26325	0.00000	-0.10994	0.00000
65	C4	DYZ	0.00000	-0.04471	0.00000	-0.30412	0.00000
66	C5	S	-0.00129	0.00000	-0.01284	0.00000	0.00479
67	C5	S	0.07479	0.00000	-0.29164	0.00000	0.23483
68	C5	PX	0.01428	0.00000	-0.09271	0.00000	0.28473
69	C5	PY	0.09426	0.00000	0.01119	0.00000	0.01024
70	C5	PZ	0.00000	-0.01748	0.00000	-0.08131	0.00000
71	C5	S	-0.66601	0.00000	1.37744	0.00000	-0.98912
72	C5	PX	0.20175	0.00000	0.26432	0.00000	-0.78882
73	C5	PY	-0.49973	0.00000	-1.20466	0.00000	0.99533
74	C5	PZ	0.00000	-0.02070	0.00000	0.05941	0.00000
75	C5	DXX	-0.01134	0.00000	-0.07592	0.00000	0.07414
76	C5	DYY	-0.05646	0.00000	0.08550	0.00000	-0.07159
77	C5	DZZ	0.08503	0.00000	-0.04297	0.00000	0.02465
78	C5	DXY	-0.04963	0.00000	0.03577	0.00000	0.00121
79	C5	DXZ	0.00000	0.30798	0.00000	0.18005	0.00000
80	C5	DYZ	0.00000	-0.06338	0.00000	-0.30973	0.00000
81	C6	S	-0.01564	0.00000	-0.02094	0.00000	0.02038
82	C6	S	0.16709	0.00000	-0.36215	0.00000	0.41215
83	C6	PX	-0.19417	0.00000	0.14815	0.00000	0.28917
84	C6	PY	0.39410	0.00000	-0.06301	0.00000	-0.04230
85	C6	PZ	0.00000	0.07717	0.00000	0.04945	0.00000
86	C6	S	-1.80798	0.00000	5.99370	0.00000	-0.13841
87	C6	PX	2.92039	0.00000	-0.16674	0.00000	-1.09720

88	C6	PY	-3.31005	0.00000	0.33309	0.00000	-1.67574
89	C6	PZ	0.00000	-0.12498	0.00000	-0.18171	0.00000
90	C6	DXX	-0.05657	0.00000	0.06072	0.00000	0.08067
91	C6	DYY	-0.04720	0.00000	0.07254	0.00000	-0.00808
92	C6	DZZ	0.09747	0.00000	-0.08619	0.00000	-0.00100
93	C6	DXY	-0.06010	0.00000	0.01974	0.00000	0.04359
94	C6	DXZ	0.00000	0.10668	0.00000	-0.18580	0.00000
95	C6	DYZ	0.00000	0.16496	0.00000	-0.03529	0.00000
96	C7	S	0.04381	0.00000	0.01866	0.00000	-0.00284
97	C7	S	0.83474	0.00000	0.11226	0.00000	-0.19352
98	C7	PX	-0.21692	0.00000	0.12044	0.00000	0.06689
99	C7	PY	0.15999	0.00000	0.20574	0.00000	-0.00639
100	C7	PZ	0.00000	-0.06268	0.00000	-0.12865	0.00000
101	C7	S	-3.45760	0.00000	-1.37941	0.00000	-0.48163
102	C7	PX	0.83051	0.00000	-2.18185	0.00000	-0.86266
103	C7	PY	-0.70204	0.00000	0.69440	0.00000	0.47067
104	C7	PZ	0.00000	0.15542	0.00000	0.07644	0.00000
105	C7	DXX	0.09430	0.00000	0.09873	0.00000	0.00439
106	C7	DYY	0.01718	0.00000	-0.03440	0.00000	-0.01474
107	C7	DZZ	-0.03555	0.00000	-0.04725	0.00000	0.02414
108	C7	DXY	0.05791	0.00000	-0.10896	0.00000	-0.05843
109	C7	DXZ	0.00000	-0.09901	0.00000	-0.21162	0.00000
110	C7	DYZ	0.00000	0.01264	0.00000	0.23441	0.00000
111	H3	S	-0.12234	0.00000	0.18169	0.00000	-0.35215
112	H3	S	-0.19015	0.00000	0.30020	0.00000	-0.64776
113	H3	PX	-0.01628	0.00000	-0.00251	0.00000	0.01010
114	H3	PY	-0.00625	0.00000	0.00095	0.00000	-0.03423
115	H3	PZ	0.00000	-0.07731	0.00000	-0.15162	0.00000
116	H4	S	0.22069	0.00000	0.16750	0.00000	-0.19237
117	H4	S	0.37220	0.00000	0.23115	0.00000	-0.39060
118	H4	PX	-0.00019	0.00000	0.00030	0.00000	-0.01944
119	H4	PY	0.00706	0.00000	0.01587	0.00000	-0.02379
120	H4	PZ	0.00000	-0.09620	0.00000	-0.15832	0.00000
121	N1	S	0.00471	0.00000	-0.00225	0.00000	0.00044
122	N1	S	0.09928	0.00000	0.18761	0.00000	-0.08806
123	N1	PX	0.15628	0.00000	-0.01977	0.00000	-0.03524
124	N1	PY	-0.33350	0.00000	0.15179	0.00000	-0.06519
125	N1	PZ	0.00000	-0.01191	0.00000	-0.02854	0.00000
126	N1	S	-0.15982	0.00000	-0.14620	0.00000	-0.42149
127	N1	PX	-0.75668	0.00000	0.35364	0.00000	0.23253
128	N1	PY	1.41658	0.00000	-1.99517	0.00000	-1.08595
129	N1	PZ	0.00000	0.01214	0.00000	0.09910	0.00000
130	N1	DXX	0.06359	0.00000	0.04519	0.00000	-0.01318
131	N1	DYY	-0.00175	0.00000	0.00075	0.00000	-0.03579
132	N1	DZZ	0.00113	0.00000	-0.00001	0.00000	0.02305
133	N1	DXY	-0.05802	0.00000	-0.01337	0.00000	0.00304
134	N1	DXZ	0.00000	0.20278	0.00000	-0.10764	0.00000
135	N1	DYZ	0.00000	-0.23406	0.00000	0.13400	0.00000
136	H6	S	-0.00172	0.00000	-0.25534	0.00000	0.56581
137	H6	S	0.08559	0.00000	-0.52950	0.00000	0.97426
138	H6	PX	-0.01493	0.00000	0.02173	0.00000	-0.04102
139	H6	PY	0.02641	0.00000	0.00877	0.00000	-0.01611
140	H6	PZ	0.00000	-0.01781	0.00000	-0.10407	0.00000
141	C8	S	-0.00205	0.00000	-0.01933	0.00000	0.00202

142	C8	S	-0.34885	0.00000	-0.47075	0.00000	-0.00898
143	C8	PX	-0.20779	0.00000	-0.44455	0.00000	-0.21274
144	C8	PY	0.33708	0.00000	-0.08884	0.00000	-0.20834
145	C8	PZ	0.00000	-0.00388	0.00000	0.01628	0.00000
146	C8	S	4.36494	0.00000	-0.45535	0.00000	-1.78246
147	C8	PX	0.58506	0.00000	3.08165	0.00000	1.64697
148	C8	PY	-4.19067	0.00000	0.40119	0.00000	1.44049
149	C8	PZ	0.00000	0.01917	0.00000	-0.03718	0.00000
150	C8	DXX	0.11733	0.00000	-0.10037	0.00000	-0.07435
151	C8	DYY	0.02887	0.00000	-0.00886	0.00000	-0.03904
152	C8	DZZ	-0.07850	0.00000	0.01934	0.00000	0.06899
153	C8	DXY	-0.01820	0.00000	0.02019	0.00000	0.00163
154	C8	DXZ	0.00000	-0.18752	0.00000	0.14082	0.00000
155	C8	DYZ	0.00000	0.37288	0.00000	-0.05044	0.00000
156	H8	S	0.12507	0.00000	0.67939	0.00000	0.26270
157	H8	S	-0.07844	0.00000	0.95111	0.00000	0.39436
158	H8	PX	0.02544	0.00000	0.03823	0.00000	0.02108
159	H8	PY	0.01667	0.00000	-0.03878	0.00000	-0.01580
160	H8	PZ	0.00000	-0.01468	0.00000	-0.14691	0.00000
161	C10	S	0.03075	0.00000	0.00390	0.00000	-0.01121
162	C10	S	0.20284	0.00000	0.16609	0.00000	-0.12054
163	C10	PX	0.09807	0.00000	0.00150	0.00000	0.00136
164	C10	PY	-0.29059	0.00000	0.11132	0.00000	0.07779
165	C10	PZ	0.00000	0.13965	0.00000	-0.02475	0.00000
166	C10	S	-4.78029	0.00000	0.23405	0.00000	1.83212
167	C10	PX	-1.26447	0.00000	-1.56879	0.00000	-0.74253
168	C10	PY	-1.68857	0.00000	0.09094	0.00000	0.81819
169	C10	PZ	0.00000	-0.10333	0.00000	0.02708	0.00000
170	C10	DXX	0.08434	0.00000	0.01743	0.00000	-0.06108
171	C10	DYY	-0.10277	0.00000	0.03004	0.00000	0.05091
172	C10	DZZ	-0.00200	0.00000	-0.01360	0.00000	0.02693
173	C10	DXY	-0.09188	0.00000	-0.09460	0.00000	-0.03470
174	C10	DXZ	0.00000	-0.17938	0.00000	0.16650	0.00000
175	C10	DYZ	0.00000	-0.32017	0.00000	0.04691	0.00000
176	H16	S	0.33587	0.00000	0.25345	0.00000	0.09543
177	H16	S	0.43461	0.00000	0.45279	0.00000	0.24638
178	H16	PX	-0.02746	0.00000	0.00459	0.00000	0.00900
179	H16	PY	-0.00259	0.00000	-0.02302	0.00000	-0.01947
180	H16	PZ	0.00000	0.02362	0.00000	0.05373	0.00000
181	H18	S	-0.10308	0.00000	-0.27759	0.00000	-0.16883
182	H18	S	-0.28653	0.00000	-0.47463	0.00000	-0.22871
183	H18	PX	-0.00794	0.00000	0.01184	0.00000	-0.00055
184	H18	PY	0.04578	0.00000	0.02161	0.00000	0.00430
185	H18	PZ	0.00000	0.13878	0.00000	-0.07727	0.00000

MO:	106	107	108	109	110
Eigenvalues:	1.67544	1.69183	1.70830	1.71739	1.75678
(ev):	45.59108	46.03698	46.48529	46.73262	47.80450

		A	A	A	A	A	
1	H1	S	0.00000	0.00000	0.00000	0.18877	0.00000
2	H1	S	0.00000	0.00000	0.00000	0.39725	0.00000
3	H1	PX	0.00000	0.00000	0.00000	0.01369	0.00000
4	H1	PY	0.00000	0.00000	0.00000	0.02313	0.00000

5	H1	PZ	-0.11533	-0.08923	-0.13202	0.00000	-0.05594
6	C1	S	0.00000	0.00000	0.00000	-0.00257	0.00000
7	C1	S	0.00000	0.00000	0.00000	0.06141	0.00000
8	C1	PX	0.00000	0.00000	0.00000	-0.01189	0.00000
9	C1	PY	0.00000	0.00000	0.00000	-0.27039	0.00000
10	C1	PZ	-0.08720	-0.05664	-0.08988	0.00000	-0.04050
11	C1	S	0.00000	0.00000	0.00000	-0.16957	0.00000
12	C1	PX	0.00000	0.00000	0.00000	-0.95131	0.00000
13	C1	PY	0.00000	0.00000	0.00000	0.46300	0.00000
14	C1	PZ	0.12742	-0.00768	0.06374	0.00000	0.07131
15	C1	DXX	0.00000	0.00000	0.00000	0.03049	0.00000
16	C1	DYY	0.00000	0.00000	0.00000	-0.02803	0.00000
17	C1	DZZ	0.00000	0.00000	0.00000	0.04741	0.00000
18	C1	DXY	0.00000	0.00000	0.00000	0.08502	0.00000
19	C1	DXZ	-0.27503	-0.15978	-0.20844	0.00000	-0.09342
20	C1	DYZ	0.15515	0.20716	-0.08253	0.00000	-0.07058
21	C2	S	0.00000	0.00000	0.00000	-0.01510	0.00000
22	C2	S	0.00000	0.00000	0.00000	-0.26223	0.00000
23	C2	PX	0.00000	0.00000	0.00000	-0.09078	0.00000
24	C2	PY	0.00000	0.00000	0.00000	0.17020	0.00000
25	C2	PZ	0.13779	-0.02831	-0.07732	0.00000	-0.00489
26	C2	S	0.00000	0.00000	0.00000	1.96870	0.00000
27	C2	PX	0.00000	0.00000	0.00000	1.18305	0.00000
28	C2	PY	0.00000	0.00000	0.00000	-0.09343	0.00000
29	C2	PZ	-0.15731	0.08355	-0.01151	0.00000	-0.05747
30	C2	DXX	0.00000	0.00000	0.00000	-0.02408	0.00000
31	C2	DYY	0.00000	0.00000	0.00000	-0.01570	0.00000
32	C2	DZZ	0.00000	0.00000	0.00000	0.02371	0.00000
33	C2	DXY	0.00000	0.00000	0.00000	0.09297	0.00000
34	C2	DXZ	-0.37765	0.06346	0.17859	0.00000	-0.01868
35	C2	DYZ	-0.12088	-0.31640	0.02135	0.00000	0.04371
36	C3	S	0.00000	0.00000	0.00000	0.01646	0.00000
37	C3	S	0.00000	0.00000	0.00000	0.28890	0.00000
38	C3	PX	0.00000	0.00000	0.00000	-0.24303	0.00000
39	C3	PY	0.00000	0.00000	0.00000	0.43542	0.00000
40	C3	PZ	0.02903	-0.02479	0.05502	0.00000	0.02598
41	C3	S	0.00000	0.00000	0.00000	-0.36275	0.00000
42	C3	PX	0.00000	0.00000	0.00000	3.64418	0.00000
43	C3	PY	0.00000	0.00000	0.00000	-4.71179	0.00000
44	C3	PZ	-0.15028	0.14342	-0.10873	0.00000	-0.14665
45	C3	DXX	0.00000	0.00000	0.00000	0.01213	0.00000
46	C3	DYY	0.00000	0.00000	0.00000	0.05542	0.00000
47	C3	DZZ	0.00000	0.00000	0.00000	-0.01514	0.00000
48	C3	DXY	0.00000	0.00000	0.00000	-0.01658	0.00000
49	C3	DXZ	-0.01274	-0.06082	0.34403	0.00000	0.22271
50	C3	DYZ	-0.06707	-0.02286	0.09469	0.00000	0.03032
51	C4	S	0.00000	0.00000	0.00000	-0.03518	0.00000
52	C4	S	0.00000	0.00000	0.00000	-0.66185	0.00000
53	C4	PX	0.00000	0.00000	0.00000	-0.10352	0.00000
54	C4	PY	0.00000	0.00000	0.00000	0.28739	0.00000
55	C4	PZ	-0.12278	-0.04437	0.02767	0.00000	0.00589
56	C4	S	0.00000	0.00000	0.00000	2.05968	0.00000
57	C4	PX	0.00000	0.00000	0.00000	-1.28250	0.00000
58	C4	PY	0.00000	0.00000	0.00000	-2.78021	0.00000

59	C4	PZ	0.05443	0.02186	-0.01387	0.00000	-0.00793
60	C4	DXX	0.00000	0.00000	0.00000	-0.03755	0.00000
61	C4	DYY	0.00000	0.00000	0.00000	-0.01356	0.00000
62	C4	DZZ	0.00000	0.00000	0.00000	0.05610	0.00000
63	C4	DXY	0.00000	0.00000	0.00000	0.06489	0.00000
64	C4	DXZ	-0.12380	0.22358	0.24843	0.00000	0.03639
65	C4	DYZ	-0.36740	-0.12138	0.00313	0.00000	-0.01615
66	C5	S	0.00000	0.00000	0.00000	0.03517	0.00000
67	C5	S	0.00000	0.00000	0.00000	0.74956	0.00000
68	C5	PX	0.00000	0.00000	0.00000	0.03968	0.00000
69	C5	PY	0.00000	0.00000	0.00000	-0.22056	0.00000
70	C5	PZ	0.06371	0.12183	0.00690	0.00000	-0.00069
71	C5	S	0.00000	0.00000	0.00000	-3.32226	0.00000
72	C5	PX	0.00000	0.00000	0.00000	-1.59912	0.00000
73	C5	PY	0.00000	0.00000	0.00000	3.19302	0.00000
74	C5	PZ	-0.01307	-0.08621	0.01572	0.00000	0.01088
75	C5	DXX	0.00000	0.00000	0.00000	-0.01023	0.00000
76	C5	DYY	0.00000	0.00000	0.00000	-0.03074	0.00000
77	C5	DZZ	0.00000	0.00000	0.00000	0.04315	0.00000
78	C5	DXY	0.00000	0.00000	0.00000	0.05761	0.00000
79	C5	DXZ	0.11412	-0.14703	-0.26506	0.00000	-0.06402
80	C5	DYZ	0.23229	0.29717	-0.06080	0.00000	-0.01869
81	C6	S	0.00000	0.00000	0.00000	-0.03676	0.00000
82	C6	S	0.00000	0.00000	0.00000	-0.65305	0.00000
83	C6	PX	0.00000	0.00000	0.00000	-0.03058	0.00000
84	C6	PY	0.00000	0.00000	0.00000	-0.20266	0.00000
85	C6	PZ	-0.05427	0.07636	-0.00733	0.00000	-0.01603
86	C6	S	0.00000	0.00000	0.00000	1.94103	0.00000
87	C6	PX	0.00000	0.00000	0.00000	2.91116	0.00000
88	C6	PY	0.00000	0.00000	0.00000	2.38710	0.00000
89	C6	PZ	0.19009	-0.23437	0.11718	0.00000	0.20531
90	C6	DXX	0.00000	0.00000	0.00000	-0.02017	0.00000
91	C6	DYY	0.00000	0.00000	0.00000	-0.11488	0.00000
92	C6	DZZ	0.00000	0.00000	0.00000	0.05800	0.00000
93	C6	DXY	0.00000	0.00000	0.00000	0.02438	0.00000
94	C6	DXZ	-0.04750	-0.08304	-0.33565	0.00000	-0.06527
95	C6	DYZ	-0.20113	0.38902	-0.04034	0.00000	-0.12448
96	C7	S	0.00000	0.00000	0.00000	0.01508	0.00000
97	C7	S	0.00000	0.00000	0.00000	0.12410	0.00000
98	C7	PX	0.00000	0.00000	0.00000	-0.01986	0.00000
99	C7	PY	0.00000	0.00000	0.00000	-0.20481	0.00000
100	C7	PZ	-0.00385	-0.04932	-0.03279	0.00000	0.06456
101	C7	S	0.00000	0.00000	0.00000	-3.26782	0.00000
102	C7	PX	0.00000	0.00000	0.00000	-0.30467	0.00000
103	C7	PY	0.00000	0.00000	0.00000	-2.43614	0.00000
104	C7	PZ	0.04210	0.02234	0.00253	0.00000	-0.10467
105	C7	DXX	0.00000	0.00000	0.00000	0.03273	0.00000
106	C7	DYY	0.00000	0.00000	0.00000	-0.05899	0.00000
107	C7	DZZ	0.00000	0.00000	0.00000	0.00418	0.00000
108	C7	DXY	0.00000	0.00000	0.00000	0.05152	0.00000
109	C7	DXZ	0.07121	-0.14705	-0.05723	0.00000	0.28102
110	C7	DYZ	0.09275	0.00454	0.04467	0.00000	0.17154
111	H3	S	0.00000	0.00000	0.00000	0.52633	0.00000
112	H3	S	0.00000	0.00000	0.00000	0.93395	0.00000

113	H3	PX	0.00000	0.00000	0.00000	0.02609	0.00000
114	H3	PY	0.00000	0.00000	0.00000	0.02738	0.00000
115	H3	PZ	-0.20349	-0.02175	0.07109	0.00000	0.00757
116	H4	S	0.00000	0.00000	0.00000	-0.52319	0.00000
117	H4	S	0.00000	0.00000	0.00000	-0.97332	0.00000
118	H4	PX	0.00000	0.00000	0.00000	0.03694	0.00000
119	H4	PY	0.00000	0.00000	0.00000	-0.02806	0.00000
120	H4	PZ	0.08027	0.18870	0.05172	0.00000	0.00870
121	N1	S	0.00000	0.00000	0.00000	0.02570	0.00000
122	N1	S	0.00000	0.00000	0.00000	0.53496	0.00000
123	N1	PX	0.00000	0.00000	0.00000	0.24219	0.00000
124	N1	PY	0.00000	0.00000	0.00000	-0.03141	0.00000
125	N1	PZ	-0.02838	0.09573	-0.02963	0.00000	-0.09685
126	N1	S	0.00000	0.00000	0.00000	-1.03275	0.00000
127	N1	PX	0.00000	0.00000	0.00000	-1.36071	0.00000
128	N1	PY	0.00000	0.00000	0.00000	1.87505	0.00000
129	N1	PZ	-0.13507	0.09192	-0.17085	0.00000	-0.14473
130	N1	DXX	0.00000	0.00000	0.00000	0.11647	0.00000
131	N1	DYY	0.00000	0.00000	0.00000	0.10846	0.00000
132	N1	DZZ	0.00000	0.00000	0.00000	0.00202	0.00000
133	N1	DXY	0.00000	0.00000	0.00000	0.00885	0.00000
134	N1	DXZ	0.11699	-0.16583	0.11267	0.00000	0.34653
135	N1	DYZ	0.08287	-0.21007	0.12886	0.00000	-0.05238
136	H6	S	0.00000	0.00000	0.00000	0.16673	0.00000
137	H6	S	0.00000	0.00000	0.00000	0.28139	0.00000
138	H6	PX	0.00000	0.00000	0.00000	-0.01158	0.00000
139	H6	PY	0.00000	0.00000	0.00000	0.00123	0.00000
140	H6	PZ	0.17994	-0.02468	-0.12280	0.00000	-0.00432
141	C8	S	0.00000	0.00000	0.00000	-0.00204	0.00000
142	C8	S	0.00000	0.00000	0.00000	-0.17247	0.00000
143	C8	PX	0.00000	0.00000	0.00000	0.13001	0.00000
144	C8	PY	0.00000	0.00000	0.00000	0.05338	0.00000
145	C8	PZ	0.00559	-0.01512	-0.01864	0.00000	-0.02693
146	C8	S	0.00000	0.00000	0.00000	2.13005	0.00000
147	C8	PX	0.00000	0.00000	0.00000	-2.81803	0.00000
148	C8	PY	0.00000	0.00000	0.00000	-0.12328	0.00000
149	C8	PZ	0.01338	0.01420	0.18985	0.00000	0.18452
150	C8	DXX	0.00000	0.00000	0.00000	0.03195	0.00000
151	C8	DYY	0.00000	0.00000	0.00000	0.01777	0.00000
152	C8	DZZ	0.00000	0.00000	0.00000	-0.01522	0.00000
153	C8	DXY	0.00000	0.00000	0.00000	-0.06177	0.00000
154	C8	DXZ	-0.12675	0.07347	-0.04130	0.00000	-0.28764
155	C8	DYZ	-0.02792	0.07264	0.19323	0.00000	0.12181
156	H8	S	0.00000	0.00000	0.00000	0.17034	0.00000
157	H8	S	0.00000	0.00000	0.00000	0.03792	0.00000
158	H8	PX	0.00000	0.00000	0.00000	-0.01419	0.00000
159	H8	PY	0.00000	0.00000	0.00000	-0.03700	0.00000
160	H8	PZ	0.02629	-0.07149	-0.04780	0.00000	0.09909
161	C10	S	0.00000	0.00000	0.00000	0.01201	0.00000
162	C10	S	0.00000	0.00000	0.00000	0.08936	0.00000
163	C10	PX	0.00000	0.00000	0.00000	0.01742	0.00000
164	C10	PY	0.00000	0.00000	0.00000	-0.06026	0.00000
165	C10	PZ	-0.02580	0.04612	0.05719	0.00000	0.02630
166	C10	S	0.00000	0.00000	0.00000	-1.07349	0.00000

167	C10	PX	0.00000	0.00000	0.00000	1.00817	0.00000
168	C10	PY	0.00000	0.00000	0.00000	-0.51510	0.00000
169	C10	PZ	0.02478	-0.05342	-0.09662	0.00000	-0.07295
170	C10	DXX	0.00000	0.00000	0.00000	0.00928	0.00000
171	C10	DYY	0.00000	0.00000	0.00000	-0.03298	0.00000
172	C10	DZZ	0.00000	0.00000	0.00000	0.01390	0.00000
173	C10	DXY	0.00000	0.00000	0.00000	0.05278	0.00000
174	C10	DXZ	-0.19235	0.20254	-0.33956	0.00000	0.45400
175	C10	DYZ	0.06200	-0.10906	-0.14789	0.00000	-0.12588
176	H16	S	0.00000	0.00000	0.00000	-0.07752	0.00000
177	H16	S	0.00000	0.00000	0.00000	-0.33391	0.00000
178	H16	PX	0.00000	0.00000	0.00000	-0.01413	0.00000
179	H16	PY	0.00000	0.00000	0.00000	0.00651	0.00000
180	H16	PZ	-0.09591	0.11699	-0.11468	0.00000	0.27146
181	H18	S	0.00000	0.00000	0.00000	0.20173	0.00000
182	H18	S	0.00000	0.00000	0.00000	0.30292	0.00000
183	H18	PX	0.00000	0.00000	0.00000	-0.00734	0.00000
184	H18	PY	0.00000	0.00000	0.00000	-0.00620	0.00000
185	H18	PZ	0.07312	-0.07348	0.19352	0.00000	-0.22480

MO:	111	112	113	114	115
Eigenvalues:	1.90008	1.98176	2.03536	2.08417	2.11203
(ev):	51.70382	53.92646	55.38507	56.71307	57.47129

		A	A	A	A	A	
1	H1	S	0.02940	0.17515	0.09118	-0.11837	0.00000
2	H1	S	0.14438	0.08649	0.17843	-0.63434	0.00000
3	H1	PX	-0.00262	0.03372	0.03374	-0.00606	0.00000
4	H1	PY	-0.06170	0.05499	-0.04336	-0.01170	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.20587
6	C1	S	-0.00964	-0.00174	-0.01986	0.03230	0.00000
7	C1	S	-0.00433	-0.11068	-0.27589	0.56810	0.00000
8	C1	PX	-0.01352	0.02930	0.03824	-0.09780	0.00000
9	C1	PY	-0.07302	0.14042	-0.00328	-0.17965	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.00250
11	C1	S	0.05080	0.14900	1.08214	-1.85854	0.00000
12	C1	PX	-0.37038	-0.33056	-0.81329	2.24590	0.00000
13	C1	PY	0.53350	-0.14059	-0.23857	-0.87888	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.48008
15	C1	DXX	0.01871	-0.09201	-0.00736	-0.14035	0.00000
16	C1	DYY	-0.12964	0.07321	0.10109	-0.04864	0.00000
17	C1	DZZ	0.15966	-0.00226	-0.12691	0.12514	0.00000
18	C1	DXY	-0.17550	0.05258	-0.09140	-0.09792	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.34103
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.42207
21	C2	S	0.00104	0.00416	-0.02034	-0.01253	0.00000
22	C2	S	0.31604	-0.05888	-0.19422	-0.52261	0.00000
23	C2	PX	0.14188	-0.04077	-0.03856	-0.20266	0.00000
24	C2	PY	-0.26215	0.04597	-0.05319	0.08971	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.01522
26	C2	S	-0.09818	0.18751	1.08387	1.07143	0.00000
27	C2	PX	-0.31860	1.26788	-0.08509	2.22179	0.00000
28	C2	PY	0.18056	1.21552	-0.93133	1.90685	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.14380

30	C2	DXX	-0.00630	0.04090	-0.00894	0.12069	0.00000
31	C2	DYY	-0.10289	0.06570	0.06111	-0.04176	0.00000
32	C2	DZZ	0.15039	-0.13318	-0.09575	-0.06630	0.00000
33	C2	DXY	0.11501	-0.15403	0.09875	0.12149	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.05656
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.20281
36	C3	S	0.02047	-0.01786	0.01937	-0.07343	0.00000
37	C3	S	0.29296	-0.28471	0.04949	-0.91219	0.00000
38	C3	PX	0.11855	0.03057	0.17901	0.21764	0.00000
39	C3	PY	-0.05758	-0.12683	0.06107	0.12365	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.04555
41	C3	S	-0.86425	3.39861	-3.17790	9.96294	0.00000
42	C3	PX	0.54557	-1.04434	0.70849	-4.36380	0.00000
43	C3	PY	1.26861	-0.06530	-0.25172	-3.25528	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.86932
45	C3	DXX	0.11577	0.04921	0.31377	0.03545	0.00000
46	C3	DYY	-0.15884	0.02215	-0.08473	-0.03810	0.00000
47	C3	DZZ	0.06128	-0.12858	-0.27590	0.15337	0.00000
48	C3	DXY	-0.29012	0.10117	0.05356	0.06636	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.01080
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01178
51	C4	S	0.00941	0.00724	-0.00239	-0.02620	0.00000
52	C4	S	0.24552	0.04898	-0.08888	-0.18904	0.00000
53	C4	PX	-0.07291	0.04056	-0.11248	-0.12492	0.00000
54	C4	PY	0.00246	-0.04635	0.08956	-0.00635	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.04257
56	C4	S	-1.32853	-0.57112	-0.11868	3.30968	0.00000
57	C4	PX	0.30213	0.27659	0.26037	-0.28252	0.00000
58	C4	PY	0.69161	0.46734	0.23824	-2.29405	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.13753
60	C4	DXX	-0.18743	0.10703	0.06213	-0.17453	0.00000
61	C4	DYY	0.04078	-0.09526	0.05877	0.06554	0.00000
62	C4	DZZ	0.15828	-0.03441	-0.18690	0.17716	0.00000
63	C4	DXY	-0.07492	0.00646	-0.03837	-0.13603	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.18362
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.11799
66	C5	S	-0.01443	-0.00687	-0.00064	0.02126	0.00000
67	C5	S	-0.08980	-0.22524	0.02461	0.40460	0.00000
68	C5	PX	0.09038	-0.03561	0.04777	0.08157	0.00000
69	C5	PY	0.08041	0.06799	-0.00656	-0.00174	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.04190
71	C5	S	0.74432	-0.54873	0.48183	-3.72751	0.00000
72	C5	PX	0.50777	0.72587	-0.45026	-0.55515	0.00000
73	C5	PY	-1.01402	-0.07987	0.31318	2.07201	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00538
75	C5	DXX	-0.19453	0.11786	0.05570	-0.19663	0.00000
76	C5	DYY	0.05276	-0.10846	0.09304	0.09085	0.00000
77	C5	DZZ	0.17750	-0.01503	-0.20972	0.07726	0.00000
78	C5	DXY	0.03836	-0.02432	0.02769	0.06622	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.11156
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.03737
81	C6	S	0.00641	0.01221	-0.00494	0.05276	0.00000
82	C6	S	0.16451	-0.05527	-0.35242	0.66161	0.00000
83	C6	PX	-0.12965	0.20537	-0.26857	0.09216	0.00000

84	C6	PY	0.08365	-0.01071	0.10788	-0.10468	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.01124
86	C6	S	2.85051	2.12872	-0.86057	-5.96872	0.00000
87	C6	PX	0.25890	-3.05906	2.60886	-5.17520	0.00000
88	C6	PY	-2.70575	-2.76494	0.66650	1.85488	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.49251
90	C6	DXX	0.05860	0.07198	0.28074	0.04098	0.00000
91	C6	DYY	-0.05791	0.18555	-0.13358	0.02239	0.00000
92	C6	DZZ	0.01835	-0.35302	-0.18986	-0.13657	0.00000
93	C6	DXY	0.30495	-0.04547	0.01114	0.03369	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.27417
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.05174
96	C7	S	0.01005	0.01926	-0.01921	0.05703	0.00000
97	C7	S	0.01090	0.47443	-0.49006	0.75172	0.00000
98	C7	PX	-0.03988	-0.01071	0.19701	0.00807	0.00000
99	C7	PY	0.08518	0.13521	0.04986	0.09658	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.02343
101	C7	S	0.12954	-2.28228	1.77772	-8.02278	0.00000
102	C7	PX	0.67999	2.26795	-1.63238	4.65758	0.00000
103	C7	PY	-0.39104	-1.10446	0.28462	-1.00422	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.61969
105	C7	DXX	-0.20204	0.06739	0.17453	0.13254	0.00000
106	C7	DYY	0.12064	0.01751	0.01897	-0.07171	0.00000
107	C7	DZZ	0.06219	-0.16725	-0.18614	-0.14434	0.00000
108	C7	DXY	0.17287	0.05864	0.18950	0.15017	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	-0.38225
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.30305
111	H3	S	-0.04368	-0.00948	-0.07350	0.24794	0.00000
112	H3	S	-0.12650	-0.19476	-0.13505	0.50404	0.00000
113	H3	PX	-0.04106	0.02859	-0.01167	-0.03247	0.00000
114	H3	PY	0.00068	-0.00418	-0.00478	0.07307	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.04617
116	H4	S	0.19260	0.16807	-0.17943	-0.11687	0.00000
117	H4	S	0.38859	0.16689	-0.23586	-0.42992	0.00000
118	H4	PX	0.02671	-0.02945	0.01889	0.09042	0.00000
119	H4	PY	0.03072	0.01270	-0.01598	0.02221	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.05559
121	N1	S	0.08565	0.08910	-0.04621	-0.04225	0.00000
122	N1	S	0.98045	1.33558	-0.55708	-0.43248	0.00000
123	N1	PX	0.03760	-0.07378	0.06332	0.03438	0.00000
124	N1	PY	-0.04858	0.09316	-0.02610	0.06970	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.03591
126	N1	S	-5.81602	-7.33317	2.92395	2.48490	0.00000
127	N1	PX	-1.75552	-1.30076	0.23340	1.17707	0.00000
128	N1	PY	-0.87967	-1.51130	1.08315	-1.01133	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.05002
130	N1	DXX	-0.04603	0.30220	-0.21267	-0.12999	0.00000
131	N1	DYY	0.29136	0.29127	0.05850	-0.02646	0.00000
132	N1	DZZ	0.08141	-0.22812	-0.05749	0.03002	0.00000
133	N1	DXY	-0.14204	-0.00832	-0.18790	0.11850	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.03257
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.25047
136	H6	S	-0.04391	0.28008	-0.09966	0.20662	0.00000
137	H6	S	-0.09299	0.40225	-0.10725	0.70521	0.00000

138	H6	PX	0.01467	-0.03041	-0.00295	0.01343	0.00000
139	H6	PY	-0.04319	0.09854	-0.04830	0.02880	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.01216
141	C8	S	0.01535	-0.02285	0.01501	-0.02609	0.00000
142	C8	S	0.10185	-0.45272	-0.08201	-0.66084	0.00000
143	C8	PX	-0.06922	0.09851	-0.07294	-0.11374	0.00000
144	C8	PY	-0.11535	-0.08615	-0.15752	-0.19249	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.02083
146	C8	S	0.10001	2.77681	-1.03706	2.03453	0.00000
147	C8	PX	-0.94532	-0.92407	-0.19404	4.09555	0.00000
148	C8	PY	3.32076	2.86887	-1.47792	3.46765	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.42237
150	C8	DXX	0.16161	0.06673	0.29160	-0.10719	0.00000
151	C8	DYY	-0.20008	0.08788	-0.03692	0.03962	0.00000
152	C8	DZZ	0.01833	-0.18769	-0.34929	0.06499	0.00000
153	C8	DXY	-0.04592	0.00779	0.06997	0.27434	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.14863
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.05066
156	H8	S	0.09455	-0.36557	0.13298	-0.28014	0.00000
157	H8	S	-0.40104	-0.70190	0.47527	-1.06420	0.00000
158	H8	PX	0.04276	-0.03650	0.07849	-0.02903	0.00000
159	H8	PY	-0.01062	0.06425	0.11473	0.13709	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	-0.27918
161	C10	S	-0.01241	-0.00095	-0.01290	-0.00471	0.00000
162	C10	S	0.07102	0.10602	-0.11128	0.06733	0.00000
163	C10	PX	0.01299	-0.00068	0.02936	0.08789	0.00000
164	C10	PY	0.25246	0.05011	-0.06122	0.11549	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.00791
166	C10	S	2.37426	1.10527	-0.50446	2.08001	0.00000
167	C10	PX	0.65192	0.70007	-0.12220	-1.78037	0.00000
168	C10	PY	0.83228	0.24483	-0.38357	0.96561	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.18896
170	C10	DXX	-0.03570	-0.01033	0.19438	-0.12890	0.00000
171	C10	DYY	-0.01321	0.03734	-0.00492	0.10434	0.00000
172	C10	DZZ	0.10981	-0.08323	-0.23412	0.02024	0.00000
173	C10	DXY	0.02910	0.02025	-0.07416	-0.15968	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00696
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.23782
176	H16	S	-0.13800	-0.11387	-0.16503	0.19646	0.00000
177	H16	S	-0.15476	-0.25671	0.01037	0.61402	0.00000
178	H16	PX	0.01717	-0.03017	-0.02351	-0.02358	0.00000
179	H16	PY	0.00567	-0.01681	0.06458	-0.01869	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.05896
181	H18	S	0.07762	0.12394	-0.11414	-0.12835	0.00000
182	H18	S	0.15755	0.15685	-0.09919	-0.60281	0.00000
183	H18	PX	-0.02789	0.00455	-0.01022	-0.00583	0.00000
184	H18	PY	0.01250	-0.02413	0.05826	-0.09602	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	-0.07617

MO:	116	117	118	119	120
Eigenvalues:	2.12691	2.14240	2.15746	2.17372	2.19360
(ev):	57.87625	58.29774	58.70737	59.15008	59.69093

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1	H1	S	0.01742	0.37347	-0.09247	0.29242	0.00000
2	H1	S	0.18940	-0.07792	-0.20469	0.31275	0.00000
3	H1	PX	-0.03467	0.13368	-0.03003	0.04406	0.00000
4	H1	PY	0.00609	0.06497	0.10831	0.10359	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.09428
6	C1	S	-0.00392	0.01150	0.00565	0.00135	0.00000
7	C1	S	-0.34964	-0.01618	0.20186	-0.25968	0.00000
8	C1	PX	0.19154	-0.01397	-0.05269	0.09260	0.00000
9	C1	PY	0.01746	-0.00701	0.02009	0.25208	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.02419
11	C1	S	0.53132	-0.60716	-0.31334	-0.22156	0.00000
12	C1	PX	-0.68750	-0.01928	0.73971	-1.04841	0.00000
13	C1	PY	0.24403	0.23005	-0.82891	0.16925	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.08162
15	C1	DXX	0.06965	-0.35439	0.00966	-0.12429	0.00000
16	C1	DYY	-0.01586	0.31288	0.00692	0.11781	0.00000
17	C1	DZZ	-0.13378	0.07588	-0.03529	0.02712	0.00000
18	C1	DXY	-0.14694	0.01810	0.24457	0.06518	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.11538
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.11178
21	C2	S	0.00809	0.00334	-0.02382	0.00701	0.00000
22	C2	S	0.00262	0.11543	-0.16572	0.28736	0.00000
23	C2	PX	-0.09164	0.09868	-0.00023	0.05482	0.00000
24	C2	PY	-0.07320	-0.15851	0.01481	-0.07285	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.03733
26	C2	S	-0.61206	0.05872	1.50775	-0.44557	0.00000
27	C2	PX	-0.19343	-0.36001	1.35445	-1.35181	0.00000
28	C2	PY	-0.01794	0.21352	0.68190	-0.64507	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.41519
30	C2	DXX	-0.03482	-0.19342	0.20738	0.29325	0.00000
31	C2	DYY	0.00613	0.11341	-0.17369	-0.28698	0.00000
32	C2	DZZ	-0.06660	0.12154	0.00876	-0.05484	0.00000
33	C2	DXY	0.21095	0.10497	0.08876	0.05256	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.35859
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.33951
36	C3	S	0.00549	0.01924	-0.02721	0.02585	0.00000
37	C3	S	0.03617	-0.23226	-0.72101	0.52035	0.00000
38	C3	PX	0.13170	0.05421	0.10131	-0.12823	0.00000
39	C3	PY	0.05849	-0.19197	0.13671	-0.27018	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00471
41	C3	S	-1.70075	0.22412	4.65998	-3.85308	0.00000
42	C3	PX	0.33738	0.32058	-1.99998	2.21387	0.00000
43	C3	PY	0.87950	0.50120	-2.12411	1.95329	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.17669
45	C3	DXX	0.07780	0.09961	-0.12605	-0.07378	0.00000
46	C3	DYY	0.01852	-0.09379	0.14237	0.00388	0.00000
47	C3	DZZ	-0.14383	0.00554	-0.07304	0.05103	0.00000
48	C3	DXY	0.10554	0.22235	-0.01445	0.31070	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.32473
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01075
51	C4	S	-0.00215	0.00942	-0.01884	0.00609	0.00000
52	C4	S	0.26979	-0.13377	-0.07337	0.24136	0.00000
53	C4	PX	-0.19624	0.00820	-0.01559	-0.17416	0.00000
54	C4	PY	-0.01472	0.03865	-0.05672	0.01216	0.00000

55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.04163
56	C4	S	-0.88120	-0.14615	1.70744	-1.39878	0.00000
57	C4	PX	0.52862	-0.18729	-0.29038	0.71316	0.00000
58	C4	PY	0.66899	-0.34480	-0.99117	0.70104	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.12790
60	C4	DXX	-0.24795	0.21109	0.08239	-0.05258	0.00000
61	C4	DYY	0.20173	-0.27708	-0.04925	-0.00101	0.00000
62	C4	DZZ	0.02491	0.10343	0.02468	0.05312	0.00000
63	C4	DXY	-0.17754	-0.22174	0.16447	0.03740	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.06279
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	-0.14790
66	C5	S	-0.01365	0.01465	0.01280	-0.01362	0.00000
67	C5	S	0.00029	-0.14755	0.15365	-0.09149	0.00000
68	C5	PX	0.21848	-0.12767	-0.06284	-0.09110	0.00000
69	C5	PY	0.08497	0.02004	-0.00301	-0.05660	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.02301
71	C5	S	0.83877	-0.09947	-2.02405	1.93913	0.00000
72	C5	PX	-0.20808	0.33478	-0.34585	0.39091	0.00000
73	C5	PY	-0.67340	-0.08526	1.38500	-0.64102	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.09400
75	C5	DXX	-0.30394	0.09110	-0.02763	-0.15004	0.00000
76	C5	DYY	0.23227	-0.13397	0.06291	0.21799	0.00000
77	C5	DZZ	0.06641	0.04671	-0.11173	-0.04758	0.00000
78	C5	DXY	0.15316	0.21340	-0.18267	-0.18986	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.21854
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	-0.15366
81	C6	S	-0.02569	0.01226	0.01697	-0.02591	0.00000
82	C6	S	-0.22715	-0.00046	0.58067	-0.08186	0.00000
83	C6	PX	-0.07954	-0.06033	0.09739	-0.06689	0.00000
84	C6	PY	0.13930	-0.05374	0.00043	0.15677	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.10351
86	C6	S	1.46429	0.41810	-3.13650	2.99920	0.00000
87	C6	PX	0.51505	0.55360	-2.09176	2.20825	0.00000
88	C6	PY	-0.66660	0.00133	0.02878	-0.92970	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.57872
90	C6	DXX	0.20101	0.15533	0.06372	-0.17317	0.00000
91	C6	DYY	-0.04649	-0.18000	-0.00689	0.05773	0.00000
92	C6	DZZ	-0.08499	0.07934	-0.10524	0.16222	0.00000
93	C6	DXY	-0.08923	0.05645	0.23303	0.12527	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	-0.04558
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.21656
96	C7	S	-0.02361	0.00750	0.02363	-0.00900	0.00000
97	C7	S	0.10695	0.24025	0.45916	-0.21567	0.00000
98	C7	PX	-0.18484	-0.09256	-0.00107	0.12410	0.00000
99	C7	PY	-0.08839	0.12970	-0.02281	0.17401	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.01998
101	C7	S	1.97028	-0.50443	-4.71436	2.72149	0.00000
102	C7	PX	-0.73801	0.40136	2.69082	-1.57631	0.00000
103	C7	PY	0.56671	-0.16564	-0.49673	-0.00121	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.12679
105	C7	DXX	0.08599	0.03052	-0.12921	0.28603	0.00000
106	C7	DYY	-0.08552	-0.12816	0.12686	-0.26589	0.00000
107	C7	DZZ	0.03514	0.18140	-0.09698	-0.00351	0.00000
108	C7	DXY	-0.22330	-0.06705	-0.13979	-0.13720	0.00000

109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.18491
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.16215
111	H3	S	-0.09472	0.38468	0.02067	-0.07433	0.00000
112	H3	S	-0.21243	0.05024	0.25429	-0.21186	0.00000
113	H3	PX	-0.13832	0.09029	0.04982	-0.02045	0.00000
114	H3	PY	0.05205	0.11025	-0.02312	-0.00323	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	-0.13255
116	H4	S	0.04142	0.24406	-0.28383	-0.24050	0.00000
117	H4	S	0.10287	0.02521	-0.28650	0.21856	0.00000
118	H4	PX	0.12114	-0.06326	0.04123	0.07270	0.00000
119	H4	PY	0.07923	0.06054	-0.09531	-0.06614	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.05147
121	N1	S	0.00474	-0.00093	0.00161	0.01045	0.00000
122	N1	S	0.07112	0.01978	-0.30916	0.40169	0.00000
123	N1	PX	-0.05743	0.11547	-0.15979	0.15101	0.00000
124	N1	PY	0.04102	0.06542	0.08349	-0.15864	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.15189
126	N1	S	-0.45473	0.15445	0.48504	-1.52365	0.00000
127	N1	PX	0.13288	-0.22824	0.29990	-0.80015	0.00000
128	N1	PY	0.01921	-0.12321	-0.66607	0.28769	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.44759
130	N1	DXX	0.28086	-0.17430	-0.23286	-0.15730	0.00000
131	N1	DYY	-0.09721	0.03841	0.17851	0.14846	0.00000
132	N1	DZZ	-0.16499	0.16304	-0.08410	0.05459	0.00000
133	N1	DXY	-0.02420	-0.15196	-0.20310	-0.05340	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.43058
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.22091
136	H6	S	0.00199	0.10496	-0.04035	-0.47999	0.00000
137	H6	S	-0.00285	-0.18365	0.42424	-0.33064	0.00000
138	H6	PX	0.01860	-0.06978	0.04534	0.14305	0.00000
139	H6	PY	-0.03033	-0.06997	-0.03733	-0.04902	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.24823
141	C8	S	-0.00714	0.01099	-0.01823	0.00744	0.00000
142	C8	S	-0.06164	0.13374	-0.20046	0.19464	0.00000
143	C8	PX	0.12178	-0.00514	0.05004	0.01403	0.00000
144	C8	PY	0.13915	0.03853	-0.12630	0.11751	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.07447
146	C8	S	0.29629	-0.11715	1.06627	-0.59982	0.00000
147	C8	PX	-0.85610	0.45738	2.01684	-1.19381	0.00000
148	C8	PY	-2.12853	0.47560	2.47951	-0.63981	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.40387
150	C8	DXX	-0.23275	-0.07741	0.12867	-0.04417	0.00000
151	C8	DYY	0.27722	-0.07699	-0.08607	0.03066	0.00000
152	C8	DZZ	-0.09188	0.18503	-0.04986	-0.00091	0.00000
153	C8	DXY	-0.24071	-0.09728	-0.24121	0.12990	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.05491
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.03811
156	H8	S	-0.14094	-0.08344	-0.14053	-0.20652	0.00000
157	H8	S	0.24746	-0.08957	-0.57794	0.43288	0.00000
158	H8	PX	-0.04384	0.00679	-0.08487	-0.04970	0.00000
159	H8	PY	-0.04813	0.03092	-0.09448	0.13107	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.04619
161	C10	S	0.00366	0.00628	-0.00850	0.00049	0.00000
162	C10	S	-0.14074	0.08254	0.07620	-0.00922	0.00000

163	C10	PX	-0.07439	-0.00217	-0.00904	0.00850	0.00000
164	C10	PY	-0.23805	0.09220	0.16679	-0.01835	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.01075
166	C10	S	-1.57266	0.27345	1.63386	-0.34240	0.00000
167	C10	PX	0.25312	-0.37596	-1.12029	0.50723	0.00000
168	C10	PY	-0.46002	0.16464	0.54687	-0.14582	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.23190
170	C10	DXX	-0.05174	-0.06585	0.10315	-0.05855	0.00000
171	C10	DYY	0.08432	-0.03125	-0.06578	0.05044	0.00000
172	C10	DZZ	-0.11644	0.15902	-0.01586	-0.01150	0.00000
173	C10	DXY	0.22905	0.10977	0.24681	-0.08766	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	-0.03228
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	-0.32286
176	H16	S	0.19392	0.20750	0.31019	-0.10703	0.00000
177	H16	S	-0.16299	0.08095	0.25155	-0.16122	0.00000
178	H16	PX	0.02709	0.05969	0.15239	-0.08540	0.00000
179	H16	PY	-0.07881	-0.02510	0.04458	-0.04363	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.09074
181	H18	S	-0.05963	-0.08658	-0.45216	0.17999	0.00000
182	H18	S	0.16481	-0.09134	-0.28434	0.09645	0.00000
183	H18	PX	0.10118	0.03001	0.12667	-0.05950	0.00000
184	H18	PY	-0.04532	-0.01909	-0.00296	0.00718	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.13287

M0:	121	122	123	124	125
Eigenvalues:	2.24660	2.27302	2.27957	2.28758	2.30563
(ev):	61.13308	61.85196	62.03024	62.24833	62.73932

			A	A	A	A	A
1	H1	S	-0.04482	0.00000	0.00000	-0.31917	-0.17840
2	H1	S	0.05061	0.00000	0.00000	-0.04154	0.00015
3	H1	PX	0.00427	0.00000	0.00000	-0.11732	-0.10293
4	H1	PY	-0.08468	0.00000	0.00000	0.17058	-0.03839
5	H1	PZ	0.00000	0.14686	-0.28243	0.00000	0.00000
6	C1	S	-0.01796	0.00000	0.00000	-0.01003	-0.00436
7	C1	S	0.05068	0.00000	0.00000	-0.19661	-0.09140
8	C1	PX	-0.07968	0.00000	0.00000	0.04517	0.07037
9	C1	PY	0.00017	0.00000	0.00000	0.03658	0.11544
10	C1	PZ	0.00000	0.02669	0.05752	0.00000	0.00000
11	C1	S	0.90026	0.00000	0.00000	0.88039	-0.64083
12	C1	PX	-0.23012	0.00000	0.00000	0.25347	0.36290
13	C1	PY	-0.26285	0.00000	0.00000	-0.82668	-0.23861
14	C1	PZ	0.00000	-0.36469	0.41287	0.00000	0.00000
15	C1	DXX	0.06010	0.00000	0.00000	0.23997	0.20338
16	C1	DYY	-0.02342	0.00000	0.00000	-0.04159	-0.02086
17	C1	DZZ	-0.02159	0.00000	0.00000	-0.24311	-0.29187
18	C1	DXY	-0.07037	0.00000	0.00000	0.32532	-0.09623
19	C1	DXZ	0.00000	0.17301	-0.30008	0.00000	0.00000
20	C1	DYZ	0.00000	-0.18267	-0.01078	0.00000	0.00000
21	C2	S	-0.01548	0.00000	0.00000	0.01677	0.01005
22	C2	S	0.10322	0.00000	0.00000	0.17969	0.11105
23	C2	PX	0.09901	0.00000	0.00000	0.03273	0.05506
24	C2	PY	0.00002	0.00000	0.00000	-0.05623	0.12098
25	C2	PZ	0.00000	0.01243	0.04865	0.00000	0.00000

26	C2	S	0.68377	0.00000	0.00000	-0.88507	0.22192
27	C2	PX	0.37682	0.00000	0.00000	0.08817	0.48929
28	C2	PY	-0.10111	0.00000	0.00000	0.71356	-0.08458
29	C2	PZ	0.00000	0.56589	0.10975	0.00000	0.00000
30	C2	DXX	-0.01186	0.00000	0.00000	-0.26523	-0.21651
31	C2	DYY	0.03079	0.00000	0.00000	0.02430	0.06114
32	C2	DZZ	0.00794	0.00000	0.00000	0.30692	0.24943
33	C2	DXY	0.03736	0.00000	0.00000	0.17144	-0.09673
34	C2	DXZ	0.00000	0.33145	0.12661	0.00000	0.00000
35	C2	DYZ	0.00000	0.17821	-0.03643	0.00000	0.00000
36	C3	S	-0.00381	0.00000	0.00000	-0.00888	-0.00588
37	C3	S	-0.07604	0.00000	0.00000	-0.31704	-0.04207
38	C3	PX	0.14157	0.00000	0.00000	0.17059	0.16417
39	C3	PY	0.14222	0.00000	0.00000	-0.11090	-0.05280
40	C3	PZ	0.00000	-0.04563	-0.05181	0.00000	0.00000
41	C3	S	-0.01404	0.00000	0.00000	-0.26916	2.39976
42	C3	PX	-0.66751	0.00000	0.00000	-1.24083	-0.36528
43	C3	PY	-0.96341	0.00000	0.00000	-0.21593	-0.83834
44	C3	PZ	0.00000	0.27051	-0.18900	0.00000	0.00000
45	C3	DXX	0.15854	0.00000	0.00000	-0.09624	-0.00391
46	C3	DYY	-0.13510	0.00000	0.00000	0.25313	-0.04569
47	C3	DZZ	-0.02006	0.00000	0.00000	-0.25164	0.13701
48	C3	DXY	-0.08131	0.00000	0.00000	-0.05309	0.27162
49	C3	DXZ	0.00000	0.01266	-0.18146	0.00000	0.00000
50	C3	DYZ	0.00000	-0.05159	-0.24541	0.00000	0.00000
51	C4	S	-0.00759	0.00000	0.00000	-0.00284	-0.02078
52	C4	S	-0.26125	0.00000	0.00000	0.17553	-0.41889
53	C4	PX	0.06120	0.00000	0.00000	0.06775	0.00376
54	C4	PY	0.11096	0.00000	0.00000	-0.16573	0.15473
55	C4	PZ	0.00000	0.03011	-0.03222	0.00000	0.00000
56	C4	S	0.09369	0.00000	0.00000	0.56127	1.47117
57	C4	PX	-0.09082	0.00000	0.00000	-0.18365	-0.07630
58	C4	PY	0.09321	0.00000	0.00000	0.14237	-0.87487
59	C4	PZ	0.00000	0.58793	-0.32698	0.00000	0.00000
60	C4	DXX	0.12253	0.00000	0.00000	0.02527	-0.16250
61	C4	DYY	0.08054	0.00000	0.00000	-0.03955	0.34097
62	C4	DZZ	-0.29662	0.00000	0.00000	0.10764	-0.24973
63	C4	DXY	0.20023	0.00000	0.00000	0.07111	0.14771
64	C4	DXZ	0.00000	-0.37428	-0.07389	0.00000	0.00000
65	C4	DYZ	0.00000	-0.22440	0.27931	0.00000	0.00000
66	C5	S	-0.00820	0.00000	0.00000	0.01920	0.00811
67	C5	S	-0.26065	0.00000	0.00000	0.17659	0.27164
68	C5	PX	-0.03398	0.00000	0.00000	0.08177	0.13530
69	C5	PY	0.11784	0.00000	0.00000	0.01648	-0.04336
70	C5	PZ	0.00000	-0.04997	-0.01728	0.00000	0.00000
71	C5	S	0.06010	0.00000	0.00000	-0.82551	-0.85701
72	C5	PX	0.13812	0.00000	0.00000	-0.27631	-0.49249
73	C5	PY	-0.00601	0.00000	0.00000	0.05575	0.72496
74	C5	PZ	0.00000	-0.69317	0.04488	0.00000	0.00000
75	C5	DXX	0.17306	0.00000	0.00000	-0.12494	0.02069
76	C5	DYY	0.00230	0.00000	0.00000	-0.10360	-0.07550
77	C5	DZZ	-0.25072	0.00000	0.00000	0.23844	0.07806
78	C5	DXY	-0.17109	0.00000	0.00000	0.16101	-0.07419
79	C5	DXZ	0.00000	-0.29365	0.20294	0.00000	0.00000

80	C5	DYZ	0.00000	0.34193	0.11716	0.00000	0.00000
81	C6	S	0.00049	0.00000	0.00000	0.00237	0.02402
82	C6	S	-0.06211	0.00000	0.00000	0.12422	0.20333
83	C6	PX	-0.06709	0.00000	0.00000	0.15000	0.12658
84	C6	PY	0.13244	0.00000	0.00000	0.07795	-0.01097
85	C6	PZ	0.00000	0.00732	-0.03614	0.00000	0.00000
86	C6	S	-0.13055	0.00000	0.00000	-0.63945	-0.70144
87	C6	PX	0.02455	0.00000	0.00000	-1.02720	-0.54390
88	C6	PY	-1.18013	0.00000	0.00000	0.86839	0.04457
89	C6	PZ	0.00000	-0.36112	-0.03163	0.00000	0.00000
90	C6	DXX	0.14104	0.00000	0.00000	0.10591	0.02827
91	C6	DYY	-0.13433	0.00000	0.00000	-0.10971	-0.19631
92	C6	DZZ	-0.02972	0.00000	0.00000	0.03519	0.12999
93	C6	DXY	0.09592	0.00000	0.00000	0.04780	-0.15114
94	C6	DXZ	0.00000	0.15467	0.20742	0.00000	0.00000
95	C6	DYZ	0.00000	-0.08030	-0.08903	0.00000	0.00000
96	C7	S	0.00370	0.00000	0.00000	-0.02091	0.02802
97	C7	S	0.07099	0.00000	0.00000	-0.46971	0.43324
98	C7	PX	-0.07777	0.00000	0.00000	0.22588	-0.03712
99	C7	PY	-0.04251	0.00000	0.00000	-0.14950	0.22072
100	C7	PZ	0.00000	-0.01659	-0.02955	0.00000	0.00000
101	C7	S	-0.35665	0.00000	0.00000	1.06709	-2.77856
102	C7	PX	0.15076	0.00000	0.00000	-0.58804	1.70973
103	C7	PY	0.09820	0.00000	0.00000	0.72667	-1.22577
104	C7	PZ	0.00000	-0.13610	-0.18055	0.00000	0.00000
105	C7	DXX	0.06858	0.00000	0.00000	0.08549	0.12275
106	C7	DYY	-0.01716	0.00000	0.00000	0.01643	-0.26680
107	C7	DZZ	-0.00336	0.00000	0.00000	-0.23913	0.13885
108	C7	DXY	0.07780	0.00000	0.00000	-0.14441	0.01774
109	C7	DXZ	0.00000	0.09768	0.28454	0.00000	0.00000
110	C7	DYZ	0.00000	0.01494	0.35362	0.00000	0.00000
111	H3	S	-0.20543	0.00000	0.00000	-0.04845	-0.24530
112	H3	S	0.03969	0.00000	0.00000	-0.01489	0.31529
113	H3	PX	0.04110	0.00000	0.00000	0.01280	-0.16811
114	H3	PY	-0.12610	0.00000	0.00000	0.01576	-0.07321
115	H3	PZ	0.00000	-0.31817	0.21713	0.00000	0.00000
116	H4	S	-0.13578	0.00000	0.00000	0.20091	-0.08643
117	H4	S	0.06720	0.00000	0.00000	-0.11430	-0.23073
118	H4	PX	-0.05360	0.00000	0.00000	0.00990	-0.05639
119	H4	PY	-0.11202	0.00000	0.00000	0.08244	-0.03054
120	H4	PZ	0.00000	0.40042	0.01069	0.00000	0.00000
121	N1	S	-0.00136	0.00000	0.00000	-0.01325	0.00678
122	N1	S	0.07285	0.00000	0.00000	-0.03042	0.44267
123	N1	PX	0.10031	0.00000	0.00000	0.16047	0.15563
124	N1	PY	0.00017	0.00000	0.00000	0.03366	0.20498
125	N1	PZ	0.00000	-0.01118	0.05343	0.00000	0.00000
126	N1	S	-0.03064	0.00000	0.00000	0.79096	-1.11553
127	N1	PX	0.11571	0.00000	0.00000	0.19695	-0.50608
128	N1	PY	-0.40695	0.00000	0.00000	-0.02978	-0.31452
129	N1	PZ	0.00000	0.10204	-0.15163	0.00000	0.00000
130	N1	DXX	-0.04190	0.00000	0.00000	-0.12990	-0.14772
131	N1	DYY	0.05590	0.00000	0.00000	0.11412	0.14137
132	N1	DZZ	0.03872	0.00000	0.00000	0.02410	0.11977
133	N1	DXY	-0.05298	0.00000	0.00000	-0.07752	-0.10783

134	N1	DXZ	0.00000	0.01547	-0.27047	0.00000	0.00000
135	N1	DYZ	0.00000	0.12359	0.22284	0.00000	0.00000
136	H6	S	0.04701	0.00000	0.00000	0.29325	0.26285
137	H6	S	0.08944	0.00000	0.00000	0.01359	0.05487
138	H6	PX	-0.02698	0.00000	0.00000	-0.09563	-0.10442
139	H6	PY	-0.05944	0.00000	0.00000	-0.04563	0.07799
140	H6	PZ	0.00000	-0.30051	-0.10156	0.00000	0.00000
141	C8	S	0.01993	0.00000	0.00000	-0.00226	0.00262
142	C8	S	-0.13174	0.00000	0.00000	-0.04224	0.03940
143	C8	PX	-0.03462	0.00000	0.00000	0.11543	0.00608
144	C8	PY	0.30904	0.00000	0.00000	0.06866	-0.15362
145	C8	PZ	0.00000	0.01170	0.09928	0.00000	0.00000
146	C8	S	-0.05569	0.00000	0.00000	-0.43860	0.94869
147	C8	PX	0.50405	0.00000	0.00000	0.04533	0.53344
148	C8	PY	-1.64793	0.00000	0.00000	-0.41818	2.07394
149	C8	PZ	0.00000	0.09768	0.48173	0.00000	0.00000
150	C8	DXX	-0.19448	0.00000	0.00000	0.01370	0.01477
151	C8	DYY	0.09712	0.00000	0.00000	0.02139	-0.14185
152	C8	DZZ	0.04365	0.00000	0.00000	-0.07637	0.19988
153	C8	DXY	0.04008	0.00000	0.00000	0.14712	0.05275
154	C8	DXZ	0.00000	0.10355	0.13947	0.00000	0.00000
155	C8	DYZ	0.00000	-0.00723	-0.08979	0.00000	0.00000
156	H8	S	0.01592	0.00000	0.00000	-0.07377	-0.20786
157	H8	S	-0.02668	0.00000	0.00000	0.29858	-0.50466
158	H8	PX	0.00318	0.00000	0.00000	-0.10963	-0.02524
159	H8	PY	-0.02693	0.00000	0.00000	-0.03831	0.12481
160	H8	PZ	0.00000	0.06640	0.17044	0.00000	0.00000
161	C10	S	0.01585	0.00000	0.00000	-0.00163	0.00407
162	C10	S	0.06933	0.00000	0.00000	-0.00954	0.13109
163	C10	PX	0.00707	0.00000	0.00000	-0.05732	0.06234
164	C10	PY	-0.04666	0.00000	0.00000	-0.00288	0.14745
165	C10	PZ	0.00000	-0.00347	-0.03266	0.00000	0.00000
166	C10	S	-1.39816	0.00000	0.00000	-0.15692	1.12298
167	C10	PX	-0.28673	0.00000	0.00000	0.42683	-0.53078
168	C10	PY	0.09852	0.00000	0.00000	0.08794	0.12259
169	C10	PZ	0.00000	-0.05135	-0.29087	0.00000	0.00000
170	C10	DXX	-0.48807	0.00000	0.00000	-0.13303	0.14170
171	C10	DYY	0.24839	0.00000	0.00000	0.09752	-0.15573
172	C10	DZZ	0.33398	0.00000	0.00000	0.04809	0.02706
173	C10	DXY	0.07743	0.00000	0.00000	-0.19936	0.06428
174	C10	DXZ	0.00000	0.00024	-0.02430	0.00000	0.00000
175	C10	DYZ	0.00000	-0.05959	-0.36960	0.00000	0.00000
176	H16	S	0.39242	0.00000	0.00000	-0.14073	0.06803
177	H16	S	0.13277	0.00000	0.00000	-0.07143	0.09161
178	H16	PX	-0.02258	0.00000	0.00000	-0.16301	0.12777
179	H16	PY	-0.27421	0.00000	0.00000	-0.14095	0.18607
180	H16	PZ	0.00000	0.00826	0.12752	0.00000	0.00000
181	H18	S	0.28862	0.00000	0.00000	0.26943	-0.21006
182	H18	S	-0.05124	0.00000	0.00000	0.11380	-0.22681
183	H18	PX	0.02691	0.00000	0.00000	-0.13227	0.06830
184	H18	PY	-0.30189	0.00000	0.00000	0.00567	0.01707
185	H18	PZ	0.00000	0.03918	0.18883	0.00000	0.00000

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Eigenvalues:	2.31922	2.35383	2.39048	2.39593	2.43253
(ev):	63.10911	64.05112	65.04840	65.19658	66.19258

		A	A	A	A	A	
1	H1	S	0.02400	-0.05257	-0.06064	0.07386	-0.07682
2	H1	S	-0.04584	-0.31394	0.07346	-0.04732	-0.03608
3	H1	PX	0.00933	0.01852	-0.03702	0.01199	-0.05109
4	H1	PY	0.00777	0.09691	-0.20188	-0.19909	-0.06050
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01541	0.02509	-0.01714	-0.00773	0.00557
7	C1	S	0.14187	0.52236	-0.16112	-0.03293	-0.04459
8	C1	PX	-0.04063	-0.20445	0.07104	0.06300	0.04492
9	C1	PY	0.05785	0.11613	-0.26290	-0.15749	-0.02599
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-1.08849	-1.31710	0.49038	-0.29791	-1.10412
12	C1	PX	0.29685	1.15189	-0.23893	0.06825	0.40258
13	C1	PY	0.56297	0.14357	0.65664	0.31447	0.35839
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00962	-0.04746	0.10253	-0.04166	0.05896
16	C1	DYY	-0.07044	-0.12826	-0.02700	0.06460	0.01252
17	C1	DZZ	0.14106	0.28220	-0.17228	-0.10957	-0.14487
18	C1	DXY	-0.09582	0.06214	-0.09287	-0.24729	0.06128
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.02783	0.01446	-0.01074	-0.00111	0.00956
22	C2	S	0.41721	0.28022	-0.10279	0.08687	-0.12014
23	C2	PX	0.14917	0.06111	-0.02587	0.09779	-0.10106
24	C2	PY	0.09296	0.07419	-0.30445	0.00122	-0.03221
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-1.21524	-1.37794	0.82655	0.83701	-0.62052
27	C2	PX	-1.49807	-0.24806	0.75570	0.40278	-0.14514
28	C2	PY	-0.65051	0.85151	1.30602	0.42939	0.36493
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.02978	-0.16804	-0.00017	0.09507	-0.03407
31	C2	DYY	-0.15868	0.03977	-0.05175	-0.15157	-0.03393
32	C2	DZZ	0.29599	0.19430	0.01608	0.13582	0.03926
33	C2	DXY	-0.23722	0.28047	0.16681	-0.11645	0.05017
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00913	0.01098	-0.01259	-0.01486	0.02077
37	C3	S	0.24403	0.01868	0.18534	-0.24254	0.30393
38	C3	PX	0.01265	0.11396	-0.10762	0.08807	-0.25064
39	C3	PY	-0.18585	-0.18140	0.02728	0.18544	-0.14087
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-1.89903	1.75029	1.60294	2.24348	0.83156
42	C3	PX	1.25809	-0.32136	0.06378	-0.81245	1.16067
43	C3	PY	1.64478	0.68957	-0.93609	-0.90895	0.40005
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.08783	0.01466	-0.19564	-0.00535	-0.33302
46	C3	DYY	0.00745	-0.12969	0.10616	-0.00638	0.04717
47	C3	DZZ	-0.02410	0.22636	0.11949	0.04114	0.35293
48	C3	DXY	-0.04897	-0.05979	-0.19475	-0.02991	0.13904
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

51	C4	S	0.02085	0.00570	-0.01888	-0.01079	-0.01029
52	C4	S	0.09585	-0.02400	-0.31732	-0.34192	-0.14514
53	C4	PX	0.02415	0.09411	0.14552	0.00457	0.05234
54	C4	PY	-0.00834	-0.06861	0.09867	0.18359	0.02251
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.48859	0.70809	-0.17340	0.19611	0.62837
57	C4	PX	0.04976	-0.55949	-0.58027	0.04394	-0.29873
58	C4	PY	0.00883	-0.03066	-0.44495	-0.99697	-0.57597
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.10444	0.08206	0.22574	0.00835	0.03779
61	C4	DYY	-0.08095	-0.09310	0.00536	0.09050	0.04638
62	C4	DZZ	0.21997	0.07468	-0.29487	-0.18298	-0.04493
63	C4	DXY	0.00732	0.27027	-0.19972	-0.14265	-0.11300
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02145	0.00693	-0.00677	0.00633	-0.00055
67	C5	S	0.39117	-0.26055	-0.15859	0.18875	0.04355
68	C5	PX	-0.05476	-0.01853	-0.14620	-0.07951	-0.05666
69	C5	PY	-0.25976	0.16931	0.06819	-0.12790	-0.03783
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.74738	-0.41822	-1.37862	-0.85248	-0.41350
72	C5	PX	0.18539	0.04232	0.48132	0.43036	-0.18110
73	C5	PY	0.10243	-0.29387	0.22279	1.03334	0.12138
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.04592	-0.01080	0.16479	0.15028	-0.01858
76	C5	DYY	-0.29155	0.03579	-0.01628	-0.16996	0.08793
77	C5	DZZ	0.42176	-0.09298	-0.22356	0.05355	-0.08788
78	C5	DXY	-0.07494	-0.11394	0.25368	-0.06913	0.14311
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00275	0.01497	0.00102	0.00392	0.02227
82	C6	S	-0.31696	0.23902	0.39062	0.26287	0.44458
83	C6	PX	-0.04718	-0.01933	0.19040	0.04526	0.22778
84	C6	PY	-0.19022	-0.03060	0.16287	-0.11937	-0.05308
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.30953	0.17929	0.09572	-0.80912	-0.17304
87	C6	PX	1.55183	-1.14658	-1.29488	-1.19125	-0.37864
88	C6	PY	2.01923	0.82293	-0.95835	-0.28778	1.31706
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.06883	0.19275	-0.25249	0.01317	-0.21232
91	C6	DYY	0.06383	-0.22362	0.09199	0.07471	-0.03687
92	C6	DZZ	0.07968	0.15253	0.13844	-0.12049	0.31688
93	C6	DXY	0.07126	0.01424	0.24987	0.25484	-0.17436
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.02066	0.01017	0.00725	0.01110	0.00887
97	C7	S	-0.41745	0.33353	-0.07702	0.40147	0.04599
98	C7	PX	0.10627	-0.11130	0.07795	-0.14995	0.11629
99	C7	PY	-0.04701	-0.01796	-0.12664	-0.10712	0.14140
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	2.29039	-0.92377	-1.61896	-2.32243	-0.70336
102	C7	PX	-1.60818	0.69152	0.78896	1.41184	-0.04463
103	C7	PY	0.31636	-0.31305	-0.34553	0.15615	-1.02757
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

105	C7	DXX	0.21210	0.04282	0.10907	-0.01716	-0.08488
106	C7	DYY	-0.11453	-0.16292	-0.10606	-0.02805	0.06059
107	C7	DZZ	-0.09331	0.12066	-0.16117	-0.00315	0.06117
108	C7	DXY	0.02784	0.05380	-0.10418	-0.21424	0.20934
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.08320	-0.09223	0.17524	0.14219	0.09092
112	H3	S	-0.01458	0.08536	0.19694	0.26734	0.17310
113	H3	PX	-0.01473	0.20077	0.05305	-0.11494	0.00039
114	H3	PY	0.01876	-0.14206	0.01868	0.04450	0.04701
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.08638	-0.02484	0.20490	-0.03144	0.02168
117	H4	S	-0.10082	0.14372	0.03747	-0.18459	-0.06340
118	H4	PX	-0.18089	0.00818	-0.07559	-0.19787	0.02458
119	H4	PY	-0.01371	-0.08526	0.02024	-0.09209	0.03058
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.02206	0.00619	0.01170	0.00431	0.02078
122	N1	S	-0.47109	0.19503	0.31108	-0.19741	-0.06058
123	N1	PX	-0.05830	0.02661	0.06649	-0.12635	-0.21449
124	N1	PY	-0.14845	0.06885	-0.23384	-0.04801	0.27645
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	2.30604	-0.73146	-1.67926	-0.02480	-0.66271
127	N1	PX	0.32939	-0.07045	-0.40807	0.22311	-0.27427
128	N1	PY	1.10545	-0.19937	-0.07041	-0.69503	0.33324
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.08537	0.24012	-0.04279	-0.10770	0.03914
131	N1	DYY	0.02630	-0.16779	0.09447	0.01971	0.03974
132	N1	DZZ	-0.03706	-0.01450	-0.06559	-0.01765	-0.07079
133	N1	DXY	-0.05662	0.01838	0.10273	-0.08063	-0.12073
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.14285	0.18737	0.09316	-0.04003	0.02647
137	H6	S	-0.43687	-0.02819	0.20793	0.11789	-0.02266
138	H6	PX	-0.02008	-0.06582	0.01133	-0.00326	0.01162
139	H6	PY	0.20070	-0.11082	-0.21931	0.09720	-0.09248
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01204	-0.02153	-0.01785	-0.01207	-0.02407
142	C8	S	-0.28035	-0.27247	-0.04869	-0.05461	-0.46380
143	C8	PX	-0.05877	0.00896	-0.03473	0.05447	-0.00188
144	C8	PY	0.04043	-0.12702	0.04173	0.00996	-0.03020
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-1.12274	0.36080	0.86075	0.59126	-0.24972
147	C8	PX	-0.42600	-0.02173	0.35245	0.96761	-0.97526
148	C8	PY	-0.16512	1.83608	0.82854	0.78784	3.01895
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.01494	-0.22312	-0.07463	-0.12076	0.41130
151	C8	DYY	0.17087	0.19206	0.09888	0.08271	-0.14758
152	C8	DZZ	-0.31549	-0.07992	-0.06138	0.03569	-0.40430
153	C8	DXY	0.00468	-0.06574	0.18156	-0.22495	-0.25645
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.00683	-0.02211	-0.17593	-0.12102	0.12301
157	H8	S	0.48318	-0.20710	-0.11012	-0.21648	-0.11692
158	H8	PX	0.02559	0.04123	-0.12540	-0.07168	0.17889

159	H8	PY	0.12029	0.12606	0.01057	-0.01186	0.25853
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.02448	-0.03219	-0.01673	-0.00978	-0.01561
162	C10	S	-0.18592	-0.25379	-0.13278	-0.07382	0.12045
163	C10	PX	0.06649	-0.03584	0.08469	-0.14618	-0.01506
164	C10	PY	-0.07453	-0.04572	-0.05343	0.01048	0.24608
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.54539	1.77216	0.66947	0.64729	2.19298
167	C10	PX	-0.30641	0.24452	-0.54573	0.31784	0.64563
168	C10	PY	0.49994	0.51108	0.22594	0.16616	1.04027
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.07704	0.14169	0.08127	0.04032	-0.15750
171	C10	DYY	0.23769	0.16417	0.06866	0.04873	0.21358
172	C10	DZZ	-0.25143	-0.50481	-0.26853	-0.14861	0.01614
173	C10	DXY	0.22302	-0.03133	0.05028	-0.10974	0.10035
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.16515	-0.23791	0.01802	-0.15587	0.00165
177	H16	S	0.11264	-0.10088	0.20543	-0.16491	-0.21629
178	H16	PX	0.10756	-0.12417	0.12222	-0.31587	-0.10020
179	H16	PY	0.01440	0.02260	0.22389	-0.29841	-0.30303
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.19514	-0.14546	-0.19796	0.03833	0.06204
182	H18	S	-0.04439	0.05447	-0.21438	0.15366	0.26595
183	H18	PX	0.18927	-0.00521	0.16114	-0.22896	-0.05106
184	H18	PY	-0.22599	0.18817	-0.14073	0.40441	-0.02772
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	131	132	133	134	135
Eigenvalues:	2.43724	2.52134	2.52181	2.56069	2.61248
(ev):	66.32070	68.60917	68.62186	69.68007	71.08919

		A	A	A	A	A	
1	H1	S	0.00000	0.00000	0.00933	0.00000	0.00000
2	H1	S	0.00000	0.00000	-0.11783	0.00000	0.00000
3	H1	PX	0.00000	0.00000	0.05784	0.00000	0.00000
4	H1	PY	0.00000	0.00000	-0.07784	0.00000	0.00000
5	H1	PZ	-0.13363	0.21529	0.00000	-0.23467	0.18022
6	C1	S	0.00000	0.00000	-0.02962	0.00000	0.00000
7	C1	S	0.00000	0.00000	-0.15863	0.00000	0.00000
8	C1	PX	0.00000	0.00000	0.05661	0.00000	0.00000
9	C1	PY	0.00000	0.00000	-0.10649	0.00000	0.00000
10	C1	PZ	-0.01006	-0.10910	0.00000	0.04925	-0.04378
11	C1	S	0.00000	0.00000	0.09679	0.00000	0.00000
12	C1	PX	0.00000	0.00000	0.26863	0.00000	0.00000
13	C1	PY	0.00000	0.00000	-1.02837	0.00000	0.00000
14	C1	PZ	0.04275	-0.11954	0.00000	0.11144	-0.00725
15	C1	DXX	0.00000	0.00000	-0.11695	0.00000	0.00000
16	C1	DYY	0.00000	0.00000	0.43344	0.00000	0.00000
17	C1	DZZ	0.00000	0.00000	-0.38986	0.00000	0.00000
18	C1	DXY	0.00000	0.00000	0.13279	0.00000	0.00000
19	C1	DXZ	0.02801	0.07069	0.00000	0.00392	-0.08212
20	C1	DYZ	0.02026	-0.05215	0.00000	0.36538	0.38216
21	C2	S	0.00000	0.00000	0.03630	0.00000	0.00000

22	C2	S	0.00000	0.00000	0.30031	0.00000	0.00000
23	C2	PX	0.00000	0.00000	0.05897	0.00000	0.00000
24	C2	PY	0.00000	0.00000	0.19739	0.00000	0.00000
25	C2	PZ	0.02912	0.05822	0.00000	0.07453	0.07395
26	C2	S	0.00000	0.00000	-0.58775	0.00000	0.00000
27	C2	PX	0.00000	0.00000	0.13407	0.00000	0.00000
28	C2	PY	0.00000	0.00000	1.13109	0.00000	0.00000
29	C2	PZ	-0.02122	0.05864	0.00000	0.08922	0.08940
30	C2	DXX	0.00000	0.00000	0.01281	0.00000	0.00000
31	C2	DYY	0.00000	0.00000	-0.36109	0.00000	0.00000
32	C2	DZZ	0.00000	0.00000	0.44815	0.00000	0.00000
33	C2	DXY	0.00000	0.00000	0.22441	0.00000	0.00000
34	C2	DXZ	0.03496	0.07806	0.00000	-0.01410	0.01289
35	C2	DYZ	-0.02226	-0.16727	0.00000	0.37430	0.41282
36	C3	S	0.00000	0.00000	-0.01666	0.00000	0.00000
37	C3	S	0.00000	0.00000	-0.41525	0.00000	0.00000
38	C3	PX	0.00000	0.00000	-0.08909	0.00000	0.00000
39	C3	PY	0.00000	0.00000	-0.22276	0.00000	0.00000
40	C3	PZ	-0.00715	-0.04010	0.00000	0.11091	0.00534
41	C3	S	0.00000	0.00000	2.01275	0.00000	0.00000
42	C3	PX	0.00000	0.00000	-2.29225	0.00000	0.00000
43	C3	PY	0.00000	0.00000	-0.55732	0.00000	0.00000
44	C3	PZ	-0.00133	-0.12949	0.00000	0.01900	-0.07404
45	C3	DXX	0.00000	0.00000	0.06478	0.00000	0.00000
46	C3	DYY	0.00000	0.00000	-0.02038	0.00000	0.00000
47	C3	DZZ	0.00000	0.00000	-0.10395	0.00000	0.00000
48	C3	DXY	0.00000	0.00000	-0.06751	0.00000	0.00000
49	C3	DXZ	0.51114	0.25624	0.00000	0.32824	0.12430
50	C3	DYZ	-0.22581	0.37128	0.00000	-0.19019	0.41583
51	C4	S	0.00000	0.00000	-0.02281	0.00000	0.00000
52	C4	S	0.00000	0.00000	-0.11859	0.00000	0.00000
53	C4	PX	0.00000	0.00000	-0.20204	0.00000	0.00000
54	C4	PY	0.00000	0.00000	0.12735	0.00000	0.00000
55	C4	PZ	-0.01595	-0.00370	0.00000	-0.07936	-0.09674
56	C4	S	0.00000	0.00000	0.84840	0.00000	0.00000
57	C4	PX	0.00000	0.00000	0.48953	0.00000	0.00000
58	C4	PY	0.00000	0.00000	-0.96939	0.00000	0.00000
59	C4	PZ	-0.05145	0.05489	0.00000	-0.10446	-0.06898
60	C4	DXX	0.00000	0.00000	0.22082	0.00000	0.00000
61	C4	DYY	0.00000	0.00000	-0.05502	0.00000	0.00000
62	C4	DZZ	0.00000	0.00000	-0.16007	0.00000	0.00000
63	C4	DXY	0.00000	0.00000	-0.11156	0.00000	0.00000
64	C4	DXZ	0.12894	0.35364	0.00000	-0.15512	-0.03353
65	C4	DYZ	-0.02468	-0.17800	0.00000	0.15777	0.04919
66	C5	S	0.00000	0.00000	0.02173	0.00000	0.00000
67	C5	S	0.00000	0.00000	0.03183	0.00000	0.00000
68	C5	PX	0.00000	0.00000	-0.14612	0.00000	0.00000
69	C5	PY	0.00000	0.00000	-0.10354	0.00000	0.00000
70	C5	PZ	0.01065	0.04800	0.00000	-0.07214	-0.06524
71	C5	S	0.00000	0.00000	-0.69980	0.00000	0.00000
72	C5	PX	0.00000	0.00000	0.40099	0.00000	0.00000
73	C5	PY	0.00000	0.00000	0.92561	0.00000	0.00000
74	C5	PZ	0.03717	0.01911	0.00000	-0.08744	-0.07857
75	C5	DXX	0.00000	0.00000	-0.23655	0.00000	0.00000

76	C5	DYY	0.00000	0.00000	0.07217	0.00000	0.00000
77	C5	DZZ	0.00000	0.00000	0.14360	0.00000	0.00000
78	C5	DXY	0.00000	0.00000	-0.24149	0.00000	0.00000
79	C5	DXZ	0.14037	0.21016	0.00000	0.24557	0.34323
80	C5	DYZ	0.05148	0.06897	0.00000	0.21756	0.24888
81	C6	S	0.00000	0.00000	0.01033	0.00000	0.00000
82	C6	S	0.00000	0.00000	0.26784	0.00000	0.00000
83	C6	PX	0.00000	0.00000	-0.12286	0.00000	0.00000
84	C6	PY	0.00000	0.00000	0.30452	0.00000	0.00000
85	C6	PZ	0.03768	-0.02035	0.00000	0.12206	0.04422
86	C6	S	0.00000	0.00000	-1.18067	0.00000	0.00000
87	C6	PX	0.00000	0.00000	-2.56225	0.00000	0.00000
88	C6	PY	0.00000	0.00000	0.22096	0.00000	0.00000
89	C6	PZ	0.05501	-0.02163	0.00000	0.15057	0.06500
90	C6	DXX	0.00000	0.00000	0.03671	0.00000	0.00000
91	C6	DYY	0.00000	0.00000	-0.06247	0.00000	0.00000
92	C6	DZZ	0.00000	0.00000	0.05467	0.00000	0.00000
93	C6	DXY	0.00000	0.00000	-0.08074	0.00000	0.00000
94	C6	DXZ	0.40408	0.43683	0.00000	-0.12382	0.06066
95	C6	DYZ	0.05399	-0.09786	0.00000	-0.23301	0.05364
96	C7	S	0.00000	0.00000	0.00705	0.00000	0.00000
97	C7	S	0.00000	0.00000	0.06385	0.00000	0.00000
98	C7	PX	0.00000	0.00000	0.04754	0.00000	0.00000
99	C7	PY	0.00000	0.00000	-0.04688	0.00000	0.00000
100	C7	PZ	-0.11001	0.09305	0.00000	-0.01461	0.06087
101	C7	S	0.00000	0.00000	-0.71747	0.00000	0.00000
102	C7	PX	0.00000	0.00000	0.97659	0.00000	0.00000
103	C7	PY	0.00000	0.00000	0.29625	0.00000	0.00000
104	C7	PZ	-0.15505	0.19656	0.00000	-0.02536	0.09791
105	C7	DXX	0.00000	0.00000	-0.26008	0.00000	0.00000
106	C7	DYY	0.00000	0.00000	0.18029	0.00000	0.00000
107	C7	DZZ	0.00000	0.00000	0.09879	0.00000	0.00000
108	C7	DXY	0.00000	0.00000	0.13087	0.00000	0.00000
109	C7	DXZ	0.12403	0.09388	0.00000	-0.12163	0.13682
110	C7	DYZ	-0.03786	0.14339	0.00000	-0.51171	0.23884
111	H3	S	0.00000	0.00000	0.11999	0.00000	0.00000
112	H3	S	0.00000	0.00000	0.14065	0.00000	0.00000
113	H3	PX	0.00000	0.00000	-0.12308	0.00000	0.00000
114	H3	PY	0.00000	0.00000	0.14389	0.00000	0.00000
115	H3	PZ	0.02575	-0.03140	0.00000	0.09579	0.15598
116	H4	S	0.00000	0.00000	-0.18521	0.00000	0.00000
117	H4	S	0.00000	0.00000	-0.08750	0.00000	0.00000
118	H4	PX	0.00000	0.00000	-0.09312	0.00000	0.00000
119	H4	PY	0.00000	0.00000	-0.20514	0.00000	0.00000
120	H4	PZ	-0.00711	-0.03715	0.00000	0.08889	0.08523
121	N1	S	0.00000	0.00000	-0.00556	0.00000	0.00000
122	N1	S	0.00000	0.00000	-0.00709	0.00000	0.00000
123	N1	PX	0.00000	0.00000	0.00958	0.00000	0.00000
124	N1	PY	0.00000	0.00000	0.09159	0.00000	0.00000
125	N1	PZ	0.01438	-0.00252	0.00000	-0.00764	0.00987
126	N1	S	0.00000	0.00000	0.07861	0.00000	0.00000
127	N1	PX	0.00000	0.00000	0.64376	0.00000	0.00000
128	N1	PY	0.00000	0.00000	-0.60885	0.00000	0.00000
129	N1	PZ	0.17542	0.11209	0.00000	-0.15096	-0.09936

130	N1	DXX	0.00000	0.00000	0.36798	0.00000	0.00000
131	N1	DYY	0.00000	0.00000	-0.13095	0.00000	0.00000
132	N1	DZZ	0.00000	0.00000	-0.17542	0.00000	0.00000
133	N1	DXY	0.00000	0.00000	0.16551	0.00000	0.00000
134	N1	DXZ	0.28263	0.13766	0.00000	-0.04888	-0.25885
135	N1	DYZ	-0.22432	0.03636	0.00000	-0.40313	0.13451
136	H6	S	0.00000	0.00000	0.06500	0.00000	0.00000
137	H6	S	0.00000	0.00000	0.11852	0.00000	0.00000
138	H6	PX	0.00000	0.00000	0.00010	0.00000	0.00000
139	H6	PY	0.00000	0.00000	0.10492	0.00000	0.00000
140	H6	PZ	0.04653	-0.03751	0.00000	-0.23215	-0.13815
141	C8	S	0.00000	0.00000	-0.00528	0.00000	0.00000
142	C8	S	0.00000	0.00000	-0.15238	0.00000	0.00000
143	C8	PX	0.00000	0.00000	0.10895	0.00000	0.00000
144	C8	PY	0.00000	0.00000	-0.06039	0.00000	0.00000
145	C8	PZ	-0.05703	0.02684	0.00000	-0.03956	0.06299
146	C8	S	0.00000	0.00000	0.29128	0.00000	0.00000
147	C8	PX	0.00000	0.00000	0.68627	0.00000	0.00000
148	C8	PY	0.00000	0.00000	0.26474	0.00000	0.00000
149	C8	PZ	-0.16443	-0.00738	0.00000	0.02903	-0.02407
150	C8	DXX	0.00000	0.00000	-0.04054	0.00000	0.00000
151	C8	DYY	0.00000	0.00000	0.02543	0.00000	0.00000
152	C8	DZZ	0.00000	0.00000	0.03006	0.00000	0.00000
153	C8	DXY	0.00000	0.00000	0.12589	0.00000	0.00000
154	C8	DXZ	0.59030	0.08955	0.00000	-0.15231	-0.09181
155	C8	DYZ	0.18479	-0.36479	0.00000	-0.27673	0.33328
156	H8	S	0.00000	0.00000	0.10583	0.00000	0.00000
157	H8	S	0.00000	0.00000	-0.37145	0.00000	0.00000
158	H8	PX	0.00000	0.00000	0.12595	0.00000	0.00000
159	H8	PY	0.00000	0.00000	-0.02791	0.00000	0.00000
160	H8	PZ	0.26040	-0.46690	0.00000	-0.07397	-0.23795
161	C10	S	0.00000	0.00000	-0.00085	0.00000	0.00000
162	C10	S	0.00000	0.00000	-0.01124	0.00000	0.00000
163	C10	PX	0.00000	0.00000	-0.01380	0.00000	0.00000
164	C10	PY	0.00000	0.00000	-0.02174	0.00000	0.00000
165	C10	PZ	0.06351	-0.10196	0.00000	-0.07262	0.11280
166	C10	S	0.00000	0.00000	0.13789	0.00000	0.00000
167	C10	PX	0.00000	0.00000	-0.18622	0.00000	0.00000
168	C10	PY	0.00000	0.00000	0.09473	0.00000	0.00000
169	C10	PZ	0.17192	-0.16267	0.00000	-0.11133	0.15985
170	C10	DXX	0.00000	0.00000	-0.01454	0.00000	0.00000
171	C10	DYY	0.00000	0.00000	0.02121	0.00000	0.00000
172	C10	DZZ	0.00000	0.00000	-0.01975	0.00000	0.00000
173	C10	DXY	0.00000	0.00000	-0.14470	0.00000	0.00000
174	C10	DXZ	0.07782	0.00772	0.00000	-0.03973	-0.02351
175	C10	DYZ	0.18327	-0.11365	0.00000	-0.04373	-0.06072
176	H16	S	0.00000	0.00000	-0.07659	0.00000	0.00000
177	H16	S	0.00000	0.00000	0.16247	0.00000	0.00000
178	H16	PX	0.00000	0.00000	0.05113	0.00000	0.00000
179	H16	PY	0.00000	0.00000	0.15767	0.00000	0.00000
180	H16	PZ	-0.32011	0.24909	0.00000	0.25278	-0.33808
181	H18	S	0.00000	0.00000	0.04937	0.00000	0.00000
182	H18	S	0.00000	0.00000	-0.10386	0.00000	0.00000
183	H18	PX	0.00000	0.00000	0.02754	0.00000	0.00000

184	H18	PY	0.00000	0.00000	-0.14848	0.00000	0.00000
185	H18	PZ	-0.02902	0.31855	0.00000	0.15261	-0.38947

MO:		136	137	138	139	140
Eigenvalues:		2.61465	2.64801	2.68326	2.70446	2.71343
(ev):		71.14828	72.05602	73.01517	73.59204	73.83611

		A	A	A	A	A	
1	H1	S	-0.09206	-0.25088	0.00000	-0.08840	0.00000
2	H1	S	0.19493	0.28337	0.00000	0.06172	0.00000
3	H1	PX	-0.11708	-0.19510	0.00000	0.07800	0.00000
4	H1	PY	0.14465	0.06234	0.00000	-0.21260	0.00000
5	H1	PZ	0.00000	0.00000	-0.11704	0.00000	-0.41877
6	C1	S	-0.03692	-0.03252	0.00000	-0.02264	0.00000
7	C1	S	-0.17754	-0.19199	0.00000	-0.07861	0.00000
8	C1	PX	-0.08620	-0.12851	0.00000	-0.02648	0.00000
9	C1	PY	-0.10895	0.07528	0.00000	0.03435	0.00000
10	C1	PZ	0.00000	0.00000	-0.02317	0.00000	0.08906
11	C1	S	1.17478	1.47144	0.00000	1.37082	0.00000
12	C1	PX	-0.51479	-0.51233	0.00000	-0.27330	0.00000
13	C1	PY	-1.04810	0.33824	0.00000	0.01394	0.00000
14	C1	PZ	0.00000	0.00000	-0.04034	0.00000	0.10352
15	C1	DXX	0.14670	0.33758	0.00000	0.02122	0.00000
16	C1	DYY	0.16207	-0.11719	0.00000	0.19067	0.00000
17	C1	DZZ	-0.37733	-0.32251	0.00000	-0.16279	0.00000
18	C1	DXY	0.24754	-0.02500	0.00000	0.09412	0.00000
19	C1	DXZ	0.00000	0.00000	0.14002	0.00000	0.17718
20	C1	DYZ	0.00000	0.00000	-0.29975	0.00000	0.31707
21	C2	S	-0.03420	-0.00885	0.00000	0.00087	0.00000
22	C2	S	-0.38728	-0.23808	0.00000	0.02558	0.00000
23	C2	PX	-0.00835	-0.02266	0.00000	0.05246	0.00000
24	C2	PY	-0.13875	0.00515	0.00000	-0.02196	0.00000
25	C2	PZ	0.00000	0.00000	0.09680	0.00000	-0.01636
26	C2	S	2.46070	1.29304	0.00000	-0.82821	0.00000
27	C2	PX	1.45002	0.63600	0.00000	0.23888	0.00000
28	C2	PY	-0.76482	0.52839	0.00000	-0.39811	0.00000
29	C2	PZ	0.00000	0.00000	0.07559	0.00000	-0.01625
30	C2	DXX	0.12751	0.21129	0.00000	0.01648	0.00000
31	C2	DYY	0.09218	-0.25571	0.00000	0.01802	0.00000
32	C2	DZZ	-0.20539	-0.00833	0.00000	-0.05893	0.00000
33	C2	DXY	-0.23642	0.14156	0.00000	-0.08795	0.00000
34	C2	DXZ	0.00000	0.00000	-0.19892	0.00000	-0.05076
35	C2	DYZ	0.00000	0.00000	-0.17584	0.00000	0.14695
36	C3	S	0.01412	-0.01576	0.00000	-0.04053	0.00000
37	C3	S	-0.03108	0.03405	0.00000	-0.23874	0.00000
38	C3	PX	0.03949	0.06444	0.00000	-0.10646	0.00000
39	C3	PY	-0.28984	-0.21388	0.00000	-0.05873	0.00000
40	C3	PZ	0.00000	0.00000	-0.03095	0.00000	0.04004
41	C3	S	0.43175	0.95389	0.00000	1.39066	0.00000
42	C3	PX	-0.66388	0.56320	0.00000	-0.67912	0.00000
43	C3	PY	-1.73162	-1.25206	0.00000	-1.04298	0.00000
44	C3	PZ	0.00000	0.00000	-0.01475	0.00000	-0.04548
45	C3	DXX	0.05738	0.16001	0.00000	0.18318	0.00000
46	C3	DYY	-0.07293	0.05620	0.00000	0.06182	0.00000

47	C3	DZZ	0.06065	-0.11470	0.00000	-0.29726	0.00000
48	C3	DXY	-0.14085	-0.02089	0.00000	-0.17911	0.00000
49	C3	DXZ	0.00000	0.00000	0.06658	0.00000	-0.09623
50	C3	DYZ	0.00000	0.00000	-0.09551	0.00000	0.19569
51	C4	S	-0.00585	0.00533	0.00000	-0.02168	0.00000
52	C4	S	-0.08371	-0.03233	0.00000	-0.01223	0.00000
53	C4	PX	-0.00698	0.02249	0.00000	-0.19518	0.00000
54	C4	PY	0.05442	0.10026	0.00000	0.02679	0.00000
55	C4	PZ	0.00000	0.00000	0.07986	0.00000	0.03600
56	C4	S	0.78756	-0.48513	0.00000	0.52772	0.00000
57	C4	PX	0.18403	-0.89441	0.00000	-0.81419	0.00000
58	C4	PY	-0.29582	0.23931	0.00000	0.50646	0.00000
59	C4	PZ	0.00000	0.00000	0.07964	0.00000	0.01630
60	C4	DXX	0.00243	0.06691	0.00000	0.28686	0.00000
61	C4	DYY	-0.02774	-0.16205	0.00000	-0.16292	0.00000
62	C4	DZZ	0.06076	0.12809	0.00000	-0.15866	0.00000
63	C4	DXY	0.00653	0.01150	0.00000	0.15462	0.00000
64	C4	DXZ	0.00000	0.00000	0.37087	0.00000	-0.12311
65	C4	DYZ	0.00000	0.00000	-0.01564	0.00000	0.45216
66	C5	S	-0.00669	0.01643	0.00000	0.02150	0.00000
67	C5	S	0.18391	0.25496	0.00000	-0.05821	0.00000
68	C5	PX	0.06035	-0.07371	0.00000	-0.12538	0.00000
69	C5	PY	-0.03672	-0.02326	0.00000	0.02490	0.00000
70	C5	PZ	0.00000	0.00000	0.10815	0.00000	0.00558
71	C5	S	-0.69566	-1.73806	0.00000	-0.37698	0.00000
72	C5	PX	-0.59483	-0.02037	0.00000	-1.05266	0.00000
73	C5	PY	0.62978	0.59455	0.00000	-0.59731	0.00000
74	C5	PZ	0.00000	0.00000	0.05773	0.00000	0.03510
75	C5	DXX	0.08059	-0.01073	0.00000	-0.23735	0.00000
76	C5	DYY	-0.03768	-0.10552	0.00000	0.08194	0.00000
77	C5	DZZ	-0.08370	0.10205	0.00000	0.19398	0.00000
78	C5	DXY	0.05249	0.16438	0.00000	-0.02018	0.00000
79	C5	DXZ	0.00000	0.00000	-0.01984	0.00000	-0.18050
80	C5	DYZ	0.00000	0.00000	0.22190	0.00000	0.18965
81	C6	S	0.00150	-0.04089	0.00000	0.04185	0.00000
82	C6	S	0.08275	-0.25181	0.00000	0.26334	0.00000
83	C6	PX	-0.05032	-0.16567	0.00000	-0.05627	0.00000
84	C6	PY	-0.12817	0.18178	0.00000	-0.17544	0.00000
85	C6	PZ	0.00000	0.00000	0.04903	0.00000	-0.04708
86	C6	S	-1.12585	0.54185	0.00000	-1.11792	0.00000
87	C6	PX	0.50935	0.23886	0.00000	-0.87857	0.00000
88	C6	PY	-1.97624	-0.52710	0.00000	0.05899	0.00000
89	C6	PZ	0.00000	0.00000	0.06809	0.00000	-0.06340
90	C6	DXX	-0.00364	0.01886	0.00000	-0.21037	0.00000
91	C6	DYY	0.05376	0.20638	0.00000	-0.02565	0.00000
92	C6	DZZ	-0.19118	-0.27908	0.00000	0.26220	0.00000
93	C6	DXY	0.20349	0.05876	0.00000	-0.00424	0.00000
94	C6	DXZ	0.00000	0.00000	0.13624	0.00000	-0.08953
95	C6	DYZ	0.00000	0.00000	-0.33636	0.00000	0.31243
96	C7	S	0.06646	0.01851	0.00000	-0.05602	0.00000
97	C7	S	0.53837	0.15280	0.00000	-0.31054	0.00000
98	C7	PX	0.05854	-0.10026	0.00000	-0.08097	0.00000
99	C7	PY	-0.09486	-0.16758	0.00000	-0.29922	0.00000
100	C7	PZ	0.00000	0.00000	-0.01205	0.00000	0.04490

101	C7	S	-3.23497	-0.61543	0.00000	1.11071	0.00000
102	C7	PX	1.84783	-0.22212	0.00000	-0.66083	0.00000
103	C7	PY	-0.57815	-1.39467	0.00000	-0.91919	0.00000
104	C7	PZ	0.00000	0.00000	-0.03867	0.00000	0.08431
105	C7	DXX	-0.30280	0.19510	0.00000	0.24090	0.00000
106	C7	DYY	-0.16183	-0.34548	0.00000	0.09636	0.00000
107	C7	DZZ	0.57237	0.21706	0.00000	-0.44906	0.00000
108	C7	DXY	0.12771	0.24901	0.00000	0.37722	0.00000
109	C7	DXZ	0.00000	0.00000	-0.08143	0.00000	0.18946
110	C7	DYZ	0.00000	0.00000	-0.08347	0.00000	0.13420
111	H3	S	-0.00854	0.12381	0.00000	-0.07845	0.00000
112	H3	S	0.02774	0.04368	0.00000	-0.04898	0.00000
113	H3	PX	-0.11012	0.38307	0.00000	-0.03131	0.00000
114	H3	PY	0.11773	-0.09853	0.00000	0.00823	0.00000
115	H3	PZ	0.00000	0.00000	-0.34926	0.00000	-0.52580
116	H4	S	-0.06628	0.15601	0.00000	0.02656	0.00000
117	H4	S	-0.23820	-0.17784	0.00000	0.02732	0.00000
118	H4	PX	0.15511	-0.22871	0.00000	0.27370	0.00000
119	H4	PY	0.12606	-0.04689	0.00000	0.16225	0.00000
120	H4	PZ	0.00000	0.00000	-0.45584	0.00000	-0.36233
121	N1	S	0.01604	-0.01205	0.00000	0.03130	0.00000
122	N1	S	0.28868	-0.28323	0.00000	0.53464	0.00000
123	N1	PX	-0.00493	-0.03443	0.00000	0.03385	0.00000
124	N1	PY	-0.18940	-0.15470	0.00000	0.04155	0.00000
125	N1	PZ	0.00000	0.00000	0.00106	0.00000	0.00422
126	N1	S	-1.49822	0.45830	0.00000	-1.60388	0.00000
127	N1	PX	-0.64756	0.34532	0.00000	-0.44114	0.00000
128	N1	PY	-0.26016	0.17271	0.00000	0.13320	0.00000
129	N1	PZ	0.00000	0.00000	-0.20641	0.00000	0.17005
130	N1	DXX	-0.30268	0.18835	0.00000	-0.12110	0.00000
131	N1	DYY	0.04876	-0.03640	0.00000	-0.17841	0.00000
132	N1	DZZ	0.22093	-0.21662	0.00000	0.35398	0.00000
133	N1	DXY	-0.05321	0.05224	0.00000	0.14733	0.00000
134	N1	DXZ	0.00000	0.00000	-0.35963	0.00000	0.27251
135	N1	DYZ	0.00000	0.00000	-0.10636	0.00000	0.13749
136	H6	S	0.00894	-0.11712	0.00000	0.09631	0.00000
137	H6	S	0.35563	0.27300	0.00000	0.10484	0.00000
138	H6	PX	0.03440	0.12657	0.00000	0.06755	0.00000
139	H6	PY	0.02180	-0.09204	0.00000	0.09041	0.00000
140	H6	PZ	0.00000	0.00000	-0.46890	0.00000	-0.02809
141	C8	S	0.00379	0.02905	0.00000	0.03256	0.00000
142	C8	S	0.11219	0.17125	0.00000	0.21766	0.00000
143	C8	PX	-0.01278	-0.01867	0.00000	-0.35182	0.00000
144	C8	PY	0.48011	-0.19099	0.00000	0.02018	0.00000
145	C8	PZ	0.00000	0.00000	0.04253	0.00000	-0.00909
146	C8	S	0.21694	-0.01755	0.00000	-0.86443	0.00000
147	C8	PX	0.86154	-0.67616	0.00000	-1.70817	0.00000
148	C8	PY	1.17511	-1.91425	0.00000	-0.16588	0.00000
149	C8	PZ	0.00000	0.00000	0.07206	0.00000	-0.06726
150	C8	DXX	-0.08392	-0.17401	0.00000	-0.24546	0.00000
151	C8	DYY	-0.09239	0.06719	0.00000	0.00436	0.00000
152	C8	DZZ	0.08676	0.20041	0.00000	0.23982	0.00000
153	C8	DXY	0.06275	-0.06662	0.00000	-0.20400	0.00000
154	C8	DXZ	0.00000	0.00000	-0.20092	0.00000	0.17058

155	C8	DYZ	0.00000	0.00000	0.08220	0.00000	-0.01544
156	H8	S	0.15711	-0.00229	0.00000	-0.07922	0.00000
157	H8	S	-0.64405	-0.07421	0.00000	0.06641	0.00000
158	H8	PX	0.16779	0.14920	0.00000	0.04767	0.00000
159	H8	PY	-0.06119	0.27364	0.00000	0.19302	0.00000
160	H8	PZ	0.00000	0.00000	0.10368	0.00000	-0.26763
161	C10	S	-0.04215	0.03573	0.00000	-0.00380	0.00000
162	C10	S	-0.18499	0.13951	0.00000	-0.01127	0.00000
163	C10	PX	0.01598	0.02293	0.00000	0.11245	0.00000
164	C10	PY	0.15744	-0.11772	0.00000	0.04355	0.00000
165	C10	PZ	0.00000	0.00000	0.04001	0.00000	-0.00579
166	C10	S	1.50496	-1.90112	0.00000	0.11564	0.00000
167	C10	PX	-0.35932	0.03218	0.00000	0.73954	0.00000
168	C10	PY	0.86383	-1.01612	0.00000	-0.13294	0.00000
169	C10	PZ	0.00000	0.00000	0.04393	0.00000	-0.00095
170	C10	DXX	-0.05676	0.03225	0.00000	-0.00204	0.00000
171	C10	DYY	0.43259	-0.27831	0.00000	0.00307	0.00000
172	C10	DZZ	-0.48699	0.30718	0.00000	-0.05968	0.00000
173	C10	DXY	-0.00133	0.06890	0.00000	0.30814	0.00000
174	C10	DXZ	0.00000	0.00000	-0.09883	0.00000	0.10578
175	C10	DYZ	0.00000	0.00000	-0.12299	0.00000	0.03998
176	H16	S	-0.05945	0.14256	0.00000	0.04006	0.00000
177	H16	S	0.22526	-0.20011	0.00000	-0.45350	0.00000
178	H16	PX	-0.11975	0.04621	0.00000	-0.00107	0.00000
179	H16	PY	-0.03603	-0.01734	0.00000	-0.17392	0.00000
180	H16	PZ	0.00000	0.00000	-0.08143	0.00000	-0.06377
181	H18	S	-0.12373	0.04471	0.00000	-0.03018	0.00000
182	H18	S	-0.09542	-0.01667	0.00000	0.30977	0.00000
183	H18	PX	0.09912	-0.05610	0.00000	0.05884	0.00000
184	H18	PY	-0.08305	0.14605	0.00000	0.29543	0.00000
185	H18	PZ	0.00000	0.00000	-0.28515	0.00000	0.15609

MO:	141	142	143	144	145
Eigenvalues:	2.72800	2.73003	2.74124	2.80231	2.80292
(ev):	74.23264	74.28780	74.59310	76.25478	76.27139

		A	A	A	A	A	
1	H1	S	0.07951	0.00000	0.00941	0.00000	0.05690
2	H1	S	-0.22101	0.00000	-0.12936	0.00000	0.16581
3	H1	PX	0.14472	0.00000	0.12504	0.00000	-0.00788
4	H1	PY	0.05354	0.00000	0.22061	0.00000	-0.44815
5	H1	PZ	0.00000	0.44587	0.00000	0.15800	0.00000
6	C1	S	0.00012	0.00000	0.00666	0.00000	0.00846
7	C1	S	0.33103	0.00000	-0.08909	0.00000	0.02845
8	C1	PX	-0.05826	0.00000	0.20044	0.00000	-0.05718
9	C1	PY	0.03976	0.00000	-0.16372	0.00000	0.18510
10	C1	PZ	0.00000	-0.02550	0.00000	-0.03798	0.00000
11	C1	S	-0.87578	0.00000	0.41085	0.00000	-0.30726
12	C1	PX	0.54749	0.00000	0.23894	0.00000	-0.39225
13	C1	PY	-0.38709	0.00000	-0.89007	0.00000	1.03366
14	C1	PZ	0.00000	-0.06795	0.00000	-0.05023	0.00000
15	C1	DXX	-0.18810	0.00000	-0.12130	0.00000	0.06113
16	C1	DYY	0.27594	0.00000	0.00275	0.00000	0.00391
17	C1	DZZ	-0.03703	0.00000	0.15248	0.00000	0.00161

18	C1	DXY	0.01032	0.00000	0.11040	0.00000	-0.03098
19	C1	DXZ	0.00000	-0.30058	0.00000	-0.08709	0.00000
20	C1	DYZ	0.00000	0.06428	0.00000	0.03195	0.00000
21	C2	S	0.02492	0.00000	-0.00904	0.00000	-0.03735
22	C2	S	0.24398	0.00000	-0.15362	0.00000	0.04382
23	C2	PX	-0.00846	0.00000	0.09906	0.00000	0.27581
24	C2	PY	0.02129	0.00000	0.05206	0.00000	0.38836
25	C2	PZ	0.00000	0.03237	0.00000	0.02993	0.00000
26	C2	S	-1.12159	0.00000	0.24962	0.00000	1.46243
27	C2	PX	-0.26596	0.00000	0.41065	0.00000	0.29138
28	C2	PY	0.71335	0.00000	0.38125	0.00000	2.09176
29	C2	PZ	0.00000	0.07224	0.00000	0.03870	0.00000
30	C2	DXX	-0.14912	0.00000	0.18666	0.00000	0.17248
31	C2	DYY	0.04720	0.00000	-0.17479	0.00000	0.22050
32	C2	DZZ	0.21501	0.00000	-0.12150	0.00000	-0.41272
33	C2	DXY	0.00954	0.00000	0.11861	0.00000	0.31598
34	C2	DXZ	0.00000	-0.31434	0.00000	0.04431	0.00000
35	C2	DYZ	0.00000	0.02044	0.00000	0.29577	0.00000
36	C3	S	0.00109	0.00000	0.00444	0.00000	-0.00809
37	C3	S	0.02857	0.00000	-0.02435	0.00000	-0.13041
38	C3	PX	-0.11174	0.00000	-0.04534	0.00000	0.02669
39	C3	PY	-0.14863	0.00000	0.21546	0.00000	0.03722
40	C3	PZ	0.00000	-0.02964	0.00000	-0.05079	0.00000
41	C3	S	0.76155	0.00000	0.85078	0.00000	1.14407
42	C3	PX	-0.02944	0.00000	-1.28556	0.00000	1.07016
43	C3	PY	-0.61299	0.00000	-1.72428	0.00000	-0.03209
44	C3	PZ	0.00000	0.08268	0.00000	0.04556	0.00000
45	C3	DXX	0.06765	0.00000	0.07073	0.00000	-0.16960
46	C3	DYY	-0.06780	0.00000	-0.16050	0.00000	0.18259
47	C3	DZZ	0.06953	0.00000	0.07691	0.00000	-0.05076
48	C3	DXY	-0.05549	0.00000	0.17597	0.00000	0.12019
49	C3	DXZ	0.00000	-0.18436	0.00000	0.12202	0.00000
50	C3	DYZ	0.00000	0.06573	0.00000	0.10945	0.00000
51	C4	S	-0.02196	0.00000	-0.07218	0.00000	0.02873
52	C4	S	-0.41984	0.00000	-0.27853	0.00000	0.06612
53	C4	PX	-0.12417	0.00000	-0.14353	0.00000	-0.08635
54	C4	PY	0.04541	0.00000	-0.21440	0.00000	0.04641
55	C4	PZ	0.00000	-0.04182	0.00000	-0.01725	0.00000
56	C4	S	1.86832	0.00000	2.64223	0.00000	-1.64901
57	C4	PX	-0.29552	0.00000	-0.89041	0.00000	0.20561
58	C4	PY	-0.79401	0.00000	-0.73911	0.00000	-0.01802
59	C4	PZ	0.00000	-0.03483	0.00000	0.00979	0.00000
60	C4	DXX	0.01671	0.00000	0.26047	0.00000	0.00112
61	C4	DYY	0.06110	0.00000	0.25221	0.00000	-0.18875
62	C4	DZZ	-0.12672	0.00000	-0.63768	0.00000	0.20128
63	C4	DXY	0.32043	0.00000	0.06615	0.00000	0.22680
64	C4	DXZ	0.00000	-0.21925	0.00000	0.12739	0.00000
65	C4	DYZ	0.00000	-0.07930	0.00000	0.02453	0.00000
66	C5	S	0.02189	0.00000	0.05951	0.00000	0.04656
67	C5	S	0.20435	0.00000	0.35880	0.00000	-0.01495
68	C5	PX	0.01184	0.00000	-0.25360	0.00000	0.15239
69	C5	PY	-0.00841	0.00000	0.11036	0.00000	0.37138
70	C5	PZ	0.00000	0.03607	0.00000	-0.00937	0.00000
71	C5	S	-1.04886	0.00000	-2.48083	0.00000	-1.97098

72	C5	PX	-0.63280	0.00000	-0.98136	0.00000	1.40965
73	C5	PY	0.28970	0.00000	0.67426	0.00000	1.27365
74	C5	PZ	0.00000	0.03277	0.00000	-0.00767	0.00000
75	C5	DXX	0.01411	0.00000	-0.32674	0.00000	0.08944
76	C5	DYY	-0.15643	0.00000	-0.05302	0.00000	-0.50192
77	C5	DZZ	0.14861	0.00000	0.50463	0.00000	0.44801
78	C5	DXY	-0.02581	0.00000	0.28957	0.00000	-0.29711
79	C5	DXZ	0.00000	-0.21524	0.00000	0.15128	0.00000
80	C5	DYZ	0.00000	0.15367	0.00000	0.30911	0.00000
81	C6	S	-0.04122	0.00000	0.01665	0.00000	-0.01424
82	C6	S	-0.42051	0.00000	0.09400	0.00000	0.01889
83	C6	PX	-0.01723	0.00000	-0.08037	0.00000	0.04998
84	C6	PY	0.12241	0.00000	-0.08050	0.00000	-0.21090
85	C6	PZ	0.00000	0.05786	0.00000	-0.01567	0.00000
86	C6	S	0.30326	0.00000	-1.34429	0.00000	1.83171
87	C6	PX	-0.40726	0.00000	-0.90460	0.00000	-0.53427
88	C6	PY	1.28408	0.00000	1.12200	0.00000	0.56502
89	C6	PZ	0.00000	-0.06221	0.00000	-0.06710	0.00000
90	C6	DXX	-0.20477	0.00000	-0.03445	0.00000	0.21249
91	C6	DYY	0.31698	0.00000	0.01030	0.00000	-0.00910
92	C6	DZZ	-0.20970	0.00000	0.06222	0.00000	-0.11386
93	C6	DXY	0.24800	0.00000	-0.01061	0.00000	-0.06752
94	C6	DXZ	0.00000	-0.26106	0.00000	0.11639	0.00000
95	C6	DYZ	0.00000	-0.05345	0.00000	0.33632	0.00000
96	C7	S	0.02128	0.00000	0.01142	0.00000	-0.00207
97	C7	S	0.08842	0.00000	0.24917	0.00000	0.03229
98	C7	PX	0.00963	0.00000	0.01890	0.00000	-0.00579
99	C7	PY	-0.00921	0.00000	0.11859	0.00000	-0.04803
100	C7	PZ	0.00000	-0.00562	0.00000	-0.03790	0.00000
101	C7	S	-0.76733	0.00000	-2.18589	0.00000	-0.78496
102	C7	PX	0.11592	0.00000	1.39910	0.00000	-0.02549
103	C7	PY	-0.38857	0.00000	0.08232	0.00000	-0.42775
104	C7	PZ	0.00000	-0.03443	0.00000	-0.08312	0.00000
105	C7	DXX	0.03400	0.00000	-0.14991	0.00000	-0.03763
106	C7	DYY	-0.14668	0.00000	0.18501	0.00000	0.03251
107	C7	DZZ	0.17218	0.00000	0.00652	0.00000	-0.03458
108	C7	DXY	-0.01386	0.00000	-0.00258	0.00000	0.00126
109	C7	DXZ	0.00000	0.03838	0.00000	-0.31451	0.00000
110	C7	DYZ	0.00000	0.20142	0.00000	0.14139	0.00000
111	H3	S	-0.14745	0.00000	-0.19907	0.00000	0.12223
112	H3	S	0.31744	0.00000	0.38344	0.00000	0.03787
113	H3	PX	-0.27722	0.00000	0.14050	0.00000	-0.27173
114	H3	PY	-0.05995	0.00000	-0.33295	0.00000	0.05676
115	H3	PZ	0.00000	0.27787	0.00000	-0.07095	0.00000
116	H4	S	0.04625	0.00000	0.19999	0.00000	0.13884
117	H4	S	-0.21203	0.00000	-0.40450	0.00000	-0.12272
118	H4	PX	0.38887	0.00000	-0.20385	0.00000	-0.13430
119	H4	PY	0.27073	0.00000	0.20700	0.00000	0.03294
120	H4	PZ	0.00000	-0.36407	0.00000	-0.20669	0.00000
121	N1	S	-0.02263	0.00000	-0.00151	0.00000	0.00580
122	N1	S	-0.69843	0.00000	-0.07506	0.00000	0.11891
123	N1	PX	-0.12177	0.00000	-0.01195	0.00000	0.04825
124	N1	PY	-0.21566	0.00000	0.05864	0.00000	-0.01411
125	N1	PZ	0.00000	-0.01279	0.00000	0.03025	0.00000

126	N1	S	1.88877	0.00000	0.70473	0.00000	-0.56244
127	N1	PX	0.67318	0.00000	0.16033	0.00000	-0.15790
128	N1	PY	0.58448	0.00000	-0.12580	0.00000	-0.38995
129	N1	PZ	0.00000	0.04591	0.00000	0.04067	0.00000
130	N1	DXX	0.10140	0.00000	-0.00863	0.00000	0.10584
131	N1	DYY	0.11649	0.00000	-0.03566	0.00000	-0.15606
132	N1	DZZ	-0.32409	0.00000	0.06002	0.00000	0.05665
133	N1	DXY	0.19719	0.00000	-0.02942	0.00000	-0.24838
134	N1	DXZ	0.00000	0.17535	0.00000	-0.02629	0.00000
135	N1	DYZ	0.00000	-0.31348	0.00000	0.35095	0.00000
136	H6	S	0.14026	0.00000	-0.06776	0.00000	-0.13289
137	H6	S	-0.10674	0.00000	0.21389	0.00000	0.14746
138	H6	PX	-0.11151	0.00000	0.21451	0.00000	0.15853
139	H6	PY	-0.37149	0.00000	0.07541	0.00000	-0.45151
140	H6	PZ	0.00000	-0.48866	0.00000	0.01617	0.00000
141	C8	S	-0.01268	0.00000	-0.00858	0.00000	0.01215
142	C8	S	-0.05399	0.00000	-0.19782	0.00000	-0.06554
143	C8	PX	0.04069	0.00000	0.04504	0.00000	0.09581
144	C8	PY	-0.14114	0.00000	0.04351	0.00000	0.01744
145	C8	PZ	0.00000	-0.04123	0.00000	-0.09450	0.00000
146	C8	S	0.44980	0.00000	0.56885	0.00000	-0.50594
147	C8	PX	0.15356	0.00000	0.96643	0.00000	0.04683
148	C8	PY	-0.65859	0.00000	1.27436	0.00000	0.92799
149	C8	PZ	0.00000	-0.01438	0.00000	0.06524	0.00000
150	C8	DXX	0.04741	0.00000	0.06827	0.00000	-0.04711
151	C8	DYY	0.11554	0.00000	-0.05051	0.00000	-0.12566
152	C8	DZZ	-0.10744	0.00000	-0.00394	0.00000	0.14054
153	C8	DXY	0.00552	0.00000	0.00825	0.00000	-0.02988
154	C8	DXZ	0.00000	0.27627	0.00000	-0.09923	0.00000
155	C8	DYZ	0.00000	-0.03819	0.00000	0.28066	0.00000
156	H8	S	0.00539	0.00000	0.01868	0.00000	0.03790
157	H8	S	-0.02613	0.00000	-0.37774	0.00000	0.01150
158	H8	PX	0.05960	0.00000	0.00481	0.00000	0.03214
159	H8	PY	0.08063	0.00000	-0.17792	0.00000	0.08916
160	H8	PZ	0.00000	0.07380	0.00000	0.46125	0.00000
161	C10	S	0.01796	0.00000	-0.01448	0.00000	-0.01100
162	C10	S	0.04967	0.00000	-0.03399	0.00000	0.02105
163	C10	PX	-0.00148	0.00000	-0.02269	0.00000	-0.03337
164	C10	PY	-0.13088	0.00000	0.07883	0.00000	0.15357
165	C10	PZ	0.00000	-0.01671	0.00000	-0.01882	0.00000
166	C10	S	-0.86119	0.00000	0.98955	0.00000	0.91813
167	C10	PX	-0.18228	0.00000	-0.29683	0.00000	-0.07597
168	C10	PY	-0.39744	0.00000	0.51295	0.00000	0.37314
169	C10	PZ	0.00000	-0.02534	0.00000	-0.08583	0.00000
170	C10	DXX	0.03922	0.00000	-0.01108	0.00000	-0.05152
171	C10	DYY	-0.17959	0.00000	0.11550	0.00000	0.12765
172	C10	DZZ	0.18052	0.00000	-0.12758	0.00000	-0.09884
173	C10	DXY	0.01050	0.00000	-0.06741	0.00000	-0.10720
174	C10	DXZ	0.00000	0.18881	0.00000	-0.17661	0.00000
175	C10	DYZ	0.00000	0.06983	0.00000	0.49385	0.00000
176	H16	S	0.07833	0.00000	-0.03637	0.00000	-0.04618
177	H16	S	0.00689	0.00000	0.19381	0.00000	0.08794
178	H16	PX	0.03185	0.00000	-0.03923	0.00000	-0.02963
179	H16	PY	-0.02550	0.00000	0.01748	0.00000	0.10737

180	H16	PZ	0.00000	-0.09590	0.00000	0.54474	0.00000
181	H18	S	-0.01562	0.00000	-0.04678	0.00000	0.01610
182	H18	S	-0.02876	0.00000	-0.08595	0.00000	-0.10962
183	H18	PX	-0.06373	0.00000	0.01572	0.00000	0.03195
184	H18	PY	0.05579	0.00000	-0.07388	0.00000	-0.13180
185	H18	PZ	0.00000	0.28722	0.00000	0.15489	0.00000

MO:	146	147	148	149	150
Eigenvalues:	2.83549	2.86871	2.88238	2.92014	2.93390
(ev):	77.15767	78.06173	78.43366	79.46111	79.83563

		A	A	A	A	A	
1	H1	S	-0.11053	0.00000	0.02070	0.02042	0.00000
2	H1	S	-0.22806	0.00000	-0.18686	-0.10142	0.00000
3	H1	PX	0.02147	0.00000	0.03877	0.13183	0.00000
4	H1	PY	-0.33753	0.00000	0.26944	0.12702	0.00000
5	H1	PZ	0.00000	0.07024	0.00000	0.00000	0.46301
6	C1	S	-0.01175	0.00000	0.01300	0.03175	0.00000
7	C1	S	0.15017	0.00000	-0.04484	0.05942	0.00000
8	C1	PX	-0.12926	0.00000	0.14938	0.19820	0.00000
9	C1	PY	0.39424	0.00000	0.03088	0.07818	0.00000
10	C1	PZ	0.00000	0.02070	0.00000	0.00000	0.00216
11	C1	S	0.79627	0.00000	-0.80424	-1.09373	0.00000
12	C1	PX	0.36224	0.00000	0.57113	0.39278	0.00000
13	C1	PY	3.02780	0.00000	-2.22389	-0.12888	0.00000
14	C1	PZ	0.00000	0.05966	0.00000	0.00000	-0.07591
15	C1	DXX	0.04076	0.00000	-0.13468	-0.09068	0.00000
16	C1	DYY	0.10053	0.00000	-0.02451	-0.13470	0.00000
17	C1	DZZ	-0.16760	0.00000	0.10571	0.23832	0.00000
18	C1	DXY	-0.55572	0.00000	0.04204	-0.06454	0.00000
19	C1	DXZ	0.00000	-0.12268	0.00000	0.00000	-0.45311
20	C1	DYZ	0.00000	0.14675	0.00000	0.00000	0.00600
21	C2	S	0.03975	0.00000	0.02124	0.00849	0.00000
22	C2	S	-0.01429	0.00000	0.06993	0.01764	0.00000
23	C2	PX	-0.14907	0.00000	-0.06280	-0.09390	0.00000
24	C2	PY	0.02230	0.00000	0.18390	-0.17506	0.00000
25	C2	PZ	0.00000	-0.01910	0.00000	0.00000	0.01093
26	C2	S	-1.30912	0.00000	0.23453	-0.68295	0.00000
27	C2	PX	0.05757	0.00000	-0.10038	-0.30532	0.00000
28	C2	PY	-0.41774	0.00000	3.41226	-0.40653	0.00000
29	C2	PZ	0.00000	-0.06268	0.00000	0.00000	-0.04349
30	C2	DXX	-0.08004	0.00000	-0.06033	-0.03836	0.00000
31	C2	DYY	-0.16029	0.00000	-0.01476	-0.07945	0.00000
32	C2	DZZ	0.30841	0.00000	0.15271	0.10547	0.00000
33	C2	DXY	-0.08100	0.00000	0.31022	-0.16441	0.00000
34	C2	DXZ	0.00000	-0.02912	0.00000	0.00000	0.45540
35	C2	DYZ	0.00000	-0.18724	0.00000	0.00000	0.16740
36	C3	S	-0.03809	0.00000	-0.03552	-0.06482	0.00000
37	C3	S	-0.17460	0.00000	-0.10277	-0.26420	0.00000
38	C3	PX	-0.04702	0.00000	-0.05147	-0.02265	0.00000
39	C3	PY	0.16156	0.00000	0.08096	0.18314	0.00000
40	C3	PZ	0.00000	0.04301	0.00000	0.00000	-0.02375
41	C3	S	2.26004	0.00000	1.11753	2.22459	0.00000
42	C3	PX	0.41988	0.00000	-2.52314	0.55554	0.00000

43	C3	PY	1.73242	0.00000	-0.81150	-0.81585	0.00000
44	C3	PZ	0.00000	-0.02495	0.00000	0.00000	0.06028
45	C3	DXX	0.13474	0.00000	0.11895	-0.07838	0.00000
46	C3	DYY	0.07947	0.00000	0.03404	0.38624	0.00000
47	C3	DZZ	-0.22205	0.00000	-0.21965	-0.43971	0.00000
48	C3	DXY	0.29211	0.00000	0.19197	-0.02802	0.00000
49	C3	DXZ	0.00000	0.25789	0.00000	0.00000	0.02258
50	C3	DYZ	0.00000	-0.23038	0.00000	0.00000	-0.14255
51	C4	S	0.01772	0.00000	0.01922	-0.01063	0.00000
52	C4	S	-0.12424	0.00000	0.04796	-0.10927	0.00000
53	C4	PX	-0.23712	0.00000	0.13826	0.10063	0.00000
54	C4	PY	0.29705	0.00000	-0.10858	-0.12421	0.00000
55	C4	PZ	0.00000	-0.02071	0.00000	0.00000	-0.01648
56	C4	S	-0.75845	0.00000	-0.17209	0.66591	0.00000
57	C4	PX	-2.94965	0.00000	2.39084	0.16565	0.00000
58	C4	PY	1.25371	0.00000	-1.18627	-0.41084	0.00000
59	C4	PZ	0.00000	-0.08589	0.00000	0.00000	0.04178
60	C4	DXX	0.04560	0.00000	-0.41867	-0.19576	0.00000
61	C4	DYY	-0.29477	0.00000	0.30920	0.22646	0.00000
62	C4	DZZ	0.22479	0.00000	0.11471	-0.07542	0.00000
63	C4	DXY	0.26703	0.00000	-0.17396	-0.09937	0.00000
64	C4	DXZ	0.00000	-0.39796	0.00000	0.00000	0.10176
65	C4	DYZ	0.00000	-0.09778	0.00000	0.00000	0.30435
66	C5	S	0.02164	0.00000	-0.01320	-0.03081	0.00000
67	C5	S	0.20728	0.00000	0.01569	0.01334	0.00000
68	C5	PX	-0.05495	0.00000	0.21065	-0.02140	0.00000
69	C5	PY	-0.17561	0.00000	0.07441	-0.11709	0.00000
70	C5	PZ	0.00000	0.02285	0.00000	0.00000	-0.02360
71	C5	S	-1.47441	0.00000	-0.65738	0.85016	0.00000
72	C5	PX	-1.77527	0.00000	2.85683	-0.08818	0.00000
73	C5	PY	-0.89437	0.00000	1.49421	-0.40465	0.00000
74	C5	PZ	0.00000	0.10040	0.00000	0.00000	0.01477
75	C5	DXX	-0.22763	0.00000	0.21183	0.10569	0.00000
76	C5	DYY	0.15597	0.00000	-0.18226	0.12168	0.00000
77	C5	DZZ	0.08029	0.00000	-0.08020	-0.23909	0.00000
78	C5	DXY	0.03135	0.00000	-0.09978	0.14188	0.00000
79	C5	DXZ	0.00000	-0.42890	0.00000	0.00000	0.03720
80	C5	DYZ	0.00000	0.10321	0.00000	0.00000	0.33771
81	C6	S	-0.00675	0.00000	-0.01934	0.00402	0.00000
82	C6	S	0.08790	0.00000	0.05945	0.02751	0.00000
83	C6	PX	-0.07532	0.00000	-0.08007	-0.03542	0.00000
84	C6	PY	0.06368	0.00000	0.15713	-0.09036	0.00000
85	C6	PZ	0.00000	-0.08007	0.00000	0.00000	-0.00529
86	C6	S	0.14539	0.00000	0.30014	-0.35577	0.00000
87	C6	PX	-0.45831	0.00000	-2.98467	-0.02692	0.00000
88	C6	PY	-0.36683	0.00000	1.20472	0.25282	0.00000
89	C6	PZ	0.00000	-0.02934	0.00000	0.00000	0.01397
90	C6	DXX	-0.20936	0.00000	-0.27942	-0.09990	0.00000
91	C6	DYY	0.19861	0.00000	0.30605	0.12970	0.00000
92	C6	DZZ	-0.11158	0.00000	-0.17132	0.02989	0.00000
93	C6	DXY	-0.22459	0.00000	-0.19267	0.15269	0.00000
94	C6	DXZ	0.00000	0.31365	0.00000	0.00000	-0.07152
95	C6	DYZ	0.00000	0.27658	0.00000	0.00000	-0.09723
96	C7	S	0.01815	0.00000	-0.02372	-0.02231	0.00000

97	C7	S	0.16284	0.00000	-0.09242	-0.03607	0.00000
98	C7	PX	0.03417	0.00000	0.10048	-0.05720	0.00000
99	C7	PY	0.09896	0.00000	0.00054	-0.26904	0.00000
100	C7	PZ	0.00000	-0.02316	0.00000	0.00000	-0.01612
101	C7	S	-0.78373	0.00000	0.54758	-0.08009	0.00000
102	C7	PX	0.78379	0.00000	0.44401	-0.68984	0.00000
103	C7	PY	0.67382	0.00000	0.02291	-1.41074	0.00000
104	C7	PZ	0.00000	0.02843	0.00000	0.00000	-0.02201
105	C7	DXX	-0.16415	0.00000	-0.05682	-0.10968	0.00000
106	C7	DYY	0.07869	0.00000	0.20335	0.09539	0.00000
107	C7	DZZ	0.10763	0.00000	-0.14787	-0.09940	0.00000
108	C7	DXY	-0.22588	0.00000	0.18032	-0.02488	0.00000
109	C7	DXZ	0.00000	0.12589	0.00000	0.00000	-0.17231
110	C7	DYZ	0.00000	-0.29412	0.00000	0.00000	-0.10595
111	H3	S	0.08370	0.00000	0.02559	-0.03274	0.00000
112	H3	S	0.04401	0.00000	0.05662	0.13767	0.00000
113	H3	PX	0.50944	0.00000	-0.08037	0.01544	0.00000
114	H3	PY	-0.21713	0.00000	-0.04681	-0.12918	0.00000
115	H3	PZ	0.00000	0.31913	0.00000	0.00000	-0.30932
116	H4	S	0.10025	0.00000	0.05204	-0.02117	0.00000
117	H4	S	0.04565	0.00000	0.08183	0.07930	0.00000
118	H4	PX	0.25186	0.00000	-0.35066	0.01850	0.00000
119	H4	PY	0.02179	0.00000	-0.24867	0.01423	0.00000
120	H4	PZ	0.00000	-0.37763	0.00000	0.00000	-0.25126
121	N1	S	0.00587	0.00000	0.02123	-0.01235	0.00000
122	N1	S	0.12488	0.00000	0.29863	-0.17324	0.00000
123	N1	PX	-0.06037	0.00000	0.01053	-0.02260	0.00000
124	N1	PY	0.03294	0.00000	-0.07011	-0.11479	0.00000
125	N1	PZ	0.00000	0.03210	0.00000	0.00000	-0.01366
126	N1	S	-0.73325	0.00000	-1.38895	0.69912	0.00000
127	N1	PX	-0.22945	0.00000	-0.28613	0.36940	0.00000
128	N1	PY	-0.24013	0.00000	0.29609	-0.05895	0.00000
129	N1	PZ	0.00000	0.13284	0.00000	0.00000	0.01844
130	N1	DXX	-0.19436	0.00000	-0.17800	0.13175	0.00000
131	N1	DYY	0.08017	0.00000	-0.02444	-0.08241	0.00000
132	N1	DZZ	0.06770	0.00000	0.17996	-0.11237	0.00000
133	N1	DXY	0.05239	0.00000	0.35028	-0.22132	0.00000
134	N1	DXZ	0.00000	0.12263	0.00000	0.00000	0.08722
135	N1	DYZ	0.00000	0.33324	0.00000	0.00000	-0.09795
136	H6	S	0.15135	0.00000	0.03734	-0.00060	0.00000
137	H6	S	0.00780	0.00000	-0.06390	-0.09426	0.00000
138	H6	PX	-0.04478	0.00000	-0.06916	-0.07071	0.00000
139	H6	PY	-0.11390	0.00000	-0.39769	0.03534	0.00000
140	H6	PZ	0.00000	0.01303	0.00000	0.00000	0.45700
141	C8	S	-0.01486	0.00000	0.00589	0.06831	0.00000
142	C8	S	-0.03676	0.00000	0.14477	0.22126	0.00000
143	C8	PX	0.02245	0.00000	-0.23703	0.21460	0.00000
144	C8	PY	0.27604	0.00000	0.28778	0.11960	0.00000
145	C8	PZ	0.00000	0.04041	0.00000	0.00000	0.03853
146	C8	S	0.23398	0.00000	-0.16856	-2.80607	0.00000
147	C8	PX	0.85264	0.00000	-0.80599	-0.78280	0.00000
148	C8	PY	1.60478	0.00000	0.97952	-0.11731	0.00000
149	C8	PZ	0.00000	-0.05577	0.00000	0.00000	-0.02889
150	C8	DXX	0.25282	0.00000	0.13283	-0.17235	0.00000

151	C8	DYY	-0.20695	0.00000	-0.19904	-0.32876	0.00000
152	C8	DZZ	-0.02660	0.00000	0.08819	0.53304	0.00000
153	C8	DXY	0.00123	0.00000	0.00886	-0.21641	0.00000
154	C8	DXZ	0.00000	-0.01865	0.00000	0.00000	-0.05179
155	C8	DYZ	0.00000	-0.12817	0.00000	0.00000	-0.35551
156	H8	S	-0.03706	0.00000	-0.04622	0.05073	0.00000
157	H8	S	-0.10747	0.00000	-0.26485	0.03968	0.00000
158	H8	PX	-0.02095	0.00000	0.07214	0.22539	0.00000
159	H8	PY	-0.16453	0.00000	-0.11975	0.59832	0.00000
160	H8	PZ	0.00000	-0.22137	0.00000	0.00000	0.13582
161	C10	S	-0.02259	0.00000	-0.01991	-0.01669	0.00000
162	C10	S	-0.02366	0.00000	-0.02737	0.07094	0.00000
163	C10	PX	-0.02346	0.00000	0.15088	-0.09240	0.00000
164	C10	PY	0.18777	0.00000	0.15387	0.35362	0.00000
165	C10	PZ	0.00000	-0.00209	0.00000	0.00000	-0.03061
166	C10	S	1.40234	0.00000	0.95979	0.82983	0.00000
167	C10	PX	-0.21179	0.00000	0.57982	0.04295	0.00000
168	C10	PY	0.82486	0.00000	0.54967	0.37128	0.00000
169	C10	PZ	0.00000	0.03283	0.00000	0.00000	0.02418
170	C10	DXX	0.01631	0.00000	0.03127	-0.09997	0.00000
171	C10	DYY	0.19631	0.00000	0.14698	0.21835	0.00000
172	C10	DZZ	-0.20595	0.00000	-0.19667	-0.14982	0.00000
173	C10	DXY	-0.04894	0.00000	0.24314	-0.15876	0.00000
174	C10	DXZ	0.00000	-0.36593	0.00000	0.00000	0.07498
175	C10	DYZ	0.00000	-0.14830	0.00000	0.00000	-0.36230
176	H16	S	-0.06568	0.00000	-0.05572	-0.03034	0.00000
177	H16	S	0.23781	0.00000	-0.20415	0.05861	0.00000
178	H16	PX	-0.09401	0.00000	-0.04464	-0.13607	0.00000
179	H16	PY	-0.05543	0.00000	-0.26661	0.16838	0.00000
180	H16	PZ	0.00000	0.19413	0.00000	0.00000	-0.24464
181	H18	S	-0.07315	0.00000	-0.05205	0.03652	0.00000
182	H18	S	-0.00403	0.00000	0.39032	-0.12180	0.00000
183	H18	PX	0.05352	0.00000	0.13395	0.07423	0.00000
184	H18	PY	-0.14544	0.00000	0.13688	-0.24902	0.00000
185	H18	PZ	0.00000	-0.41611	0.00000	0.00000	-0.09047

MO:	151	152	153	154	155
Eigenvalues:	2.96574	2.96810	2.99339	3.03725	3.06360
(ev):	80.70196	80.76604	81.45435	82.64784	83.36496

		A	A	A	A	A	
1	H1	S	0.00000	-0.10144	0.00000	0.04284	0.00000
2	H1	S	0.00000	-0.11324	0.00000	0.17261	0.00000
3	H1	PX	0.00000	-0.09024	0.00000	0.11166	0.00000
4	H1	PY	0.00000	0.40790	0.00000	0.05196	0.00000
5	H1	PZ	-0.15647	0.00000	-0.11844	0.00000	0.03771
6	C1	S	0.00000	-0.05191	0.00000	-0.04369	0.00000
7	C1	S	0.00000	-0.10363	0.00000	-0.00939	0.00000
8	C1	PX	0.00000	-0.10425	0.00000	-0.02531	0.00000
9	C1	PY	0.00000	0.10925	0.00000	0.12020	0.00000
10	C1	PZ	-0.02838	0.00000	-0.02798	0.00000	-0.00284
11	C1	S	0.00000	1.71595	0.00000	1.53881	0.00000
12	C1	PX	0.00000	0.16162	0.00000	-0.92773	0.00000
13	C1	PY	0.00000	-2.17107	0.00000	0.25103	0.00000

14	C1	PZ	0.02592	0.00000	-0.03000	0.00000	0.02778
15	C1	DXX	0.00000	-0.02236	0.00000	-0.06557	0.00000
16	C1	DYY	0.00000	0.25909	0.00000	0.36377	0.00000
17	C1	DZZ	0.00000	-0.38132	0.00000	-0.30895	0.00000
18	C1	DXY	0.00000	-0.27671	0.00000	-0.15871	0.00000
19	C1	DXZ	0.18877	0.00000	0.18216	0.00000	-0.04412
20	C1	DYZ	-0.23595	0.00000	-0.31624	0.00000	-0.33397
21	C2	S	0.00000	-0.01022	0.00000	-0.05875	0.00000
22	C2	S	0.00000	-0.05522	0.00000	-0.18888	0.00000
23	C2	PX	0.00000	0.18988	0.00000	0.04327	0.00000
24	C2	PY	0.00000	-0.11444	0.00000	0.07653	0.00000
25	C2	PZ	0.02393	0.00000	0.01196	0.00000	0.03006
26	C2	S	0.00000	0.52893	0.00000	2.70376	0.00000
27	C2	PX	0.00000	1.24496	0.00000	1.30402	0.00000
28	C2	PY	0.00000	1.86673	0.00000	-0.13977	0.00000
29	C2	PZ	-0.00583	0.00000	0.05621	0.00000	-0.04853
30	C2	DXX	0.00000	0.18905	0.00000	-0.08356	0.00000
31	C2	DYY	0.00000	-0.01558	0.00000	0.46878	0.00000
32	C2	DZZ	0.00000	-0.08034	0.00000	-0.36962	0.00000
33	C2	DXY	0.00000	-0.23079	0.00000	0.27140	0.00000
34	C2	DXZ	0.01751	0.00000	-0.15279	0.00000	0.27508
35	C2	DYZ	0.21857	0.00000	0.40058	0.00000	0.21049
36	C3	S	0.00000	-0.03275	0.00000	-0.00457	0.00000
37	C3	S	0.00000	-0.34128	0.00000	-0.09168	0.00000
38	C3	PX	0.00000	-0.11207	0.00000	-0.04710	0.00000
39	C3	PY	0.00000	0.17962	0.00000	0.00541	0.00000
40	C3	PZ	0.02410	0.00000	-0.01896	0.00000	0.06416
41	C3	S	0.00000	2.11260	0.00000	0.91562	0.00000
42	C3	PX	0.00000	-4.82807	0.00000	0.74212	0.00000
43	C3	PY	0.00000	-1.08913	0.00000	-1.74685	0.00000
44	C3	PZ	-0.00372	0.00000	0.05096	0.00000	-0.03779
45	C3	DXX	0.00000	0.44416	0.00000	-0.13317	0.00000
46	C3	DYY	0.00000	-0.38000	0.00000	0.08884	0.00000
47	C3	DZZ	0.00000	-0.09534	0.00000	-0.01270	0.00000
48	C3	DXY	0.00000	0.06614	0.00000	-0.19480	0.00000
49	C3	DXZ	0.03137	0.00000	-0.26892	0.00000	-0.22822
50	C3	DYZ	-0.21544	0.00000	-0.06126	0.00000	-0.37732
51	C4	S	0.00000	0.02872	0.00000	0.01229	0.00000
52	C4	S	0.00000	-0.13876	0.00000	-0.14923	0.00000
53	C4	PX	0.00000	0.03195	0.00000	-0.26108	0.00000
54	C4	PY	0.00000	0.22814	0.00000	0.14696	0.00000
55	C4	PZ	0.01822	0.00000	0.01947	0.00000	0.02708
56	C4	S	0.00000	0.19396	0.00000	-0.75450	0.00000
57	C4	PX	0.00000	1.16070	0.00000	-0.37138	0.00000
58	C4	PY	0.00000	-0.12232	0.00000	0.13414	0.00000
59	C4	PZ	-0.04182	0.00000	0.02323	0.00000	-0.01835
60	C4	DXX	0.00000	-0.33762	0.00000	-0.13492	0.00000
61	C4	DYY	0.00000	0.03980	0.00000	-0.05329	0.00000
62	C4	DZZ	0.00000	0.24775	0.00000	0.14327	0.00000
63	C4	DXY	0.00000	-0.01116	0.00000	0.23034	0.00000
64	C4	DXZ	0.08035	0.00000	0.29317	0.00000	0.17027
65	C4	DYZ	-0.37152	0.00000	-0.25675	0.00000	-0.16704
66	C5	S	0.00000	-0.00863	0.00000	0.00862	0.00000
67	C5	S	0.00000	0.10571	0.00000	-0.00114	0.00000

68	C5	PX	0.00000	0.14428	0.00000	0.23784	0.00000
69	C5	PY	0.00000	0.04240	0.00000	0.26828	0.00000
70	C5	PZ	-0.01240	0.00000	-0.02241	0.00000	-0.02698
71	C5	S	0.00000	-1.02078	0.00000	-1.33898	0.00000
72	C5	PX	0.00000	1.06245	0.00000	-0.07048	0.00000
73	C5	PY	0.00000	0.79549	0.00000	0.81322	0.00000
74	C5	PZ	0.03577	0.00000	-0.03929	0.00000	0.03701
75	C5	DXX	0.00000	0.44152	0.00000	-0.15202	0.00000
76	C5	DYY	0.00000	-0.28717	0.00000	-0.10911	0.00000
77	C5	DZZ	0.00000	-0.08350	0.00000	0.09974	0.00000
78	C5	DXY	0.00000	-0.12237	0.00000	-0.10523	0.00000
79	C5	DXZ	0.06405	0.00000	0.32563	0.00000	0.10034
80	C5	DYZ	0.27076	0.00000	0.12999	0.00000	0.30742
81	C6	S	0.00000	0.10305	0.00000	-0.00559	0.00000
82	C6	S	0.00000	0.56397	0.00000	0.34486	0.00000
83	C6	PX	0.00000	-0.05613	0.00000	0.01152	0.00000
84	C6	PY	0.00000	-0.23620	0.00000	-0.19959	0.00000
85	C6	PZ	-0.06014	0.00000	-0.02313	0.00000	0.01563
86	C6	S	0.00000	-3.58581	0.00000	-0.32536	0.00000
87	C6	PX	0.00000	-4.50515	0.00000	0.75300	0.00000
88	C6	PY	0.00000	-0.19446	0.00000	-1.28102	0.00000
89	C6	PZ	-0.03933	0.00000	-0.11830	0.00000	0.08571
90	C6	DXX	0.00000	-0.27285	0.00000	-0.03142	0.00000
91	C6	DYY	0.00000	-0.18120	0.00000	0.02864	0.00000
92	C6	DZZ	0.00000	0.53563	0.00000	-0.12846	0.00000
93	C6	DXY	0.00000	0.13179	0.00000	0.36253	0.00000
94	C6	DXZ	0.07812	0.00000	-0.27489	0.00000	-0.25148
95	C6	DYZ	0.35065	0.00000	0.39160	0.00000	-0.14895
96	C7	S	0.00000	-0.03662	0.00000	0.02820	0.00000
97	C7	S	0.00000	0.04462	0.00000	0.11934	0.00000
98	C7	PX	0.00000	-0.04877	0.00000	0.05715	0.00000
99	C7	PY	0.00000	0.13532	0.00000	-0.02290	0.00000
100	C7	PZ	0.00247	0.00000	-0.00689	0.00000	-0.03787
101	C7	S	0.00000	-0.22510	0.00000	-2.09646	0.00000
102	C7	PX	0.00000	1.46601	0.00000	0.79725	0.00000
103	C7	PY	0.00000	1.06762	0.00000	-1.31788	0.00000
104	C7	PZ	0.01222	0.00000	0.01396	0.00000	0.01458
105	C7	DXX	0.00000	-0.09703	0.00000	-0.18103	0.00000
106	C7	DYY	0.00000	0.33667	0.00000	-0.04162	0.00000
107	C7	DZZ	0.00000	-0.29153	0.00000	0.14290	0.00000
108	C7	DXY	0.00000	-0.05327	0.00000	-0.27058	0.00000
109	C7	DXZ	-0.06288	0.00000	-0.05128	0.00000	0.57538
110	C7	DYZ	-0.26491	0.00000	0.09523	0.00000	-0.18475
111	H3	S	0.00000	-0.05944	0.00000	0.04009	0.00000
112	H3	S	0.00000	-0.16897	0.00000	0.15083	0.00000
113	H3	PX	0.00000	0.12912	0.00000	0.06635	0.00000
114	H3	PY	0.00000	-0.00557	0.00000	-0.18536	0.00000
115	H3	PZ	0.28542	0.00000	0.07657	0.00000	0.05714
116	H4	S	0.00000	0.03677	0.00000	-0.01463	0.00000
117	H4	S	0.00000	-0.00869	0.00000	-0.16682	0.00000
118	H4	PX	0.00000	0.11944	0.00000	-0.20603	0.00000
119	H4	PY	0.00000	0.13334	0.00000	-0.14506	0.00000
120	H4	PZ	-0.19676	0.00000	0.07134	0.00000	-0.18163
121	N1	S	0.00000	0.01693	0.00000	0.05541	0.00000

122	N1	S	0.00000	0.16854	0.00000	0.52274	0.00000
123	N1	PX	0.00000	-0.02211	0.00000	-0.12490	0.00000
124	N1	PY	0.00000	0.16218	0.00000	-0.09806	0.00000
125	N1	PZ	0.01334	0.00000	0.02656	0.00000	-0.02219
126	N1	S	0.00000	-0.74065	0.00000	-3.07246	0.00000
127	N1	PX	0.00000	0.51101	0.00000	-1.30857	0.00000
128	N1	PY	0.00000	-1.14779	0.00000	0.57033	0.00000
129	N1	PZ	0.05277	0.00000	0.22610	0.00000	-0.09833
130	N1	DXX	0.00000	0.15558	0.00000	-0.20476	0.00000
131	N1	DYY	0.00000	-0.17958	0.00000	-0.33474	0.00000
132	N1	DZZ	0.00000	0.06813	0.00000	0.43451	0.00000
133	N1	DXY	0.00000	-0.04375	0.00000	0.35997	0.00000
134	N1	DXZ	-0.01015	0.00000	0.45485	0.00000	-0.12157
135	N1	DYZ	0.41492	0.00000	0.01900	0.00000	-0.21226
136	H6	S	0.00000	0.10623	0.00000	0.05143	0.00000
137	H6	S	0.00000	0.51394	0.00000	0.21081	0.00000
138	H6	PX	0.00000	0.14074	0.00000	-0.08697	0.00000
139	H6	PY	0.00000	-0.30450	0.00000	0.27370	0.00000
140	H6	PZ	0.01403	0.00000	-0.15292	0.00000	0.24045
141	C8	S	0.00000	-0.02702	0.00000	-0.07298	0.00000
142	C8	S	0.00000	-0.23954	0.00000	0.34454	0.00000
143	C8	PX	0.00000	0.05140	0.00000	-0.12440	0.00000
144	C8	PY	0.00000	-0.15670	0.00000	0.18281	0.00000
145	C8	PZ	0.01989	0.00000	0.01777	0.00000	-0.01743
146	C8	S	0.00000	1.21776	0.00000	2.60202	0.00000
147	C8	PX	0.00000	1.00556	0.00000	-1.29474	0.00000
148	C8	PY	0.00000	0.43033	0.00000	0.41593	0.00000
149	C8	PZ	0.00224	0.00000	-0.08052	0.00000	-0.00761
150	C8	DXX	0.00000	-0.11052	0.00000	0.28949	0.00000
151	C8	DYY	0.00000	0.23182	0.00000	0.12765	0.00000
152	C8	DZZ	0.00000	-0.14178	0.00000	-0.56500	0.00000
153	C8	DXY	0.00000	-0.11705	0.00000	-0.19037	0.00000
154	C8	DXZ	-0.37980	0.00000	0.27175	0.00000	0.17945
155	C8	DYZ	-0.03058	0.00000	-0.43575	0.00000	0.43524
156	H8	S	0.00000	-0.12214	0.00000	-0.06083	0.00000
157	H8	S	0.00000	-0.34744	0.00000	-0.24039	0.00000
158	H8	PX	0.00000	-0.02252	0.00000	0.07237	0.00000
159	H8	PY	0.00000	-0.06383	0.00000	0.34047	0.00000
160	H8	PZ	-0.04280	0.00000	0.06751	0.00000	-0.48019
161	C10	S	0.00000	0.00382	0.00000	0.02250	0.00000
162	C10	S	0.00000	-0.00751	0.00000	0.05040	0.00000
163	C10	PX	0.00000	-0.12974	0.00000	-0.00120	0.00000
164	C10	PY	0.00000	-0.14261	0.00000	-0.19090	0.00000
165	C10	PZ	-0.00752	0.00000	-0.03865	0.00000	0.05357
166	C10	S	0.00000	-0.02518	0.00000	-0.72831	0.00000
167	C10	PX	0.00000	-0.17086	0.00000	0.25212	0.00000
168	C10	PY	0.00000	-0.11269	0.00000	-0.46899	0.00000
169	C10	PZ	-0.00289	0.00000	0.02384	0.00000	0.00966
170	C10	DXX	0.00000	-0.05039	0.00000	0.06227	0.00000
171	C10	DYY	0.00000	-0.04216	0.00000	-0.12340	0.00000
172	C10	DZZ	0.00000	0.05897	0.00000	0.16063	0.00000
173	C10	DXY	0.00000	-0.13092	0.00000	-0.04720	0.00000
174	C10	DXZ	0.54568	0.00000	-0.32601	0.00000	-0.11700
175	C10	DYZ	-0.09663	0.00000	-0.34041	0.00000	0.37589

176	H16	S	0.00000	-0.02897	0.00000	-0.01474	0.00000
177	H16	S	0.00000	0.09915	0.00000	-0.12304	0.00000
178	H16	PX	0.00000	0.06655	0.00000	0.13063	0.00000
179	H16	PY	0.00000	0.18169	0.00000	0.05427	0.00000
180	H16	PZ	-0.44118	0.00000	0.07480	0.00000	0.22197
181	H18	S	0.00000	0.03815	0.00000	0.04505	0.00000
182	H18	S	0.00000	-0.15009	0.00000	-0.00462	0.00000
183	H18	PX	0.00000	-0.12762	0.00000	-0.09543	0.00000
184	H18	PY	0.00000	-0.01797	0.00000	-0.05951	0.00000
185	H18	PZ	0.40063	0.00000	-0.38140	0.00000	0.02721

MO:	156	157	158	159	160
Eigenvalues:	3.10168	3.10809	3.11390	3.16425	3.24038
(ev):	84.40116	84.57542	84.73346	86.10363	88.17531

		A	A	A	A	A	
1	H1	S	-0.00322	0.00000	-0.04597	-0.01196	-0.09994
2	H1	S	-0.15890	0.00000	-0.16606	-0.24728	-0.30053
3	H1	PX	0.02673	0.00000	0.06031	-0.08548	0.22357
4	H1	PY	-0.30717	0.00000	-0.21101	-0.07393	0.17606
5	H1	PZ	0.00000	0.36050	0.00000	0.00000	0.00000
6	C1	S	0.04125	0.00000	0.01112	0.06330	0.02191
7	C1	S	0.07058	0.00000	0.15812	0.26671	0.26050
8	C1	PX	0.10409	0.00000	-0.03724	-0.01326	0.19840
9	C1	PY	0.13156	0.00000	0.24268	-0.01008	-0.20173
10	C1	PZ	0.00000	0.04923	0.00000	0.00000	0.00000
11	C1	S	-1.28251	0.00000	-0.02531	-2.66589	-1.04844
12	C1	PX	0.60734	0.00000	0.42022	1.41180	0.89961
13	C1	PY	0.97524	0.00000	0.19250	-0.33898	-0.46952
14	C1	PZ	0.00000	-0.08933	0.00000	0.00000	0.00000
15	C1	DXX	-0.02826	0.00000	0.00391	0.06583	0.04286
16	C1	DYY	-0.19698	0.00000	0.05079	-0.40344	-0.17438
17	C1	DZZ	0.23389	0.00000	0.00630	0.36397	0.12182
18	C1	DXY	0.10764	0.00000	-0.05254	0.09605	-0.08715
19	C1	DXZ	0.00000	-0.43738	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.09539	0.00000	0.00000	0.00000
21	C2	S	0.02293	0.00000	-0.05404	0.06037	-0.02617
22	C2	S	0.01676	0.00000	-0.19790	-0.02246	-0.27082
23	C2	PX	-0.08253	0.00000	0.13550	0.07686	0.11069
24	C2	PY	-0.16510	0.00000	-0.18715	-0.06714	0.21419
25	C2	PZ	0.00000	-0.03927	0.00000	0.00000	0.00000
26	C2	S	-0.81393	0.00000	1.73662	-1.67105	1.81534
27	C2	PX	-0.38890	0.00000	1.18042	0.18006	1.44266
28	C2	PY	-0.05239	0.00000	-0.38072	1.39754	1.25117
29	C2	PZ	0.00000	0.09654	0.00000	0.00000	0.00000
30	C2	DXX	0.00213	0.00000	0.00274	0.11343	-0.03517
31	C2	DYY	-0.19009	0.00000	0.18787	-0.42597	0.15909
32	C2	DZZ	0.17262	0.00000	-0.27975	0.39768	-0.13436
33	C2	DXY	-0.09044	0.00000	0.13370	0.08322	-0.01967
34	C2	DXZ	0.00000	-0.40548	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.01191	0.00000	0.00000	0.00000
36	C3	S	-0.04235	0.00000	-0.07093	-0.08090	-0.09009
37	C3	S	-0.17615	0.00000	-0.33415	-0.39548	-0.33235
38	C3	PX	-0.01254	0.00000	-0.06052	0.11433	0.11798

39	C3	PY	0.02019	0.00000	-0.09878	-0.06949	-0.11918
40	C3	PZ	0.00000	0.00768	0.00000	0.00000	0.00000
41	C3	S	2.09528	0.00000	4.08087	5.82234	6.45633
42	C3	PX	0.49522	0.00000	-1.84799	-1.66564	-1.54905
43	C3	PY	0.61423	0.00000	-0.50432	-0.43890	-2.74243
44	C3	PZ	0.00000	0.11095	0.00000	0.00000	0.00000
45	C3	DXX	-0.10352	0.00000	0.29947	0.35423	0.11113
46	C3	DYY	0.24893	0.00000	0.07236	0.11462	0.40470
47	C3	DZZ	-0.22275	0.00000	-0.37963	-0.41860	-0.46393
48	C3	DXY	0.37350	0.00000	0.12303	0.02405	-0.53749
49	C3	DXZ	0.00000	0.05878	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	-0.44161	0.00000	0.00000	0.00000
51	C4	S	0.01699	0.00000	0.04695	-0.00668	-0.05287
52	C4	S	0.01233	0.00000	0.01255	-0.14008	-0.11793
53	C4	PX	0.12411	0.00000	-0.01567	0.27153	-0.01992
54	C4	PY	-0.17368	0.00000	-0.03977	-0.15174	-0.00035
55	C4	PZ	0.00000	-0.03188	0.00000	0.00000	0.00000
56	C4	S	-0.33354	0.00000	-0.57012	1.38104	2.18715
57	C4	PX	-0.33354	0.00000	0.09424	0.49144	-0.24912
58	C4	PY	-0.11986	0.00000	0.07792	-1.15662	-1.31832
59	C4	PZ	0.00000	0.10216	0.00000	0.00000	0.00000
60	C4	DXX	-0.12745	0.00000	-0.17278	0.13662	0.14923
61	C4	DYY	0.13042	0.00000	-0.07085	0.02638	0.03269
62	C4	DZZ	0.08886	0.00000	0.32872	-0.06268	-0.27438
63	C4	DXY	-0.00190	0.00000	0.26265	-0.04613	-0.21354
64	C4	DXZ	0.00000	0.17304	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.35937	0.00000	0.00000	0.00000
66	C5	S	-0.02902	0.00000	-0.02830	-0.03205	0.05079
67	C5	S	0.06425	0.00000	-0.01662	-0.04290	0.06270
68	C5	PX	-0.06981	0.00000	0.11137	-0.20752	0.02193
69	C5	PY	-0.08972	0.00000	0.25504	-0.05078	0.01596
70	C5	PZ	0.00000	0.03668	0.00000	0.00000	0.00000
71	C5	S	0.57436	0.00000	-0.07607	0.04880	-3.04164
72	C5	PX	0.00183	0.00000	0.01575	0.49385	0.01201
73	C5	PY	-0.39285	0.00000	0.46330	0.14777	1.39279
74	C5	PZ	0.00000	-0.09728	0.00000	0.00000	0.00000
75	C5	DXX	0.07121	0.00000	0.18386	0.25499	-0.14874
76	C5	DYY	0.12105	0.00000	-0.11081	-0.04797	-0.07546
77	C5	DZZ	-0.21268	0.00000	-0.18496	-0.25533	0.26723
78	C5	DXY	0.21764	0.00000	0.11072	0.16587	-0.22383
79	C5	DXZ	0.00000	0.18686	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	-0.34047	0.00000	0.00000	0.00000
81	C6	S	-0.00908	0.00000	0.10178	0.00925	0.04947
82	C6	S	0.07951	0.00000	-0.04393	0.62688	0.12751
83	C6	PX	0.00846	0.00000	0.06759	-0.28121	0.11157
84	C6	PY	-0.01090	0.00000	0.50266	-0.20110	0.13432
85	C6	PZ	0.00000	-0.01967	0.00000	0.00000	0.00000
86	C6	S	0.58673	0.00000	-5.76230	-0.00973	-3.24897
87	C6	PX	-0.11432	0.00000	-1.09587	-3.37468	-2.05486
88	C6	PY	-0.11872	0.00000	0.14105	-0.09466	0.55783
89	C6	PZ	0.00000	-0.13925	0.00000	0.00000	0.00000
90	C6	DXX	-0.05376	0.00000	-0.21346	-0.17079	-0.15397
91	C6	DYY	0.05404	0.00000	-0.44723	0.14276	-0.20357
92	C6	DZZ	-0.04648	0.00000	0.73808	-0.13097	0.29166

93	C6	DXY	-0.00577	0.00000	0.05389	-0.04725	-0.49792
94	C6	DXZ	0.00000	0.08339	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.38642	0.00000	0.00000	0.00000
96	C7	S	0.01605	0.00000	0.03402	0.04915	0.09019
97	C7	S	0.23941	0.00000	0.23356	0.32288	0.36790
98	C7	PX	0.26477	0.00000	0.10023	0.00719	0.11069
99	C7	PY	-0.08866	0.00000	-0.10118	-0.01316	-0.27843
100	C7	PZ	0.00000	-0.04943	0.00000	0.00000	0.00000
101	C7	S	-0.83841	0.00000	-2.37353	-3.46258	-6.25763
102	C7	PX	0.36948	0.00000	1.72114	2.01881	2.97569
103	C7	PY	-0.20222	0.00000	0.00340	-0.76300	-1.31094
104	C7	PZ	0.00000	-0.03343	0.00000	0.00000	0.00000
105	C7	DXX	-0.05764	0.00000	-0.01128	0.00828	-0.09776
106	C7	DYY	0.15337	0.00000	-0.12721	-0.35403	-0.55861
107	C7	DZZ	0.05526	0.00000	0.17619	0.27660	0.49323
108	C7	DXY	0.06834	0.00000	0.00441	-0.10255	-0.17683
109	C7	DXZ	0.00000	0.22047	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	-0.33537	0.00000	0.00000	0.00000
111	H3	S	0.05756	0.00000	0.03369	0.03430	0.05916
112	H3	S	0.16952	0.00000	0.04692	0.20507	0.24678
113	H3	PX	-0.04403	0.00000	-0.15997	-0.28442	0.07163
114	H3	PY	-0.09571	0.00000	-0.05899	0.12869	0.02929
115	H3	PZ	0.00000	-0.34578	0.00000	0.00000	0.00000
116	H4	S	0.01783	0.00000	-0.05998	0.00408	0.02810
117	H4	S	0.03928	0.00000	-0.22584	-0.02261	-0.11353
118	H4	PX	-0.06636	0.00000	-0.18104	0.08906	0.06196
119	H4	PY	0.03660	0.00000	0.09539	0.15599	-0.12937
120	H4	PZ	0.00000	0.32986	0.00000	0.00000	0.00000
121	N1	S	0.00454	0.00000	-0.05960	0.05590	-0.01917
122	N1	S	0.18266	0.00000	-0.56776	0.66226	0.00088
123	N1	PX	0.00373	0.00000	0.08124	-0.15597	0.08372
124	N1	PY	-0.00546	0.00000	0.24194	0.10313	0.27558
125	N1	PZ	0.00000	0.02770	0.00000	0.00000	0.00000
126	N1	S	-0.72344	0.00000	3.10952	-3.41948	0.74553
127	N1	PX	-0.28230	0.00000	1.01652	-0.59193	0.17181
128	N1	PY	-0.09522	0.00000	0.64783	-0.97566	-0.02562
129	N1	PZ	0.00000	0.11492	0.00000	0.00000	0.00000
130	N1	DXX	-0.24318	0.00000	0.04700	-0.02675	-0.18554
131	N1	DYY	0.10829	0.00000	0.54385	-0.51917	0.42993
132	N1	DZZ	0.06965	0.00000	-0.51752	0.42630	-0.15170
133	N1	DXY	-0.04444	0.00000	0.37258	0.23637	-0.03138
134	N1	DXZ	0.00000	0.07056	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.30658	0.00000	0.00000	0.00000
136	H6	S	0.00298	0.00000	0.04950	0.17861	0.15467
137	H6	S	-0.10159	0.00000	0.35087	0.28963	0.43785
138	H6	PX	-0.01064	0.00000	0.09662	0.23647	0.18111
139	H6	PY	-0.00188	0.00000	0.33856	0.01263	-0.22004
140	H6	PZ	0.00000	-0.34321	0.00000	0.00000	0.00000
141	C8	S	-0.05967	0.00000	0.01364	-0.06436	-0.03949
142	C8	S	-0.09970	0.00000	-0.24738	0.04290	-0.32184
143	C8	PX	-0.03978	0.00000	0.08714	-0.11029	0.16807
144	C8	PY	0.07901	0.00000	-0.10270	-0.00720	0.08995
145	C8	PZ	0.00000	0.00448	0.00000	0.00000	0.00000
146	C8	S	2.42604	0.00000	-0.13320	2.39262	2.56910

147	C8	PX	0.06228	0.00000	1.50871	0.39479	1.75605
148	C8	PY	-0.60326	0.00000	1.04923	2.31403	1.67437
149	C8	PZ	0.00000	-0.01927	0.00000	0.00000	0.00000
150	C8	DXX	-0.35880	0.00000	0.12320	0.35817	0.15328
151	C8	DYY	0.46327	0.00000	-0.05137	0.03302	0.01193
152	C8	DZZ	-0.31850	0.00000	0.14309	-0.40734	-0.13484
153	C8	DXY	-0.00848	0.00000	0.13459	-0.22565	0.28424
154	C8	DXZ	0.00000	-0.07840	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.08896	0.00000	0.00000	0.00000
156	H8	S	-0.05925	0.00000	-0.09298	-0.07079	-0.04414
157	H8	S	-0.24367	0.00000	-0.47330	-0.45966	-0.66728
158	H8	PX	0.41702	0.00000	0.09157	-0.08755	-0.04037
159	H8	PY	-0.12922	0.00000	-0.14110	0.02542	0.15366
160	H8	PZ	0.00000	-0.21987	0.00000	0.00000	0.00000
161	C10	S	-0.00099	0.00000	-0.01047	0.02393	-0.01117
162	C10	S	0.17826	0.00000	-0.07830	-0.00965	0.21426
163	C10	PX	-0.05225	0.00000	0.02077	-0.07469	0.07284
164	C10	PY	-0.34341	0.00000	0.08186	-0.03435	-0.04373
165	C10	PZ	0.00000	0.01073	0.00000	0.00000	0.00000
166	C10	S	-1.20736	0.00000	0.98471	0.74886	0.61043
167	C10	PX	-0.13353	0.00000	-0.56742	-0.13367	-0.77235
168	C10	PY	-0.99874	0.00000	0.67954	0.31012	0.00806
169	C10	PZ	0.00000	0.00647	0.00000	0.00000	0.00000
170	C10	DXX	-0.28977	0.00000	0.10996	0.21716	-0.09622
171	C10	DYY	0.10114	0.00000	-0.05400	-0.22159	0.12323
172	C10	DZZ	0.02573	0.00000	-0.06537	0.15508	-0.07270
173	C10	DXY	-0.00460	0.00000	0.02189	-0.09338	0.06203
174	C10	DXZ	0.00000	0.06394	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.06004	0.00000	0.00000	0.00000
176	H16	S	0.04791	0.00000	0.04060	-0.01524	0.07862
177	H16	S	-0.17566	0.00000	0.30116	0.13444	0.07815
178	H16	PX	0.37724	0.00000	-0.15243	-0.08655	0.21017
179	H16	PY	0.32928	0.00000	-0.14818	-0.06172	-0.00707
180	H16	PZ	0.00000	-0.01993	0.00000	0.00000	0.00000
181	H18	S	0.05697	0.00000	-0.14609	-0.04314	-0.13272
182	H18	S	-0.28223	0.00000	-0.01586	-0.06191	-0.32399
183	H18	PX	-0.35839	0.00000	0.08820	0.00657	-0.20229
184	H18	PY	0.31383	0.00000	-0.05096	-0.23020	0.17741
185	H18	PZ	0.00000	0.05755	0.00000	0.00000	0.00000

MO:	161	162	163	164	165
Eigenvalues:	3.29653	3.32987	3.34927	3.43269	3.46974
(ev):	89.70315	90.61046	91.13834	93.40837	94.41652

		A	A	A	A	A	
1	H1	S	-0.15350	0.01250	0.08817	0.00796	0.06530
2	H1	S	-0.36332	-0.02323	0.24145	-0.01352	0.06404
3	H1	PX	0.31966	0.02270	-0.29923	-0.07341	-0.11664
4	H1	PY	-0.23776	0.03528	0.02582	0.14223	-0.38469
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02741	0.01585	0.04578	0.01242	0.01975
7	C1	S	0.08992	-0.02318	-0.23086	-0.15274	-0.24367
8	C1	PX	0.23780	0.13337	-0.06956	0.08287	0.10408
9	C1	PY	-0.11591	0.00457	-0.15211	0.07035	-0.25322

10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.59282	-0.59426	-0.58915	0.20250	-0.20480
12	C1	PX	0.45979	0.11605	0.02477	0.11023	-0.01204
13	C1	PY	-0.20390	0.88140	-0.51450	-0.02954	0.86265
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.09553	-0.01958	0.06797	-0.01004	-0.11315
16	C1	DYY	0.17327	-0.13241	-0.30492	-0.14543	-0.06803
17	C1	DZZ	-0.16876	0.08830	0.31523	0.09489	0.15036
18	C1	DXY	0.35859	-0.15126	0.09781	-0.29773	0.58569
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02052	0.00496	-0.04218	-0.03023	-0.01386
22	C2	S	-0.13333	0.09227	0.20781	0.27321	0.08513
23	C2	PX	-0.15250	0.14006	-0.06023	0.06655	0.02196
24	C2	PY	-0.16866	0.03928	0.15293	0.11701	-0.16386
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.96541	-0.31572	0.79520	0.26396	0.19828
27	C2	PX	0.85092	-0.06667	0.06330	0.49551	0.15963
28	C2	PY	1.06183	-0.48785	0.69813	-0.40607	-0.12562
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.01956	0.05765	-0.09232	0.05267	0.11838
31	C2	DYY	0.06808	0.00128	0.32372	0.16484	0.06268
32	C2	DZZ	-0.09290	0.01310	-0.29108	-0.20682	-0.08278
33	C2	DXY	-0.33154	-0.09737	0.08121	0.32252	-0.49657
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03576	-0.00679	-0.02900	-0.06186	0.00114
37	C3	S	-0.11275	0.00455	0.00138	0.17992	-0.34157
38	C3	PX	-0.00864	0.10885	-0.02706	0.16854	-0.00132
39	C3	PY	-0.44068	0.07839	0.09708	-0.15075	-0.03355
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	3.04173	0.78799	1.57568	2.11372	1.48077
42	C3	PX	-2.06096	1.35193	-0.33333	-0.97750	0.80941
43	C3	PY	-0.57655	0.00349	-1.38563	-0.72389	-0.28917
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.10243	-0.44341	0.19850	-0.29826	0.06811
46	C3	DYY	0.17968	0.36485	-0.09008	0.52613	-0.09516
47	C3	DZZ	-0.17930	-0.02351	-0.13518	-0.33720	0.00559
48	C3	DXY	-0.31032	0.11829	0.25848	0.15830	0.13516
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01590	-0.01945	-0.06707	-0.03076	-0.01707
52	C4	S	0.09558	-0.11077	0.21917	-0.08680	0.18219
53	C4	PX	-0.03399	0.06377	0.06119	0.05502	0.17493
54	C4	PY	-0.19231	0.00928	0.01629	0.04645	-0.22744
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.35903	0.53529	1.37813	0.84599	0.14093
57	C4	PX	-0.00243	-0.81142	0.10658	-0.40801	-0.83880
58	C4	PY	-0.27256	-0.04688	-0.44526	0.01549	0.01393
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.27100	-0.06282	0.24549	-0.04807	-0.23275
61	C4	DYY	0.25093	0.09354	-0.00129	-0.01550	0.42150
62	C4	DZZ	0.10443	-0.10416	-0.42202	-0.15999	-0.13939
63	C4	DXY	-0.10333	-0.19037	-0.23745	-0.18198	-0.38278

64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00927	0.01668	0.07296	0.01787	0.02310
67	C5	S	0.13383	0.06177	-0.17640	-0.23567	0.21174
68	C5	PX	0.07784	0.00760	0.07265	0.16726	0.00644
69	C5	PY	-0.11591	-0.01245	-0.00079	0.14539	-0.08595
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.12274	-0.44307	-1.67115	-0.44870	-0.95802
72	C5	PX	0.61914	-0.71979	0.14460	-0.57596	-0.46947
73	C5	PY	0.41292	-0.17076	0.58693	-0.20408	0.01447
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.16859	0.14086	-0.21494	0.22553	0.02055
76	C5	DYY	0.22376	-0.13786	-0.04598	-0.35021	0.10768
77	C5	DZZ	-0.06676	0.08269	0.45090	0.14632	0.09098
78	C5	DXY	0.12780	-0.15753	-0.27181	-0.26827	-0.11895
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.03560	-0.00397	0.02889	0.01568	0.03297
82	C6	S	0.52476	-0.02148	-0.25684	0.46219	-0.30892
83	C6	PX	-0.02330	0.16326	0.07921	-0.10495	0.05663
84	C6	PY	-0.40097	-0.04282	0.12638	-0.23903	-0.00011
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.95007	0.57949	-1.51037	-0.99512	-0.52507
87	C6	PX	-2.65540	0.85778	-0.22479	-1.04399	0.22076
88	C6	PY	-1.17200	0.20465	1.39559	-0.92208	0.32633
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.31399	0.39724	-0.20977	-0.07988	0.42165
91	C6	DYY	0.22681	-0.31841	-0.01152	0.20551	-0.48399
92	C6	DZZ	0.05143	0.00339	0.24512	-0.02832	0.19200
93	C6	DXY	0.16418	0.07943	0.06386	0.52308	0.41867
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.03160	0.01509	-0.01163	0.02560	0.02527
97	C7	S	0.11683	0.15291	0.29685	0.07942	0.02078
98	C7	PX	0.03170	0.41012	0.02209	0.23103	-0.13463
99	C7	PY	-0.30416	-0.12011	-0.07357	-0.27227	0.16294
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-2.39291	-0.99403	-1.31882	-1.82148	-1.20207
102	C7	PX	1.72229	0.34972	0.71644	1.18299	0.13798
103	C7	PY	0.33382	-0.62139	-0.89049	0.02997	-0.61554
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.29399	-0.09258	0.14452	0.30127	-0.19635
106	C7	DYY	-0.47797	0.09671	0.00377	-0.44644	0.05955
107	C7	DZZ	0.16134	0.04196	-0.10314	0.12287	0.12247
108	C7	DXY	0.35035	-0.18312	0.10827	0.32852	-0.11304
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.08444	0.02843	-0.07601	-0.00187	0.01423
112	H3	S	0.21282	0.07503	-0.14272	-0.04132	0.10277
113	H3	PX	0.12149	0.15995	0.11716	0.10307	0.32832
114	H3	PY	-0.21864	-0.07406	0.23478	-0.05667	-0.10061
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.06930	-0.00754	0.08485	0.04890	-0.03284
117	H4	S	0.12196	-0.03135	0.11489	0.07752	0.00439

118	H4	PX	-0.19353	0.19731	0.11151	0.31415	0.01347
119	H4	PY	-0.20095	0.11918	-0.22160	0.02106	0.09501
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.01447	-0.01202	0.00183	0.00615	0.00918
122	N1	S	0.13431	0.21212	-0.12057	-0.12232	-0.07086
123	N1	PX	-0.10501	0.13382	-0.06998	-0.06891	0.05901
124	N1	PY	-0.04973	-0.00269	0.07663	-0.13660	0.05185
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.21387	-0.20524	0.56860	-0.13166	0.03326
127	N1	PX	0.16704	-0.24063	-0.25106	0.42186	0.02039
128	N1	PY	-1.60835	0.12980	1.14930	-1.16450	0.51675
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.05878	-0.02278	-0.37090	0.43144	0.29892
131	N1	DYY	-0.27040	0.01200	0.34185	-0.54677	-0.13572
132	N1	DZZ	0.09477	-0.00577	-0.00686	0.05066	-0.02417
133	N1	DXY	-0.42377	-0.01754	0.40234	-0.24028	0.50544
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.02994	0.01560	-0.05948	-0.04244	-0.05017
137	H6	S	0.16892	0.04075	-0.21190	0.09026	0.01045
138	H6	PX	-0.12559	0.07214	-0.25445	-0.19984	-0.10998
139	H6	PY	-0.22205	-0.04895	-0.09113	0.27789	-0.25362
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.00963	-0.04106	-0.01918	0.03772	-0.00445
142	C8	S	-0.23524	0.32831	0.10703	-0.45811	-0.05951
143	C8	PX	-0.03187	0.05416	-0.16692	0.02955	-0.00482
144	C8	PY	-0.35682	-0.37166	-0.05181	0.03425	0.14501
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	1.26253	0.59943	0.77477	0.18426	0.01231
147	C8	PX	1.79922	-0.10886	-0.54972	1.30781	-0.37546
148	C8	PY	0.66722	0.61663	0.89622	0.09797	0.80932
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.17396	-0.27988	-0.09313	0.26459	0.38239
151	C8	DYY	0.31136	0.49460	0.23928	-0.31416	-0.32175
152	C8	DZZ	-0.07638	-0.30170	-0.12774	0.25559	-0.01243
153	C8	DXY	-0.08769	0.41237	-0.54034	0.10545	0.05318
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.07237	-0.15894	-0.13012	-0.12353	0.14036
157	H8	S	-0.37773	-0.33238	-0.38204	-0.34802	0.09030
158	H8	PX	-0.09386	0.50974	0.23870	0.07544	-0.23154
159	H8	PY	-0.35364	-0.00697	-0.07686	-0.40334	0.20059
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.03059	0.04314	0.00743	-0.01664	-0.02349
162	C10	S	-0.20512	-0.38286	-0.12624	0.25233	0.20270
163	C10	PX	-0.17032	0.25320	-0.33737	0.08754	0.18019
164	C10	PY	-0.11175	-0.23178	-0.02450	0.08453	0.05615
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.06988	-0.17063	0.30687	0.24374	0.80198
167	C10	PX	-0.66070	0.18803	-0.19731	-0.37685	0.18752
168	C10	PY	0.08631	0.15535	0.25173	-0.06297	0.21733
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.17769	0.29651	0.07036	-0.04717	0.03968
171	C10	DYY	-0.34047	-0.63107	-0.19185	0.27335	0.19792

172	C10	DZZ	0.21792	0.34571	0.07461	-0.16318	-0.18326
173	C10	DXY	-0.07733	-0.05894	-0.01310	-0.01545	-0.03749
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.12676	-0.02277	0.14841	-0.07009	-0.17748
177	H16	S	0.36952	0.02822	0.30165	-0.02791	-0.20534
178	H16	PX	-0.27041	-0.21083	-0.31556	0.25104	0.28307
179	H16	PY	0.03922	-0.29136	0.24491	-0.08649	-0.18474
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.04755	0.14403	-0.11938	-0.06214	-0.04428
182	H18	S	-0.21612	0.33750	-0.11315	-0.22557	0.04895
183	H18	PX	0.06885	0.49516	-0.10027	-0.15058	-0.06845
184	H18	PY	-0.18021	0.01090	-0.26191	0.05852	0.02625
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	166	167	168	169	170
Eigenvalues:	3.54727	3.62575	3.69588	3.72333	3.78343
(ev):	96.52618	98.66173	100.57002	101.31713	102.95245

		A	A	A	A	A	
1	H1	S	0.19929	0.31260	0.37230	0.15946	-0.00208
2	H1	S	0.14116	0.24642	0.21759	0.16398	-0.00950
3	H1	PX	-0.42429	-0.49980	-0.56892	-0.21944	-0.00054
4	H1	PY	-0.00630	-0.03664	-0.04023	0.17623	0.24033
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.03496	0.01121	0.01578	0.00113	0.01121
7	C1	S	-0.03505	-0.23979	-0.22025	-0.00092	0.08178
8	C1	PX	-0.31594	-0.26166	-0.29377	-0.19065	-0.05725
9	C1	PY	0.01901	-0.10225	-0.12548	0.10104	0.23689
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.63181	0.00643	-0.26220	-0.18162	-0.24905
12	C1	PX	0.35182	-0.28212	-0.10134	-0.20973	0.13035
13	C1	PY	-0.96076	0.11780	0.22997	-0.32517	-0.71151
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.10523	-0.33369	-0.43654	-0.12306	0.08508
16	C1	DYY	0.00736	0.17356	0.22088	0.11572	-0.03551
17	C1	DZZ	0.19440	0.09957	0.13302	0.00093	0.02099
18	C1	DXY	-0.01677	0.05598	0.00634	-0.31369	-0.46100
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.04293	0.01436	-0.01050	-0.00275	-0.01414
22	C2	S	0.02680	-0.16649	0.24096	0.00538	-0.09589
23	C2	PX	-0.29112	0.27086	-0.33669	-0.17252	-0.05847
24	C2	PY	-0.13189	-0.03885	0.18035	-0.14951	-0.31280
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.87199	-0.22163	0.24772	0.12844	0.56538
27	C2	PX	0.67767	0.00834	-0.09036	-0.24127	0.34276
28	C2	PY	1.36433	-0.33763	-0.15434	0.32363	0.84374
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.05837	-0.28006	0.45278	0.16649	0.03517
31	C2	DYY	0.00431	0.12080	-0.21889	-0.15567	-0.05528
32	C2	DZZ	-0.23268	0.10525	-0.11598	-0.00870	-0.02902
33	C2	DXY	-0.14082	-0.03806	0.24193	-0.34671	-0.57960
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.06065	0.01669	-0.02498	0.01253	-0.03615
37	C3	S	-0.40806	0.01497	-0.02656	0.13810	0.06888
38	C3	PX	-0.16093	-0.02596	-0.03724	0.14569	0.24625
39	C3	PY	0.20294	-0.04771	-0.09970	-0.04197	-0.00388
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	4.17211	-0.84778	0.86146	-0.76839	1.41301
42	C3	PX	-2.76744	0.42856	-0.02928	0.23215	-0.99482
43	C3	PY	-1.29753	0.12760	-0.13553	-0.03559	-0.89633
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.53988	-0.02537	-0.03605	-0.26409	-0.35432
46	C3	DYY	-0.36991	-0.00004	0.07181	0.22946	0.38132
47	C3	DZZ	-0.21003	0.05270	-0.13678	0.03766	-0.17464
48	C3	DXY	0.14459	-0.03596	-0.18655	-0.14509	0.08231
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.02329	0.03745	0.01467	0.01647	-0.00709
52	C4	S	0.02644	-0.34147	-0.22111	-0.17365	-0.08678
53	C4	PX	-0.10878	-0.17564	-0.14612	-0.27536	-0.22811
54	C4	PY	0.00754	-0.49872	-0.29661	-0.06461	0.13858
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.83767	-0.50604	0.02048	-0.31238	0.29034
57	C4	PX	0.56183	-0.22863	-0.42373	0.37640	0.60492
58	C4	PY	-0.72697	-0.12437	-0.27799	-0.28656	-0.51560
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.27319	0.06584	0.02047	0.26313	0.29188
61	C4	DYY	-0.21300	-0.31786	-0.16732	-0.40710	-0.36302
62	C4	DZZ	-0.12001	0.24004	0.12877	0.14115	0.00794
63	C4	DXY	0.14672	-0.42960	-0.37151	0.03688	0.26485
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02583	0.03076	-0.02467	-0.00843	0.01087
67	C5	S	-0.10727	-0.33205	0.23788	0.14348	0.06925
68	C5	PX	-0.09161	0.23462	-0.18968	-0.26449	-0.22718
69	C5	PY	-0.10581	-0.42795	0.41669	-0.02974	-0.20947
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.29631	-0.08167	0.03517	0.23514	-0.54784
72	C5	PX	0.72863	-0.02125	-0.44720	0.37371	0.64862
73	C5	PY	0.70797	-0.42198	0.27893	0.30643	0.58022
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.31144	0.10548	0.04116	-0.24986	-0.31649
76	C5	DYY	0.26958	-0.31890	0.09854	0.38330	0.42169
77	C5	DZZ	0.13157	0.20666	-0.17792	-0.09780	0.00302
78	C5	DXY	0.18737	0.38318	-0.49517	0.03614	0.25202
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.06913	0.00517	0.00068	-0.00258	0.01829
82	C6	S	0.46877	-0.13601	0.11234	-0.12774	-0.06467
83	C6	PX	-0.21107	0.03272	-0.03642	0.15715	0.17931
84	C6	PY	-0.41393	0.03436	0.11183	0.03295	-0.02282
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-2.10320	0.07274	-0.28463	0.43288	-0.75468
87	C6	PX	-3.40082	0.57973	-0.05225	0.18043	-1.11371
88	C6	PY	-0.20494	-0.04959	-0.12628	0.31209	0.14102

89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.51797	0.06935	-0.06476	0.31289	0.38819
91	C6	DYY	0.43976	-0.02611	0.02890	-0.29982	-0.43817
92	C6	DZZ	0.19550	0.03601	0.01711	0.02648	0.08392
93	C6	DXY	0.26381	-0.01003	-0.28319	-0.04829	0.29077
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.02500	0.00203	0.03704	-0.04848	0.01372
97	C7	S	0.36116	-0.14235	-0.13561	0.07556	-0.02796
98	C7	PX	0.13167	-0.05748	-0.12692	0.17981	0.09664
99	C7	PY	0.19447	0.00054	-0.03257	-0.21284	-0.12537
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-2.95775	0.52761	-0.99876	0.98802	-1.11660
102	C7	PX	2.08368	-0.43144	0.31465	-0.25686	0.75910
103	C7	PY	0.10740	0.06396	-0.02317	-0.30635	-0.14160
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.24827	-0.00753	-0.09056	0.21784	0.11434
106	C7	DYY	0.17338	0.04987	-0.01529	-0.22031	-0.21121
107	C7	DZZ	0.04149	0.02669	0.21137	-0.23382	0.06821
108	C7	DXY	-0.43494	0.06041	0.11954	0.03340	0.16858
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	0.02048	0.54539	0.37102	0.24814	0.04926
112	H3	S	0.08450	0.40519	0.32970	0.17702	0.06765
113	H3	PX	-0.19687	-0.33972	-0.10980	-0.30026	-0.25063
114	H3	PY	0.09069	-0.83254	-0.54938	-0.26326	0.05860
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.09002	0.50698	-0.45953	-0.18032	-0.00524
117	H4	S	0.08449	0.40309	-0.39979	-0.13379	-0.00934
118	H4	PX	-0.15184	0.45008	-0.20691	-0.27156	-0.23244
119	H4	PY	-0.25618	-0.69774	0.67507	0.14957	-0.12953
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	-0.00867	0.00525	-0.00190	-0.01432	0.04032
122	N1	S	-0.04785	-0.08667	0.09092	0.16837	-0.03542
123	N1	PX	-0.02964	0.00733	-0.00422	0.06359	0.03255
124	N1	PY	-0.15740	-0.00093	0.08664	0.07106	0.10700
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.15696	0.24117	-0.09068	-0.05567	-0.52834
127	N1	PX	0.60147	0.00264	-0.07990	-0.12925	0.07256
128	N1	PY	-1.54851	0.23525	-0.04485	0.26101	0.08527
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.27477	0.00884	-0.12465	-0.09344	0.28417
131	N1	DYY	-0.36522	0.09359	0.11420	0.01749	-0.06940
132	N1	DZZ	-0.02307	0.00207	0.00032	-0.04749	0.12026
133	N1	DXY	-0.53248	0.02839	-0.04816	0.19051	0.39847
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.11853	0.26492	-0.39071	-0.15597	0.00293
137	H6	S	0.02024	0.16395	-0.24530	-0.14821	0.09171
138	H6	PX	-0.35776	0.46542	-0.62525	-0.19180	-0.00874
139	H6	PY	-0.10921	0.05576	0.04389	-0.22171	-0.29369
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.01281	0.00394	-0.02988	0.04906	-0.03066
142	C8	S	-0.22456	0.02008	-0.02205	0.12402	-0.22115

143	C8	PX	0.32005	-0.01506	-0.02188	-0.09536	-0.08344
144	C8	PY	-0.15121	0.00823	0.04720	-0.14264	0.22127
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.76611	-0.23245	0.91722	-1.30028	1.37025
147	C8	PX	1.86570	-0.23655	0.32899	-0.57046	0.08155
148	C8	PY	1.17629	-0.36989	-0.04426	0.51055	0.03199
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.00778	-0.02722	-0.06968	0.01598	0.28781
151	C8	DYY	0.06687	0.00363	0.03658	0.10108	-0.31739
152	C8	DZZ	-0.00403	0.00767	-0.14330	0.21747	-0.12876
153	C8	DXY	0.51769	-0.02261	0.01682	-0.12069	-0.09119
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.13179	0.07691	0.17820	-0.23725	-0.03135
157	H8	S	-0.52537	0.14028	0.03733	-0.14474	-0.22992
158	H8	PX	0.16804	-0.08641	-0.25173	0.29484	-0.02498
159	H8	PY	0.09913	0.02785	0.07758	-0.14574	-0.13596
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00055	0.00384	0.03658	-0.08374	0.07049
162	C10	S	0.02612	-0.04401	-0.21470	0.46573	-0.32505
163	C10	PX	0.36630	-0.02407	-0.05531	-0.18136	0.03292
164	C10	PY	-0.06161	0.01805	0.13436	-0.38983	0.44107
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.69723	-0.23932	-0.61033	1.46613	-0.98182
167	C10	PX	-0.27519	0.05217	-0.17705	0.10389	-0.05229
168	C10	PY	0.21645	-0.05637	-0.11000	0.25074	-0.08473
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	0.03240	-0.03548	-0.22935	0.62584	-0.52658
171	C10	DYY	-0.06507	0.01704	0.07767	-0.34991	0.44732
172	C10	DZZ	0.02137	0.02515	0.23187	-0.51318	0.38636
173	C10	DXY	-0.20779	0.02623	0.09016	0.06524	0.08218
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	-0.17989	0.03772	0.24128	-0.34319	0.34631
177	H16	S	-0.04822	0.00863	0.18129	-0.25153	0.25110
178	H16	PX	0.25739	-0.05010	-0.24295	0.30576	-0.31171
179	H16	PY	-0.27707	0.04511	0.23717	-0.41000	0.41411
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.12973	0.01688	0.12348	-0.51295	0.32499
182	H18	S	-0.00395	0.03630	0.04001	-0.28306	0.22572
183	H18	PX	0.24940	0.01640	0.15351	-0.61504	0.36059
184	H18	PY	0.16941	0.01452	0.15910	-0.50812	0.36662
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	171	172	173	174	175
Eigenvalues:	3.88398	3.98232	4.02097	4.25472	4.46388
(ev):	105.68842	108.36459	109.41620	115.77675	121.46844

		A	A	A	A	A	
1	H1	S	0.59034	0.05615	0.05647	0.42830	0.07508
2	H1	S	0.39235	-0.07394	-0.01733	0.28936	0.11206
3	H1	PX	-0.76336	-0.08529	-0.07023	-0.46160	-0.02514
4	H1	PY	-0.06689	0.10558	0.00531	-0.07468	-0.03939
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

6	C1	S	0.06418	0.04317	0.03132	0.07110	-0.07626
7	C1	S	-0.34516	-0.09970	-0.07621	-0.36666	0.39465
8	C1	PX	-0.46223	-0.03457	-0.02877	-0.31267	-0.01946
9	C1	PY	0.01129	0.20484	0.11593	0.05771	-0.10133
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.62372	-0.79347	-0.54824	-0.28202	0.45218
12	C1	PX	-0.30999	0.41614	0.23188	-0.35629	-0.44302
13	C1	PY	0.02359	-0.19158	0.05157	0.08527	0.34701
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.63061	0.00177	-0.01493	-0.44538	-0.26257
16	C1	DYY	0.59294	0.06387	0.08342	0.82106	-0.20371
17	C1	DZZ	0.37581	0.17795	0.12727	0.32592	-0.28311
18	C1	DXY	-0.05641	-0.29967	-0.11061	-0.03350	0.11796
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.06603	-0.00960	-0.02362	-0.07581	-0.10285
22	C2	S	-0.37893	-0.02346	0.06421	0.38150	0.70404
23	C2	PX	0.47143	-0.00026	-0.06725	-0.31610	0.04109
24	C2	PY	0.05203	-0.05130	-0.08057	-0.10813	-0.07035
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.64883	0.30250	0.33791	0.45894	0.13882
27	C2	PX	0.30034	0.24266	0.23989	-0.25976	0.03217
28	C2	PY	-0.03625	0.37484	0.16118	-0.07416	-0.00899
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.63932	-0.03137	0.09317	0.43778	-0.42584
31	C2	DYY	0.59466	0.01699	-0.13671	-0.82421	-0.40407
32	C2	DZZ	0.38776	-0.02897	-0.10625	-0.34314	-0.40358
33	C2	DXY	-0.08102	-0.04900	-0.04400	0.05957	-0.08131
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.02014	-0.08595	-0.04896	0.02343	-0.23305
37	C3	S	0.06905	0.18835	-0.05620	-0.09635	1.56394
38	C3	PX	-0.04090	0.01142	-0.04680	0.02487	-0.03944
39	C3	PY	-0.11900	-0.01875	0.08525	-0.16670	-0.04418
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.23046	2.32965	1.99853	-0.13560	0.25003
42	C3	PX	0.13417	-0.52148	-0.35558	0.36216	0.52545
43	C3	PY	-0.05941	-0.58608	-0.36894	-0.21081	0.08535
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.14872	-0.41568	-0.16521	-0.11920	-0.82759
46	C3	DYY	0.09105	0.27408	0.04851	0.20472	-0.95089
47	C3	DZZ	-0.10848	-0.38913	-0.19068	0.08222	-0.92920
48	C3	DXY	-0.17410	0.28146	0.19780	-0.44109	-0.00883
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.05028	-0.02647	-0.02028	-0.04782	0.02433
52	C4	S	0.27790	0.00009	0.01389	0.20908	-0.00810
53	C4	PX	-0.03009	-0.03395	0.04568	0.12753	0.02620
54	C4	PY	0.27500	0.16671	0.14314	0.33746	-0.05693
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.36015	0.78649	0.53193	0.31824	-0.76093
57	C4	PX	0.10540	0.12401	-0.05612	0.03584	-0.04416
58	C4	PY	0.14098	-0.38512	-0.16387	0.33416	0.39589
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

60	C4	DXX	-0.28760	-0.01186	-0.08480	-0.59997	0.05103
61	C4	DYY	0.23842	-0.04272	0.08947	0.39016	0.07771
62	C4	DZZ	-0.26456	-0.10897	-0.10199	-0.24349	0.08540
63	C4	DXY	0.27674	0.20446	0.20279	0.59986	-0.04829
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.04957	0.00915	0.01832	0.04255	0.00110
67	C5	S	0.27709	0.01675	-0.06554	-0.15875	-0.02869
68	C5	PX	-0.00546	-0.01214	0.03572	0.15230	-0.02976
69	C5	PY	0.26320	-0.04591	-0.11770	-0.32178	-0.04637
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.38019	-0.59832	-0.55902	-0.41161	0.16381
72	C5	PX	-0.18784	0.10552	0.00668	0.08554	0.06845
73	C5	PY	0.10074	0.34149	0.08338	-0.28855	-0.20530
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.27194	-0.05049	0.07775	0.48639	0.03665
76	C5	DYY	0.22823	0.02425	-0.05683	-0.31855	0.07830
77	C5	DZZ	-0.26365	0.03848	0.09234	0.21941	0.00162
78	C5	DXY	-0.30605	0.08768	0.21125	0.68704	0.02356
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.02084	0.00504	0.01628	-0.01357	-0.17415
82	C6	S	0.06277	0.11397	0.15550	0.03019	1.05593
83	C6	PX	0.06151	0.10376	-0.04615	0.01617	0.11900
84	C6	PY	-0.11070	0.03590	-0.11035	0.16472	0.19743
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.34788	-0.96863	-0.57361	0.03931	2.10205
87	C6	PX	-0.06300	-0.72095	-0.71702	0.40513	0.02730
88	C6	PY	-0.13085	0.29444	-0.18641	0.15700	-1.01721
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.14449	-0.01576	0.04044	0.21402	-0.58775
91	C6	DYY	0.08675	-0.08555	0.01676	-0.24109	-0.83274
92	C6	DZZ	-0.11561	0.02508	0.01984	-0.02634	-0.68537
93	C6	DXY	0.12266	0.04862	0.15355	-0.37847	-0.11895
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00221	0.11860	0.09284	-0.04129	-0.16804
97	C7	S	-0.06143	-0.50894	-0.38771	0.19465	1.16955
98	C7	PX	0.09793	-0.51158	-0.09702	0.08760	-0.06287
99	C7	PY	-0.13547	0.02873	0.18409	-0.21577	0.14217
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.02249	-2.35246	-1.93986	0.01880	0.25270
102	C7	PX	-0.00130	0.54071	0.70653	0.08710	0.00926
103	C7	PY	-0.04627	-0.22219	-0.17838	-0.22583	-0.37670
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.14484	-0.38889	-0.35298	0.11943	-0.74651
106	C7	DYY	-0.13173	0.44292	0.45946	-0.39601	-0.56063
107	C7	DZZ	-0.01335	0.62636	0.42693	-0.17084	-0.66489
108	C7	DXY	0.00927	0.79797	0.11895	-0.04265	-0.01335
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.32588	-0.10895	-0.15600	-0.48800	0.00372
112	H3	S	-0.22466	-0.01452	-0.03977	-0.28079	-0.06119
113	H3	PX	0.25879	0.00043	0.06202	0.26245	0.01022

114	H3	PY	0.35099	0.17178	0.19649	0.45826	-0.01685
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.32844	0.04346	0.15978	0.49097	0.00057
117	H4	S	-0.22956	-0.02438	0.08295	0.27369	0.06636
118	H4	PX	-0.29476	-0.01747	0.08437	0.29150	-0.00226
119	H4	PY	0.32502	-0.08041	-0.17635	-0.43655	0.02172
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.01284	0.00508	-0.01174	0.00373	0.34116
122	N1	S	-0.12080	-0.03385	0.08131	0.11228	-0.28589
123	N1	PX	-0.02233	-0.02570	0.09055	0.02522	0.20610
124	N1	PY	-0.07838	0.04012	-0.09382	0.16536	0.13989
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-0.02228	0.07332	-0.03474	-0.03722	-4.34292
127	N1	PX	0.07847	-0.01978	0.18444	-0.15872	-0.94587
128	N1	PY	-0.16738	-0.03095	-0.47980	0.28956	-0.30025
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.09572	-0.18571	0.19715	-0.11058	1.02900
131	N1	DYY	-0.01607	0.21717	-0.20243	0.15281	1.13932
132	N1	DZZ	0.03688	0.01399	-0.02740	0.01662	1.08366
133	N1	DXY	-0.11962	0.02731	-0.17836	0.14863	0.00893
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	0.60353	0.02922	-0.07821	-0.42958	0.08036
137	H6	S	0.40042	0.05113	0.02885	-0.27004	-0.03173
138	H6	PX	0.79459	0.00799	-0.11685	-0.47491	0.05893
139	H6	PY	0.00574	-0.02948	-0.00335	0.00943	0.00655
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.01522	-0.02050	-0.02037	0.00141	-0.06109
142	C8	S	-0.08253	0.04808	-0.00522	-0.00330	0.50255
143	C8	PX	0.02085	-0.08420	0.00377	-0.03489	0.11977
144	C8	PY	-0.01722	-0.19453	-0.10216	0.04772	-0.05327
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.14649	0.75765	0.52804	0.11644	0.80602
147	C8	PX	0.13426	0.37708	0.83956	-0.21032	-0.84051
148	C8	PY	-0.21952	0.59195	0.47097	0.14438	0.65665
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.02192	-0.42340	-0.10368	0.08795	-0.32010
151	C8	DYY	-0.00865	0.43779	0.08416	-0.05339	-0.23515
152	C8	DZZ	0.07195	-0.11627	-0.08690	0.00420	-0.28104
153	C8	DXY	0.04375	-0.25231	0.66129	-0.15708	0.16768
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.08100	0.70495	0.31812	-0.14606	0.11677
157	H8	S	-0.05492	0.24695	-0.00644	-0.13622	-0.13297
158	H8	PX	0.10490	-0.89229	-0.36824	0.14730	-0.08586
159	H8	PY	-0.07810	0.23517	0.22412	-0.08769	0.06053
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	0.00286	-0.02927	-0.00087	0.00187	-0.06292
162	C10	S	0.00094	0.02682	-0.02708	0.01746	0.38173
163	C10	PX	-0.04952	0.32397	-0.67028	0.08039	-0.00772
164	C10	PY	0.01891	-0.33768	-0.06290	0.04366	0.00063
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	-0.13940	0.49656	0.25883	0.03086	0.40621
167	C10	PX	-0.10602	0.10427	-0.64659	0.05060	0.24562

168	C10	PY	-0.05041	0.04639	0.08032	0.02507	0.08804
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.01019	0.18573	0.23353	-0.05444	-0.20394
171	C10	DYY	0.01466	-0.27872	-0.24437	0.06244	-0.26946
172	C10	DZZ	0.01105	-0.12648	0.00439	0.00466	-0.25136
173	C10	DXY	0.07594	-0.61583	1.13621	-0.15819	0.07822
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.06164	-0.42027	0.60406	-0.06233	0.02846
177	H16	S	0.04650	-0.21493	0.31589	-0.01303	-0.10496
178	H16	PX	-0.05301	0.42632	-0.65728	0.07727	-0.04912
179	H16	PY	0.03735	-0.32898	0.24241	-0.00777	0.00458
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	-0.03844	0.17016	-0.67512	0.08783	-0.00067
182	H18	S	-0.05157	0.03839	-0.38174	0.03975	0.04448
183	H18	PX	-0.04677	0.25429	-0.74796	0.09871	-0.00529
184	H18	PY	-0.00718	-0.02941	-0.23735	0.03213	-0.02596
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	176	177	178	179	180
Eigenvalues:	4.53682	4.57047	4.59613	4.69338	4.75434
(ev):	123.45324	124.36886	125.06718	127.71346	129.37231

		A	A	A	A	A	
1	H1	S	-0.09646	0.10324	0.25826	0.14374	-0.03927
2	H1	S	0.10343	-0.09816	-0.03282	-0.07107	0.16213
3	H1	PX	0.07219	-0.08441	-0.21510	-0.14349	0.08311
4	H1	PY	0.01085	-0.00538	-0.04588	-0.00727	-0.00951
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.14675	-0.12126	-0.24252	-0.16089	0.02456
7	C1	S	-1.06979	0.82845	1.53514	0.98790	-0.23429
8	C1	PX	0.11204	-0.06672	-0.07989	-0.04067	0.01375
9	C1	PY	-0.05517	0.10726	-0.08857	-0.03914	0.18083
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.19065	0.16009	0.49313	0.65862	-0.16162
12	C1	PX	-0.05704	0.11019	-0.20112	-0.09429	-0.33667
13	C1	PY	0.05911	-0.12435	0.22780	-0.14008	0.22278
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.61192	-0.54553	-1.15482	-0.76776	0.26172
16	C1	DYY	0.56877	-0.42185	-0.84782	-0.62844	0.15974
17	C1	DZZ	0.56557	-0.47306	-0.91418	-0.59755	0.05830
18	C1	DXY	0.01522	-0.09719	0.10904	0.05077	-0.11352
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.17721	0.11847	0.19925	-0.02320	0.16455
22	C2	S	-1.20482	-0.68126	-1.28310	0.04546	-0.91281
23	C2	PX	-0.12227	-0.02044	-0.06950	-0.00392	-0.07676
24	C2	PY	-0.06186	0.11980	-0.06470	-0.12801	0.00367
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.44595	-0.50451	-0.37224	0.54517	-0.66376
27	C2	PX	0.06732	-0.01814	-0.22684	0.13763	-0.02069
28	C2	PY	0.17629	0.04831	-0.21131	-0.10321	0.38648
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.74395	0.54868	0.90563	-0.09054	0.80462

31	C2	DYY	0.60840	0.40777	0.70097	-0.08283	0.51304
32	C2	DZZ	0.67781	0.44168	0.77076	-0.06617	0.59088
33	C2	DXY	0.00134	0.12411	-0.00444	-0.10993	0.07461
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.03012	-0.00086	-0.20616	0.01662	0.12411
37	C3	S	-0.25626	0.01436	1.33267	-0.12099	-0.78958
38	C3	PX	0.04068	0.11113	0.03568	-0.03189	-0.01608
39	C3	PY	-0.15051	-0.06493	0.06708	0.18067	0.01403
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.28159	0.31725	0.02027	-0.66372	0.31757
42	C3	PX	-0.33093	-0.61602	0.44105	0.03015	0.67873
43	C3	PY	0.22401	0.13430	0.24372	-0.08322	-0.08444
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.07940	-0.08300	-0.85898	0.14214	0.46020
46	C3	DYY	0.20890	0.19249	-0.81878	-0.05530	0.49797
47	C3	DZZ	0.10116	-0.01716	-0.80062	0.07089	0.46913
48	C3	DXY	-0.06975	0.00951	0.03365	0.03860	-0.02131
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.23452	-0.20900	-0.02781	0.00259	-0.20533
52	C4	S	-1.53175	1.30500	0.25072	0.03482	1.25910
53	C4	PX	0.07090	-0.01294	0.14961	0.09268	-0.00406
54	C4	PY	0.10789	-0.03563	-0.09012	-0.07213	0.03570
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.61983	0.60094	-0.01096	0.14973	0.16723
57	C4	PX	0.03543	-0.00615	-0.17221	-0.05696	-0.03600
58	C4	PY	0.11244	-0.11586	0.11001	0.00466	0.01713
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.80192	-0.79007	-0.22560	-0.06386	-0.90411
61	C4	DYY	1.02454	-0.87390	0.05489	0.11896	-0.98016
62	C4	DZZ	0.89552	-0.80324	-0.12758	0.00079	-0.76481
63	C4	DXY	0.07825	-0.00922	-0.00966	-0.02583	-0.00378
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.24109	-0.11128	0.18517	0.15616	0.01224
67	C5	S	-1.66554	0.61856	-1.11946	-0.86677	-0.37327
68	C5	PX	-0.06445	0.11895	0.07138	-0.01325	0.07757
69	C5	PY	0.11620	0.05202	0.05154	-0.02974	0.12352
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.41257	0.32642	-0.43963	-0.74807	0.10037
72	C5	PX	0.09537	0.01506	-0.22168	-0.17742	0.32364
73	C5	PY	-0.07233	-0.12947	0.05867	0.29240	-0.43067
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.89924	-0.32994	0.75947	0.62104	0.28193
76	C5	DYY	1.06339	-0.57035	0.65706	0.67945	0.06465
77	C5	DZZ	0.92432	-0.41176	0.72195	0.58116	0.04852
78	C5	DXY	-0.08777	0.02982	0.01050	0.01247	-0.01484
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.11157	0.21541	0.02355	-0.13067	0.05387
82	C6	S	-0.68331	-1.15261	-0.25327	0.73657	-0.35716
83	C6	PX	0.02439	0.00886	0.08082	-0.01432	0.04908
84	C6	PY	-0.06831	-0.07241	-0.06460	0.03899	0.05050

85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.24850	-0.94401	-0.28638	-0.09879	3.43723
87	C6	PX	-0.51715	-0.78531	0.60220	0.47812	-0.45773
88	C6	PY	-0.33285	-0.15847	0.33571	0.14062	-2.00711
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.36610	0.77994	0.25647	-0.48859	0.13149
91	C6	DYY	0.44826	0.86930	0.05532	-0.57892	0.17671
92	C6	DZZ	0.40256	0.80167	0.11450	-0.47437	0.17117
93	C6	DXY	0.05472	0.08959	0.04421	-0.01659	-0.06792
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.09248	-0.14115	-0.02591	0.23406	0.12455
97	C7	S	0.60747	0.91248	0.12828	-1.49879	-0.60281
98	C7	PX	-0.03551	-0.07649	-0.00719	0.05606	0.08950
99	C7	PY	-0.06194	-0.07699	0.13806	-0.02003	0.00705
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00615	0.02154	0.62715	-0.43901	-1.07655
102	C7	PX	0.30350	0.10049	-0.54417	-0.13811	0.87506
103	C7	PY	0.19750	0.50579	-0.12662	0.17331	-0.93742
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.39286	-0.58446	-0.10847	1.16403	0.40173
106	C7	DYY	-0.43187	-0.62263	0.01122	0.96977	0.40238
107	C7	DZZ	-0.34714	-0.51654	-0.09428	0.87581	0.44407
108	C7	DXY	0.09379	0.17392	-0.07896	-0.12125	-0.10114
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.20534	0.14297	-0.04290	-0.03834	0.19215
112	H3	S	0.09488	-0.07922	-0.03785	-0.01238	-0.05794
113	H3	PX	0.07913	-0.06295	0.02816	0.01894	-0.08738
114	H3	PY	0.14211	-0.09327	0.05175	0.03363	-0.15771
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	-0.19754	0.12483	-0.09171	-0.12562	0.03320
117	H4	S	0.17226	-0.00821	0.03543	-0.02645	0.23660
118	H4	PX	-0.09275	0.05806	-0.03282	-0.06048	-0.00244
119	H4	PY	0.13879	-0.09532	0.04218	0.08182	0.00973
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.09750	-0.03737	-0.10463	-0.05350	0.42714
122	N1	S	-0.10825	-0.01838	0.09944	-0.00382	0.03316
123	N1	PX	0.04087	-0.00435	-0.06340	0.01412	0.09877
124	N1	PY	-0.06291	-0.14105	-0.01494	0.05080	0.07676
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.34729	0.46832	1.42741	0.98601	-7.45202
127	N1	PX	-0.22781	0.32543	0.18176	0.22912	-1.90282
128	N1	PY	-0.38098	-0.46593	0.34556	0.31769	-0.76575
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	0.33214	0.01877	-0.38181	-0.09565	1.01913
131	N1	DYY	0.23381	-0.21646	-0.31315	-0.08047	1.10704
132	N1	DZZ	0.31604	-0.12033	-0.32783	-0.18792	1.37750
133	N1	DXY	-0.10283	-0.16550	0.05146	0.07077	0.04110
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.12205	-0.11276	-0.20411	0.01306	-0.15321
137	H6	S	0.14034	0.06845	-0.00081	0.00630	0.09052

138	H6	PX	-0.09824	-0.10749	-0.15430	0.02680	-0.17614
139	H6	PY	0.01388	0.01322	0.01075	-0.00111	-0.00377
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	-0.11737	-0.23710	0.11829	-0.02599	0.16283
142	C8	S	0.70204	1.46049	-0.72003	0.31437	-1.02233
143	C8	PX	0.03685	0.01645	-0.01890	-0.07688	0.01627
144	C8	PY	-0.04748	-0.05757	0.11132	-0.19928	-0.07200
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	0.73946	0.54671	-0.84897	-0.31634	1.32489
147	C8	PX	0.17772	0.78505	-0.22347	0.08524	-1.41885
148	C8	PY	0.39701	-0.11390	-0.50348	-0.39783	2.05031
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	-0.46638	-0.90228	0.49914	-0.15656	0.57231
151	C8	DYY	-0.41684	-0.91846	0.41230	-0.06981	0.81696
152	C8	DZZ	-0.45562	-0.89968	0.45993	-0.12166	0.56807
153	C8	DXY	0.08023	0.08635	-0.05392	-0.10460	0.01099
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	0.07619	0.18680	0.02914	-0.23466	-0.20060
157	H8	S	-0.11536	0.01148	0.12320	0.19759	-0.35687
158	H8	PX	-0.09251	-0.16221	0.01522	0.22777	0.10780
159	H8	PY	-0.01097	-0.01186	0.03447	-0.09573	0.01496
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.08014	-0.14746	0.15507	-0.30794	-0.00734
162	C10	S	0.56024	1.07811	-1.02702	1.96607	-0.07654
163	C10	PX	-0.00128	0.00287	-0.00174	0.01060	-0.02292
164	C10	PY	0.06015	0.16225	-0.07283	0.07021	-0.15474
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	0.29898	0.18037	-0.58047	0.73985	1.09728
167	C10	PX	-0.05004	-0.28503	0.04943	-0.00520	0.64915
168	C10	PY	0.02405	-0.10034	-0.07518	0.02021	0.33854
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.35381	-0.71155	0.70280	-1.47805	0.07542
171	C10	DYY	-0.32299	-0.56167	0.64545	-1.33227	-0.17315
172	C10	DZZ	-0.30351	-0.54988	0.58037	-1.12627	-0.02902
173	C10	DXY	0.02089	0.02209	-0.01630	-0.03279	0.02512
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.06503	0.15520	-0.11933	0.23648	-0.08920
177	H16	S	-0.02420	-0.00668	0.06113	-0.16586	-0.21073
178	H16	PX	-0.04901	-0.09081	0.09648	-0.19269	-0.00665
179	H16	PY	0.02128	0.04950	-0.04986	0.12946	-0.00741
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.04497	0.09874	-0.10251	0.26991	0.00896
182	H18	S	-0.07461	-0.21323	0.10409	-0.15885	0.20361
183	H18	PX	0.03348	0.07378	-0.09074	0.24256	-0.00760
184	H18	PY	0.00978	0.03840	-0.03536	0.10963	-0.03015
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

MO:	181	182	183	184	185
Eigenvalues:	4.86203	4.88576	5.04654	5.28033	0.00000
(ev):	132.30270	132.94838	137.32340	143.68525	0.00000

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1	H1	S	-0.00313	0.25367	0.06797	-0.21258	0.00000
2	H1	S	0.04847	0.04260	-0.11924	0.04590	0.00000
3	H1	PX	0.01114	-0.24467	-0.09210	0.22936	0.00000
4	H1	PY	-0.02417	-0.01295	-0.00890	-0.01060	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.04057	-0.23752	-0.04869	0.17493	0.00000
7	C1	S	-0.27385	1.33181	0.37159	-1.07533	0.00000
8	C1	PX	0.01476	0.04918	0.00108	-0.06938	0.00000
9	C1	PY	-0.15118	-0.02790	-0.09380	-0.03666	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.37526	1.41893	-0.28652	-0.91727	0.00000
12	C1	PX	0.00558	-0.54508	0.32339	0.26349	0.00000
13	C1	PY	0.29788	0.07785	0.01723	-0.13797	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.15572	-1.18125	-0.34653	1.01811	0.00000
16	C1	DYY	0.21248	-1.05767	-0.26480	1.00925	0.00000
17	C1	DZZ	0.15770	-0.85104	-0.16517	0.57101	0.00000
18	C1	DXY	0.14458	-0.00038	0.09100	0.07709	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.06772	-0.23027	0.14392	-0.13268	0.00000
22	C2	S	-0.35772	1.38673	-0.93128	0.82945	0.00000
23	C2	PX	-0.00872	-0.05196	0.01059	-0.05380	0.00000
24	C2	PY	0.16324	0.02600	0.08611	-0.01730	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.16015	1.53411	-0.44593	0.71019	0.00000
27	C2	PX	0.05007	0.70403	0.16539	0.36744	0.00000
28	C2	PY	-0.01483	0.32703	0.05195	0.41553	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.40911	-1.12560	0.87688	-0.75043	0.00000
31	C2	DYY	0.26025	-1.12767	0.72188	-0.78444	0.00000
32	C2	DZZ	0.22318	-0.83381	0.48424	-0.43466	0.00000
33	C2	DXY	0.15873	0.05973	0.05644	0.00520	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.20263	0.09926	-0.03300	-0.24852	0.00000
37	C3	S	1.19534	-0.69620	0.06703	1.34366	0.00000
38	C3	PX	0.03086	0.10038	-0.02462	-0.00731	0.00000
39	C3	PY	0.04209	0.03028	0.11750	0.11288	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.41304	0.50046	0.89614	3.53678	0.00000
42	C3	PX	0.02412	-0.17882	-0.36204	-0.86575	0.00000
43	C3	PY	0.39903	-0.22782	0.50537	-0.98022	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.90452	0.29572	-0.03939	-1.04713	0.00000
46	C3	DYY	-0.97493	0.67450	-0.26120	-1.43542	0.00000
47	C3	DZZ	-0.74281	0.36468	-0.10141	-0.83969	0.00000
48	C3	DXY	-0.05959	0.02773	-0.01143	-0.11698	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.15826	0.13547	0.12173	-0.13827	0.00000
52	C4	S	-0.98363	-0.77670	-0.82036	0.86294	0.00000
53	C4	PX	-0.02621	0.12689	0.01880	-0.05605	0.00000
54	C4	PY	0.02358	-0.05919	-0.01897	0.05410	0.00000

55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-1.00805	-1.16812	-0.34896	1.04117	0.00000
57	C4	PX	0.12690	0.06877	0.08030	-0.05654	0.00000
58	C4	PY	0.20703	0.35696	-0.08654	-0.31856	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.77445	0.56486	0.66701	-0.77045	0.00000
61	C4	DYY	0.74126	0.78377	0.68658	-0.81867	0.00000
62	C4	DZZ	0.56990	0.46371	0.42153	-0.44981	0.00000
63	C4	DXY	0.03222	-0.03327	0.01845	0.00580	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.22184	0.03586	-0.16331	0.12009	0.00000
67	C5	S	1.30153	-0.28080	1.01789	-0.77289	0.00000
68	C5	PX	0.01932	-0.12750	0.05468	-0.04095	0.00000
69	C5	PY	0.03215	-0.05939	0.05374	-0.04185	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	1.10151	-0.50032	0.66645	-1.14590	0.00000
72	C5	PX	0.27718	0.31229	0.09328	0.02565	0.00000
73	C5	PY	-0.33332	0.09208	-0.08073	0.27012	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-1.00610	0.15372	-0.82428	0.69928	0.00000
76	C5	DYY	-1.07997	0.37082	-0.92607	0.71734	0.00000
77	C5	DZZ	-0.79822	0.10266	-0.56097	0.38810	0.00000
78	C5	DXY	0.02374	0.03582	0.01653	0.00411	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.17013	0.26217	-0.03969	0.17596	0.00000
82	C6	S	-1.03366	-1.48003	0.40761	-0.96418	0.00000
83	C6	PX	0.05146	-0.04931	0.07236	0.02296	0.00000
84	C6	PY	-0.05442	0.01955	0.04275	-0.04008	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.07785	0.24556	0.38298	-1.73173	0.00000
87	C6	PX	-0.28095	-0.82911	-0.60168	-1.23639	0.00000
88	C6	PY	-0.96370	-1.61530	-0.82374	0.14888	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.83159	0.99258	-0.24438	0.83462	0.00000
91	C6	DYY	0.75634	1.31575	-0.40814	0.90714	0.00000
92	C6	DZZ	0.61082	0.91663	-0.14713	0.59339	0.00000
93	C6	DXY	-0.00568	-0.08317	-0.02080	-0.06601	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.05846	0.04544	0.22163	0.19461	0.00000
97	C7	S	-0.24707	-0.17701	-1.37586	-0.89381	0.00000
98	C7	PX	0.03850	0.03332	-0.00837	-0.03366	0.00000
99	C7	PY	0.16866	-0.07107	-0.01960	0.13767	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.15862	-1.00633	-1.01258	-3.04260	0.00000
102	C7	PX	0.13555	0.79838	0.42604	1.30880	0.00000
103	C7	PY	-0.26203	-0.38683	0.10776	-0.38530	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.21180	0.10673	1.29698	1.04895	0.00000
106	C7	DYY	0.31180	0.06151	0.97812	0.90205	0.00000
107	C7	DZZ	0.19487	0.17645	0.77058	0.61991	0.00000
108	C7	DXY	-0.21544	0.07098	-0.06610	-0.23490	0.00000

109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	H3	S	-0.13743	-0.15941	-0.13881	0.17994	0.00000
112	H3	S	0.03333	-0.00770	0.07809	0.00335	0.00000
113	H3	PX	0.06801	0.07946	0.06219	-0.07709	0.00000
114	H3	PY	0.12818	0.15029	0.14419	-0.18022	0.00000
115	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	H4	S	0.22772	-0.05769	0.19583	-0.13888	0.00000
117	H4	S	0.02822	0.08872	-0.03784	0.04240	0.00000
118	H4	PX	0.11558	-0.05562	0.10976	-0.08166	0.00000
119	H4	PY	-0.18582	0.07004	-0.18590	0.14738	0.00000
120	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
121	N1	S	0.04920	0.19371	0.11360	-0.00700	0.00000
122	N1	S	0.20026	0.09766	-0.13615	-0.00499	0.00000
123	N1	PX	-0.09423	-0.02345	0.13465	-0.04264	0.00000
124	N1	PY	-0.04509	-0.10365	0.05577	-0.07893	0.00000
125	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	N1	S	-1.64116	-4.00911	-1.74496	-0.01352	0.00000
127	N1	PX	-0.52122	-0.99044	-0.14603	0.09288	0.00000
128	N1	PY	-0.23040	-0.76611	-0.41672	-0.37291	0.00000
129	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
130	N1	DXX	-0.08313	0.40982	0.53266	-0.00762	0.00000
131	N1	DYY	-0.09393	0.31997	0.47186	-0.13917	0.00000
132	N1	DZZ	0.21708	0.65931	0.27643	0.00453	0.00000
133	N1	DXY	0.05586	-0.11671	-0.06808	-0.10717	0.00000
134	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	H6	S	-0.09881	0.24340	-0.18538	0.17624	0.00000
137	H6	S	0.03868	0.07839	0.14597	0.03417	0.00000
138	H6	PX	-0.12112	0.20935	-0.21430	0.16453	0.00000
139	H6	PY	-0.00432	0.00562	-0.00388	-0.00126	0.00000
140	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
141	C8	S	0.20104	-0.00143	-0.23473	-0.11992	0.00000
142	C8	S	-1.20376	-0.07961	1.48166	0.61555	0.00000
143	C8	PX	-0.05542	-0.00884	-0.00156	-0.02494	0.00000
144	C8	PY	-0.12113	0.01588	0.08119	0.01526	0.00000
145	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	C8	S	-0.53717	1.22147	1.57225	1.34958	0.00000
147	C8	PX	-0.42589	-0.36816	0.19320	0.81979	0.00000
148	C8	PY	0.50031	1.33811	0.25965	0.88479	0.00000
149	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
150	C8	DXX	0.87956	-0.02404	-1.13088	-0.48419	0.00000
151	C8	DYY	1.05073	0.04558	-1.35618	-0.66673	0.00000
152	C8	DZZ	0.71376	-0.00932	-0.82714	-0.39590	0.00000
153	C8	DXY	-0.05602	-0.00966	-0.07904	-0.09133	0.00000
154	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	H8	S	-0.11675	-0.05438	-0.30948	-0.30118	0.00000
157	H8	S	-0.06051	-0.25349	0.01688	-0.22109	0.00000
158	H8	PX	0.10451	-0.01136	0.26973	0.26994	0.00000
159	H8	PY	-0.00246	-0.00033	-0.12496	-0.09187	0.00000
160	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
161	C10	S	-0.17714	0.06308	0.15128	0.05280	0.00000
162	C10	S	1.04887	-0.40904	-0.87231	-0.25962	0.00000

163	C10	PX	-0.01469	-0.01284	0.01351	0.01602	0.00000
164	C10	PY	-0.11327	-0.02687	0.17490	0.12488	0.00000
165	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	C10	S	1.02964	0.41767	-0.68464	0.13520	0.00000
167	C10	PX	0.23955	0.25656	-0.01149	-0.25174	0.00000
168	C10	PY	0.18239	0.14806	-0.09156	0.09552	0.00000
169	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
170	C10	DXX	-0.86353	0.35620	0.77480	0.25097	0.00000
171	C10	DYY	-0.95991	0.25482	0.93492	0.37078	0.00000
172	C10	DZZ	-0.60740	0.21925	0.47818	0.15830	0.00000
173	C10	DXY	-0.00864	-0.00258	-0.04170	-0.05519	0.00000
174	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	H16	S	0.12646	-0.10467	-0.17749	-0.05409	0.00000
177	H16	S	-0.18393	-0.06110	0.09690	0.10788	0.00000
178	H16	PX	-0.14189	0.05672	0.16302	0.07216	0.00000
179	H16	PY	0.10084	-0.04215	-0.10881	-0.04117	0.00000
180	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
181	H18	S	0.18276	-0.04689	-0.13611	-0.05442	0.00000
182	H18	S	-0.03400	0.09450	0.09712	-0.06220	0.00000
183	H18	PX	0.15962	-0.06151	-0.13698	-0.04004	0.00000
184	H18	PY	0.07652	-0.04122	-0.08140	-0.01938	0.00000
185	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

Atomic Charges from Electrostatic Potential

Resolution: 1 points per atomic unit

6696 of 15903 gridpoints used in calculation

Atom	Charge
----	-----
H 1	0.182682
C 2	-0.282027
C 3	-0.427477
C 4	0.157576
C 5	-0.155004
C 6	-0.019853
C 7	0.637866
C 8	-0.505415
H 9	0.137409
H 10	0.125546
N 11	-0.720030
H 12	0.197534
C 13	0.477692
H 14	0.237911
C 15	-0.429961
H 16	0.177680
H 17	0.207870

Total Charge = 0.000000

RMS fit: 1.283698
RRMS fit: 0.177393

Dipole moment from formal charges:

x = 2.1987, y = 0.5541, z = 0.0000 = 2.2675 debye

Q-minus(elesta) = -0.7200

Q-plus(elesta) = 0.2379

Mulliken Population Analysis

AO	atom type		Occupancy
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1	H1	S	0.534227
2	H1	S	0.293930
3	H1	PX	0.010027
4	H1	PY	0.001556
5	H1	PZ	0.002424
6	C1	S	1.996538
7	C1	S	0.673068
8	C1	PX	0.731242
9	C1	PY	0.741701
10	C1	PZ	0.520173
11	C1	S	0.451915
12	C1	PX	0.308437
13	C1	PY	0.165618
14	C1	PZ	0.451393
15	C1	DXX	0.018907
16	C1	DYY	0.020693
17	C1	DZZ	-0.018414
18	C1	DXY	0.013999
19	C1	DXZ	0.003430
20	C1	DYZ	0.008192
21	C2	S	1.996536
22	C2	S	0.672240
23	C2	PX	0.730798
24	C2	PY	0.744021
25	C2	PZ	0.532194
26	C2	S	0.467023
27	C2	PX	0.306340
28	C2	PY	0.159501
29	C2	PZ	0.465732
30	C2	DXX	0.018030
31	C2	DYY	0.020448
32	C2	DZZ	-0.017929
33	C2	DXY	0.014807
34	C2	DXZ	0.003257
35	C2	DYZ	0.006821
36	C3	S	1.996655
37	C3	S	0.671935

38	C3	PX	0.714603
39	C3	PY	0.760397
40	C3	PZ	0.544646
41	C3	S	0.440812
42	C3	PX	0.210980
43	C3	PY	0.233561
44	C3	PZ	0.466911
45	C3	DXX	0.019466
46	C3	DYY	0.030938
47	C3	DZZ	-0.017152
48	C3	DXY	0.013298
49	C3	DXZ	0.003656
50	C3	DYZ	0.010067
51	C4	S	1.996540
52	C4	S	0.669391
53	C4	PX	0.718668
54	C4	PY	0.746079
55	C4	PZ	0.524657
56	C4	S	0.489691
57	C4	PX	0.199828
58	C4	PY	0.294507
59	C4	PZ	0.474817
60	C4	DXX	0.020150
61	C4	DYY	0.019471
62	C4	DZZ	-0.018519
63	C4	DXY	0.014098
64	C4	DXZ	0.005439
65	C4	DYZ	0.005240
66	C5	S	1.996582
67	C5	S	0.674128
68	C5	PX	0.722416
69	C5	PY	0.754860
70	C5	PZ	0.499870
71	C5	S	0.499096
72	C5	PX	0.212127
73	C5	PY	0.293392
74	C5	PZ	0.453126
75	C5	DXX	0.019682
76	C5	DYY	0.019518
77	C5	DZZ	-0.018988
78	C5	DXY	0.014776
79	C5	DXZ	0.005484
80	C5	DYZ	0.005965
81	C6	S	1.996741
82	C6	S	0.693344
83	C6	PX	0.723360
84	C6	PY	0.756907
85	C6	PZ	0.480469
86	C6	S	0.345409
87	C6	PX	0.184739
88	C6	PY	0.130464
89	C6	PZ	0.365449
90	C6	DXX	0.021562
91	C6	DYY	0.034517

92	C6	DZZ	-0.020076
93	C6	DXY	0.024653
94	C6	DXZ	0.006464
95	C6	DYZ	0.015544
96	C7	S	1.996678
97	C7	S	0.676646
98	C7	PX	0.724481
99	C7	PY	0.751110
100	C7	PZ	0.511160
101	C7	S	0.445210
102	C7	PX	0.309117
103	C7	PY	0.200439
104	C7	PZ	0.458662
105	C7	DXX	0.021581
106	C7	DYY	0.016439
107	C7	DZZ	-0.017967
108	C7	DXY	0.016389
109	C7	DXZ	0.002856
110	C7	DYZ	0.008651
111	H3	S	0.535714
112	H3	S	0.297733
113	H3	PX	0.003041
114	H3	PY	0.008358
115	H3	PZ	0.002458
116	H4	S	0.536095
117	H4	S	0.294211
118	H4	PX	0.003646
119	H4	PY	0.007816
120	H4	PZ	0.002259
121	N1	S	1.996235
122	N1	S	0.785459
123	N1	PX	0.913388
124	N1	PY	0.778246
125	N1	PZ	0.672021
126	N1	S	0.964114
127	N1	PX	0.571462
128	N1	PY	0.314826
129	N1	PZ	0.552948
130	N1	DXX	-0.000187
131	N1	DYY	0.013831
132	N1	DZZ	-0.011239
133	N1	DXY	0.017646
134	N1	DXZ	0.006469
135	N1	DYZ	0.009289
136	H6	S	0.531044
137	H6	S	0.282647
138	H6	PX	0.010177
139	H6	PY	0.001499
140	H6	PZ	0.002415
141	C8	S	1.996653
142	C8	S	0.680637
143	C8	PX	0.667464
144	C8	PY	0.769201
145	C8	PZ	0.537599

146	C8	S	0.375689
147	C8	PX	0.126334
148	C8	PY	0.093261
149	C8	PZ	0.429449
150	C8	DXX	0.019140
151	C8	DYY	0.030685
152	C8	DZZ	-0.019127
153	C8	DXY	0.025934
154	C8	DXZ	0.009133
155	C8	DYZ	0.010716
156	H8	S	0.530976
157	H8	S	0.287277
158	H8	PX	0.009214
159	H8	PY	0.002740
160	H8	PZ	0.002486
161	C10	S	1.996645
162	C10	S	0.679880
163	C10	PX	0.726621
164	C10	PY	0.770854
165	C10	PZ	0.463199
166	C10	S	0.565019
167	C10	PX	0.369295
168	C10	PY	0.236050
169	C10	PZ	0.444426
170	C10	DXX	0.011825
171	C10	DYY	0.018859
172	C10	DZZ	-0.020377
173	C10	DXY	0.013621
174	C10	DXZ	0.000145
175	C10	DYZ	0.007897
176	H16	S	0.533171
177	H16	S	0.306004
178	H16	PX	0.007270
179	H16	PY	0.004369
180	H16	PZ	0.002240
181	H18	S	0.529085
182	H18	S	0.288122
183	H18	PX	0.008764
184	H18	PY	0.003094
185	H18	PZ	0.002105

Atom	Occupancy	Charge
-----	-----	-----
H1	0.842164	0.157836
C1	6.086893	-0.086893
C2	6.119819	-0.119819
C3	6.100773	-0.100773
C4	6.160057	-0.160057
C5	6.152032	-0.152032
C6	5.759546	0.240454
C7	6.121452	-0.121452
H3	0.847304	0.152696
H4	0.844027	0.155973

N1	7.584508	-0.584508
H6	0.827782	0.172218
C8	5.752768	0.247232
H8	0.832693	0.167307
C10	6.283960	-0.283960
H16	0.853054	0.146946
H18	0.831169	0.168831

Total Charge = 0.000000

Natural Atomic Orbital Populations

Nao	Atom	Type	Basis	Occupancy
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1	H1	S	MIN	0.762232
2	H1	S	RYD	0.000660
3	H1	PX	RYD	0.000584
4	H1	PY	RYD	0.000022
5	H1	PZ	RYD	0.000084
6	C1	S	MIN	1.999001
7	C1	S	MIN	0.946432
8	C1	S	RYD	0.000872
9	C1	S	RYD	0.000017
10	C1	PX	MIN	1.202635
11	C1	PX	RYD	0.005762
12	C1	PY	MIN	1.048784
13	C1	PY	RYD	0.006172
14	C1	PZ	MIN	0.978641
15	C1	PZ	RYD	0.001737
16	C1	DXY	RYD	0.001645
17	C1	DXZ	RYD	0.000736
18	C1	DYZ	RYD	0.000962
19	C1	DXX-YY	RYD	0.001647
20	C1	D3ZZ-RR	RYD	0.001200
21	C2	S	MIN	1.998979
22	C2	S	MIN	0.958145
23	C2	S	RYD	0.001101
24	C2	S	RYD	0.000030
25	C2	PX	MIN	1.208579
26	C2	PX	RYD	0.005767
27	C2	PY	MIN	1.052169
28	C2	PY	RYD	0.007106
29	C2	PZ	MIN	1.005452
30	C2	PZ	RYD	0.001993
31	C2	DXY	RYD	0.001815
32	C2	DXZ	RYD	0.000747
33	C2	DYZ	RYD	0.000851
34	C2	DXX-YY	RYD	0.001530
35	C2	D3ZZ-RR	RYD	0.001217
36	C3	S	MIN	1.998972
37	C3	S	MIN	0.885307
38	C3	S	RYD	0.001378

39	C3	S	RYD	0.000049
40	C3	PX	MIN	1.074367
41	C3	PX	RYD	0.008200
42	C3	PY	MIN	1.115619
43	C3	PY	RYD	0.004436
44	C3	PZ	MIN	1.037130
45	C3	PZ	RYD	0.001083
46	C3	DXY	RYD	0.001228
47	C3	DXZ	RYD	0.000292
48	C3	DYZ	RYD	0.001438
49	C3	DXX-YY	RYD	0.001830
50	C3	D3ZZ-RR	RYD	0.001064
51	C4	S	MIN	1.999075
52	C4	S	MIN	0.958946
53	C4	S	RYD	0.000696
54	C4	S	RYD	0.000025
55	C4	PX	MIN	1.067538
56	C4	PX	RYD	0.005994
57	C4	PY	MIN	1.183150
58	C4	PY	RYD	0.006385
59	C4	PZ	MIN	1.008590
60	C4	PZ	RYD	0.001893
61	C4	DXY	RYD	0.001657
62	C4	DXZ	RYD	0.000548
63	C4	DYZ	RYD	0.001053
64	C4	DXX-YY	RYD	0.001705
65	C4	D3ZZ-RR	RYD	0.001256
66	C5	S	MIN	1.999086
67	C5	S	MIN	0.962389
68	C5	S	RYD	0.000636
69	C5	S	RYD	0.000028
70	C5	PX	MIN	1.077615
71	C5	PX	RYD	0.005832
72	C5	PY	MIN	1.176961
73	C5	PY	RYD	0.006360
74	C5	PZ	MIN	0.961742
75	C5	PZ	RYD	0.001598
76	C5	DXY	RYD	0.001718
77	C5	DXZ	RYD	0.000546
78	C5	DYZ	RYD	0.001159
79	C5	DXX-YY	RYD	0.001678
80	C5	D3ZZ-RR	RYD	0.001280
81	C6	S	MIN	1.999157
82	C6	S	MIN	0.838809
83	C6	S	RYD	0.003640
84	C6	S	RYD	0.000105
85	C6	PX	MIN	1.009691
86	C6	PX	RYD	0.010802
87	C6	PY	MIN	0.972122
88	C6	PY	RYD	0.007625
89	C6	PZ	MIN	0.864754
90	C6	PZ	RYD	0.001134
91	C6	DXY	RYD	0.002288
92	C6	DXZ	RYD	0.000670

93	C6	DYZ	RVD	0.002295
94	C6	DXX-YY	RVD	0.002404
95	C6	D3ZZ-RR	RVD	0.001021
96	C7	S	MIN	1.998878
97	C7	S	MIN	0.958603
98	C7	S	RVD	0.000707
99	C7	S	RVD	0.000040
100	C7	PX	MIN	1.176245
101	C7	PX	RVD	0.004635
102	C7	PY	MIN	1.069483
103	C7	PY	RVD	0.005020
104	C7	PZ	MIN	0.959855
105	C7	PZ	RVD	0.001440
106	C7	DXY	RVD	0.001665
107	C7	DXZ	RVD	0.000509
108	C7	DYZ	RVD	0.001260
109	C7	DXX-YY	RVD	0.001580
110	C7	D3ZZ-RR	RVD	0.001232
111	H3	S	MIN	0.763667
112	H3	S	RVD	0.000525
113	H3	PX	RVD	0.000134
114	H3	PY	RVD	0.000474
115	H3	PZ	RVD	0.000083
116	H4	S	MIN	0.763460
117	H4	S	RVD	0.000544
118	H4	PX	RVD	0.000181
119	H4	PY	RVD	0.000442
120	H4	PZ	RVD	0.000072
121	N1	S	MIN	1.999380
122	N1	S	MIN	1.378795
123	N1	S	RVD	0.000485
124	N1	S	RVD	0.000015
125	N1	PX	MIN	1.623516
126	N1	PX	RVD	0.004276
127	N1	PY	MIN	1.254374
128	N1	PY	RVD	0.003891
129	N1	PZ	MIN	1.246202
130	N1	PZ	RVD	0.001303
131	N1	DXY	RVD	0.003892
132	N1	DXZ	RVD	0.002985
133	N1	DYZ	RVD	0.001751
134	N1	DXX-YY	RVD	0.002990
135	N1	D3ZZ-RR	RVD	0.002863
136	H6	S	MIN	0.751460
137	H6	S	RVD	0.000765
138	H6	PX	RVD	0.000571
139	H6	PY	RVD	0.000022
140	H6	PZ	RVD	0.000077
141	C8	S	MIN	1.999041
142	C8	S	MIN	0.865816
143	C8	S	RVD	0.002880
144	C8	S	RVD	0.000109
145	C8	PX	MIN	0.937354

146	C8	PX	RYD	0.009642
147	C8	PY	MIN	1.062377
148	C8	PY	RYD	0.007632
149	C8	PZ	MIN	1.009711
150	C8	PZ	RYD	0.001605
151	C8	DXY	RYD	0.002139
152	C8	DXZ	RYD	0.001079
153	C8	DYZ	RYD	0.001641
154	C8	DXX-YY	RYD	0.002298
155	C8	D3ZZ-RR	RYD	0.001107
156	H8	S	MIN	0.760888
157	H8	S	RYD	0.000440
158	H8	PX	RYD	0.000538
159	H8	PY	RYD	0.000083
160	H8	PZ	RYD	0.000088
161	C10	S	MIN	1.998994
162	C10	S	MIN	1.046941
163	C10	S	RYD	0.001135
164	C10	S	RYD	0.000016
165	C10	PX	MIN	1.220922
166	C10	PX	RYD	0.004335
167	C10	PY	MIN	1.127537
168	C10	PY	RYD	0.003594
169	C10	PZ	MIN	0.889253
170	C10	PZ	RYD	0.002249
171	C10	DXY	RYD	0.001857
172	C10	DXZ	RYD	0.000047
173	C10	DYZ	RYD	0.001501
174	C10	DXX-YY	RYD	0.002020
175	C10	D3ZZ-RR	RYD	0.001518
176	H16	S	MIN	0.782447
177	H16	S	RYD	0.000416
178	H16	PX	RYD	0.000420
179	H16	PY	RYD	0.000203
180	H16	PZ	RYD	0.000087
181	H18	S	MIN	0.764824
182	H18	S	RYD	0.000813
183	H18	PX	RYD	0.000526
184	H18	PY	RYD	0.000101
185	H18	PZ	RYD	0.000072

Total MIN occupancy: 67.762094
Total RYD occupancy: 0.237906
Total occupancy: 68.000000

Natural Atomic Populations and Charges

Atom	Occupancy	Charge
-----	-----	-----
H1	0.763582	0.236418
C1	6.196243	-0.196243
C2	6.245483	-0.245483

C3	6.132393	-0.132393
C4	6.238510	-0.238510
C5	6.198625	-0.198625
C6	5.716518	0.283482
C7	6.181153	-0.181153
H3	0.764883	0.235117
H4	0.764701	0.235299
N1	7.526719	-0.526719
H6	0.752895	0.247105
C8	5.904430	0.095570
H8	0.762037	0.237963
C10	6.301918	-0.301918
H16	0.783574	0.216426
H18	0.766336	0.233664

Total Charge = 0.000000

Q-minus(NAO) = -0.5267

Q-plus(NAO) = 0.2471

Reason for exit: Normal completion

Wall Time: 000:00:00

CPU Time: 000:00:00

Job WF28826 started on DESKTOP-T7TL8TH at Thu Mar 09 16:34:24 2023
Jaguar version 3.5, release 42

Job name: Ic
Task: Geometry optimization

Stoichiometry: C10NH90
Molecular weight: 159.07 amu
Molecular charge: 0
Spin multiplicity: 1
Point Group: Cs

SCF method: RHF
Basis set: 6-31G**
Basis functions: 225

Total electrons: 84
Alpha electrons: 42
Beta electrons: 42
Total orbitals: 225
Core orbitals: 42
Open-shell orbitals: 0
Occupied orbitals: 42
Shells: 1

Non-default options chosen:

Geometry will be optimized in redundant internal coordinates
Initial Hessian: from previous calculation

WARNING: Hessian has too many zero eigenvalues
Some coordinates may be inadvertently frozen

Iter	Energy	Gmax	Grms	Dmax	Drms
1	-513.167325 *	0.05664	0.01460	0.09735	0.03556
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
2	-513.181510 .	0.01790	0.00458	0.03899	0.01180
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
3	-513.183031 .	0.00552	0.00168	0.01433	0.00419
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
4	-513.183221 .	0.00361	0.00073	0.00674	0.00161
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
5	-513.183208 *	0.00068	0.00017 *	0.00124 *	0.00045 *
WARNING: Hessian has too many zero eigenvalues Some coordinates may be inadvertently frozen					
6	-513.183207 #	0.00023 *	0.00006 *	0.00070 *	0.00015 #

 ** Geometry optimization complete **

Final energy -513.18320745742

Job WF28826 completed on DESKTOP-T7TL8TH at Thu Mar 09 16:36:12 2023

Wall Time: 000:01:47

CPU Time: 000:00:00

TITAN Properties Program: (PC/x86)

Release 6.0.2

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-20.60019	-15.54147	-11.31105	-11.28860	-11.27098
(ev):		-560.55981	-422.90511	-307.78945	-307.17847	-306.69918
		A	A	A	A	A
1	H1 S	-0.00001	-0.00005	0.00007	0.00003	-0.00006
2	H1 S	-0.00020	-0.00039	-0.00029	0.00013	-0.00068
3	H1 PX	0.00001	0.00000	-0.00013	-0.00001	0.00000
4	H1 PY	0.00002	0.00001	0.00003	0.00002	0.00004
5	H1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1 S	0.00002	0.00003	0.00919	0.00000	0.00007
7	C1 S	0.00013	0.00012	0.00016	0.00016	0.00031
8	C1 PX	0.00001	-0.00003	0.00008	0.00000	-0.00008
9	C1 PY	-0.00003	-0.00001	0.00005	-0.00012	-0.00006
10	C1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1 S	-0.00169	-0.00136	0.00161	-0.00311	-0.00240
12	C1 PX	0.00083	0.00120	-0.00013	0.00049	0.00174
13	C1 PY	-0.00028	0.00004	0.00003	0.00039	0.00018
14	C1 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1 DXX	0.00002	0.00000	-0.00037	0.00004	-0.00005
16	C1 DYY	-0.00010	0.00002	-0.00038	-0.00013	-0.00006
17	C1 DZZ	0.00002	0.00006	-0.00002	0.00001	0.00014
18	C1 DXY	0.00005	0.00000	-0.00004	0.00002	0.00002
19	C1 DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1 DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2 S	0.00001	-0.00002	-0.00026	0.00004	-0.01405
22	C2 S	0.00003	-0.00005	-0.00052	0.00016	-0.00066
23	C2 PX	0.00001	-0.00001	-0.00007	0.00001	0.00014
24	C2 PY	0.00000	0.00004	-0.00004	-0.00006	-0.00001
25	C2 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2 S	-0.00023	0.00058	0.00426	-0.00241	-0.00107
27	C2 PX	0.00007	0.00032	0.00295	-0.00124	-0.00053
28	C2 PY	-0.00030	-0.00064	0.00034	-0.00086	-0.00083
29	C2 PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2 DXX	0.00000	-0.00013	0.00005	0.00000	0.00055
31	C2 DYY	0.00001	0.00003	0.00018	-0.00003	0.00055
32	C2 DZZ	0.00001	-0.00002	-0.00021	0.00005	0.00010

33	C2	DXY	-0.00001	-0.00002	0.00001	-0.00002	-0.00027
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.00001	-0.00040	-0.00002	-0.01165
37	C3	S	0.00000	0.00002	-0.00014	-0.00006	-0.00028
38	C3	PX	0.00002	-0.00003	0.00012	0.00001	-0.00004
39	C3	PY	0.00000	-0.00003	-0.00019	-0.00007	-0.00002
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00012	0.00005	-0.00315	-0.00002	-0.00731
42	C3	PX	-0.00034	-0.00120	-0.00315	0.00013	0.00169
43	C3	PY	0.00070	0.00083	0.00468	0.00225	0.00292
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.00002	0.00005	-0.00005	0.00047
46	C3	DYY	0.00001	-0.00006	0.00009	0.00005	0.00036
47	C3	DZZ	0.00000	0.00001	-0.00004	-0.00003	0.00018
48	C3	DXY	0.00002	0.00005	0.00000	0.00003	0.00020
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00001	-0.00001	0.99568	0.00071	-0.00010
52	C4	S	0.00031	-0.00007	0.02680	-0.00021	-0.00015
53	C4	PX	0.00000	0.00000	-0.00004	-0.00014	-0.00002
54	C4	PY	0.00033	-0.00001	0.00124	-0.00006	-0.00004
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00105	0.00170	-0.00590	0.00034	0.00314
57	C4	PX	0.00094	0.00008	0.00006	0.00309	0.00002
58	C4	PY	-0.00073	-0.00055	0.00413	0.00151	-0.00112
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00001	0.00001	-0.00131	0.00006	0.00006
61	C4	DYY	-0.00011	0.00002	-0.00063	0.00024	0.00008
62	C4	DZZ	-0.00009	-0.00002	-0.00235	-0.00006	-0.00002
63	C4	DXY	-0.00002	0.00000	-0.00018	0.00003	0.00001
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00001	0.00002	0.00599	0.00001	0.00044
67	C5	S	0.00003	0.00007	0.00048	-0.00021	0.00044
68	C5	PX	0.00000	0.00003	-0.00002	0.00004	0.00009
69	C5	PY	0.00002	-0.00003	-0.00003	0.00009	-0.00011
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00061	-0.00036	0.00017	0.00393	-0.00080
72	C5	PX	-0.00022	-0.00077	0.00025	0.00137	-0.00177
73	C5	PY	-0.00018	0.00028	0.00074	-0.00141	0.00094
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00005	0.00001	-0.00051	-0.00001	-0.00005
76	C5	DYY	-0.00003	0.00002	-0.00044	0.00004	-0.00013
77	C5	DZZ	-0.00002	0.00005	-0.00008	-0.00007	0.00016
78	C5	DXY	-0.00005	-0.00002	-0.00028	0.00002	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00005	-0.00005	-0.00003	-0.99550
82	C6	S	0.00002	-0.00028	0.00015	-0.00005	-0.02755
83	C6	PX	-0.00001	-0.00002	-0.00003	-0.00002	-0.00007
84	C6	PY	0.00001	-0.00011	0.00004	-0.00001	0.00016
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.00016	-0.00438	-0.00240	0.00110	0.00835

87	C6	PX	0.00011	-0.00032	0.00124	0.00018	0.00333
88	C6	PY	-0.00030	0.00147	-0.00380	0.00049	0.00370
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.00003	0.00000	0.00003	0.00176
91	C6	DYY	0.00000	0.00065	-0.00007	-0.00002	0.00099
92	C6	DZZ	0.00001	0.00003	0.00001	-0.00001	0.00243
93	C6	DXY	0.00000	0.00001	0.00001	-0.00004	0.00018
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	-0.00002	-0.00009	-0.00001	0.00121
97	C7	S	-0.00003	-0.00006	-0.00035	-0.00006	-0.00028
98	C7	PX	0.00000	-0.00004	-0.00003	0.00000	0.00006
99	C7	PY	0.00002	-0.00004	0.00006	0.00005	-0.00002
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00078	0.00171	0.00671	0.00146	0.00615
102	C7	PX	-0.00038	-0.00124	-0.00256	-0.00093	-0.00422
103	C7	PY	0.00008	0.00079	0.00184	0.00008	0.00002
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00001	-0.00001	0.00002	-0.00010
106	C7	DYY	0.00001	0.00000	0.00007	0.00000	-0.00004
107	C7	DZZ	-0.00001	-0.00001	-0.00012	-0.00001	-0.00016
108	C7	DXY	0.00000	0.00002	0.00001	-0.00001	0.00008
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.99462	0.00000	0.00000	-0.00011	0.00001
112	O1	S	0.02130	0.00002	0.00116	0.00043	0.00006
113	O1	PX	0.00106	0.00001	0.00000	0.00027	0.00001
114	O1	PY	-0.00076	-0.00001	-0.00026	0.00004	-0.00002
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00409	-0.00009	-0.00476	-0.00013	-0.00018
117	O1	PX	-0.00088	-0.00003	0.00023	-0.00118	-0.00003
118	O1	PY	0.00026	0.00009	0.00320	0.00029	0.00022
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00419	0.00002	0.00051	-0.00058	0.00005
121	O1	DYY	-0.00417	-0.00001	-0.00067	-0.00018	-0.00002
122	O1	DZZ	-0.00394	0.00002	0.00080	0.00025	0.00005
123	O1	DXY	-0.00007	0.00000	-0.00015	-0.00032	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00002	-0.00006	-0.00007	0.00008	-0.00012
127	H4	S	-0.00019	-0.00028	-0.00006	0.00042	-0.00085
128	H4	PX	-0.00001	0.00000	0.00006	0.00001	0.00003
129	H4	PY	0.00003	0.00002	-0.00005	0.00002	0.00002
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	-0.99524	0.00001	-0.00001	0.00032
132	N1	S	0.00000	-0.02514	0.00002	-0.00002	-0.00071
133	N1	PX	0.00000	-0.00166	0.00001	-0.00002	0.00008
134	N1	PY	0.00000	-0.00131	-0.00003	0.00001	-0.00007
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.00010	0.00724	-0.00108	0.00018	0.00525
137	N1	PX	0.00005	0.00263	0.00009	0.00010	0.00106
138	N1	PY	-0.00005	0.00147	-0.00026	0.00001	0.00232
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00001	0.00291	0.00005	0.00000	0.00014

141	N1	DYY	0.00000	0.00252	0.00003	0.00000	0.00013
142	N1	DZZ	0.00000	0.00308	-0.00001	-0.00002	-0.00047
143	N1	DXY	0.00000	-0.00012	-0.00001	0.00000	0.00004
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00001	-0.00001	0.00008	-0.00003	-0.00007
147	H6	S	0.00001	0.00002	0.00096	-0.00035	-0.00021
148	H6	PX	0.00000	0.00002	-0.00001	0.00000	-0.00010
149	H6	PY	0.00001	0.00005	0.00002	0.00002	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.00001	0.00004	0.00000	-0.00040
152	C8	S	0.00002	-0.00038	0.00013	0.00000	0.00030
153	C8	PX	0.00000	0.00016	-0.00006	0.00000	0.00010
154	C8	PY	0.00000	-0.00008	0.00005	-0.00003	0.00005
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.00029	-0.00284	-0.00122	-0.00071	-0.00342
157	C8	PX	-0.00006	0.00211	0.00006	-0.00023	0.00031
158	C8	PY	-0.00023	-0.00161	-0.00227	0.00013	-0.00500
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00001	0.00030	-0.00001	-0.00001	-0.00018
161	C8	DYY	0.00000	0.00009	-0.00001	0.00000	-0.00009
162	C8	DZZ	0.00001	0.00009	0.00004	0.00000	0.00005
163	C8	DXY	-0.00001	-0.00014	-0.00003	-0.00001	0.00009
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00001	0.00007	-0.00003	0.00003	0.00016
167	H8	S	0.00009	0.00039	0.00053	0.00027	0.00119
168	H8	PX	0.00000	-0.00001	0.00000	0.00000	-0.00002
169	H8	PY	0.00000	-0.00002	-0.00006	0.00000	0.00001
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	-0.00001	-0.00001	0.00000	0.00000
172	C10	S	0.00000	0.00000	0.00000	-0.00002	-0.00003
173	C10	PX	0.00000	0.00000	-0.00003	-0.00001	0.00006
174	C10	PY	0.00000	0.00000	-0.00006	0.00001	-0.00008
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.00007	-0.00063	-0.00124	0.00036	-0.00255
177	C10	PX	0.00007	-0.00071	0.00049	0.00006	0.00015
178	C10	PY	-0.00001	-0.00027	-0.00027	0.00019	-0.00075
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.00002	-0.00003	0.00000	-0.00007
181	C10	DYY	0.00000	-0.00005	-0.00001	0.00001	0.00002
182	C10	DZZ	0.00000	0.00001	-0.00002	0.00000	-0.00003
183	C10	DXY	0.00000	-0.00011	0.00000	0.00000	0.00002
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.00001	0.00005	-0.00004	-0.00002	0.00006
187	H16	S	-0.00003	0.00029	-0.00008	-0.00003	0.00008
188	H16	PX	0.00000	0.00001	-0.00001	0.00000	-0.00003
189	H16	PY	0.00000	0.00000	0.00000	0.00000	0.00001
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00001	-0.00003	0.00006	0.00000	-0.00001
192	H18	S	0.00002	-0.00020	0.00020	0.00004	0.00009
193	H18	PX	0.00000	0.00003	0.00001	0.00000	0.00002
194	H18	PY	0.00000	0.00002	0.00001	0.00000	0.00000

195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00000	-0.00071	0.99583	-0.00002
197	C9	S	0.00025	0.00001	-0.00018	0.02763	0.00000
198	C9	PX	-0.00038	-0.00001	-0.00004	-0.00097	-0.00001
199	C9	PY	-0.00017	0.00000	-0.00001	-0.00069	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00016	-0.00002	-0.00022	-0.01224	-0.00003
202	C9	PX	0.00021	0.00001	0.00029	-0.00044	0.00004
203	C9	PY	-0.00015	-0.00001	-0.00074	0.00088	-0.00009
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00008	0.00000	0.00002	-0.00138	-0.00001
206	C9	DYY	0.00004	0.00001	0.00020	-0.00148	0.00001
207	C9	DZZ	0.00003	0.00001	0.00005	-0.00156	0.00001
208	C9	DXY	0.00005	0.00000	0.00015	0.00006	0.00001
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.00001	0.00000	0.00009	-0.00007	0.00001
212	H3	S	-0.00004	0.00000	0.00025	0.00182	0.00005
213	H3	PX	0.00003	0.00000	0.00004	-0.00001	0.00000
214	H3	PY	0.00007	0.00000	0.00006	0.00014	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00007	0.00000	-0.00009	0.00013	-0.00001
217	H5	S	-0.00013	0.00001	-0.00001	0.00251	0.00002
218	H5	PX	0.00004	0.00000	-0.00003	0.00007	0.00000
219	H5	PY	0.00002	0.00000	0.00005	-0.00007	0.00000
220	H5	PZ	-0.00004	0.00000	-0.00001	-0.00006	0.00000
221	H7	S	-0.00007	0.00000	-0.00009	0.00013	-0.00001
222	H7	S	-0.00013	0.00001	-0.00001	0.00251	0.00002
223	H7	PX	0.00004	0.00000	-0.00003	0.00007	0.00000
224	H7	PY	0.00002	0.00000	0.00005	-0.00007	0.00000
225	H7	PZ	0.00004	0.00000	0.00001	0.00006	0.00000

MO: 6 7 8 9 10
Eigenvalues: -11.25727 -11.24891 -11.24274 -11.24199 -11.23919
(ev): -306.32603 -306.09843 -305.93066 -305.91030 -305.83416

			A	A	A	A	A
1	H1	S	0.00007	-0.00007	0.00000	-0.00004	-0.00004
2	H1	S	0.00072	-0.00076	0.00002	-0.00079	-0.00029
3	H1	PX	0.00000	-0.00001	0.00000	-0.00003	-0.00010
4	H1	PY	-0.00003	-0.00002	0.00001	-0.00001	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00006	0.00151	0.00001	-0.00018	0.03839
7	C1	S	-0.00015	0.00042	-0.00005	0.00039	0.00120
8	C1	PX	0.00004	-0.00004	0.00000	0.00000	0.00005
9	C1	PY	0.00004	-0.00004	0.00000	0.00004	0.00022
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00158	-0.00395	0.00045	-0.00657	0.00164
12	C1	PX	-0.00210	0.00227	-0.00015	0.00303	0.00048
13	C1	PY	0.00055	0.00105	-0.00017	0.00130	-0.00106
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	-0.00013	-0.00001	-0.00008	-0.00045
16	C1	DYY	-0.00006	-0.00012	0.00002	-0.00008	-0.00082
17	C1	DZZ	-0.00007	0.00014	-0.00002	0.00012	-0.00022

18	C1	DXY	-0.00001	0.00004	0.00000	-0.00002	-0.00017
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00024	-0.11731	0.00107	0.98857	0.00315
22	C2	S	0.00012	-0.00312	0.00003	0.02750	-0.00008
23	C2	PX	0.00003	0.00003	0.00001	0.00033	-0.00004
24	C2	PY	-0.00007	0.00016	-0.00001	0.00003	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.00051	-0.00008	0.00000	-0.01013	0.00102
27	C2	PX	-0.00074	0.00054	-0.00001	-0.00046	0.00065
28	C2	PY	-0.00083	-0.00066	-0.00026	-0.00021	0.00034
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00001	0.00064	0.00000	-0.00155	0.00008
31	C2	DYY	0.00004	0.00054	0.00001	-0.00141	0.00006
32	C2	DZZ	0.00006	0.00032	0.00000	-0.00246	-0.00006
33	C2	DXY	0.00003	0.00000	-0.00001	0.00013	-0.00002
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00036	0.00037	0.00043	-0.00331	0.98854
37	C3	S	0.00009	-0.00006	0.00007	-0.00020	0.02762
38	C3	PX	-0.00005	-0.00001	0.00001	0.00007	-0.00019
39	C3	PY	-0.00006	-0.00003	0.00004	-0.00013	0.00005
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00293	0.00105	-0.00167	-0.00070	-0.01350
42	C3	PX	0.00324	-0.00119	-0.00021	-0.00124	0.00071
43	C3	PY	0.00072	0.00328	0.00050	0.00582	0.00114
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00003	0.00001	0.00001	0.00007	-0.00182
46	C3	DYY	0.00020	0.00006	-0.00004	0.00007	-0.00118
47	C3	DZZ	0.00009	0.00001	0.00001	-0.00001	-0.00234
48	C3	DXY	-0.00007	0.00001	0.00000	0.00004	-0.00015
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00622	0.00001	0.00089	-0.00001
52	C4	S	0.00012	-0.00010	0.00004	-0.00028	-0.00027
53	C4	PX	0.00000	-0.00008	0.00000	0.00001	0.00002
54	C4	PY	0.00000	-0.00004	0.00000	0.00000	0.00003
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.00268	-0.00152	-0.00021	0.00195	0.00081
57	C4	PX	-0.00053	0.00173	-0.00004	0.00153	0.00006
58	C4	PY	0.00130	-0.00142	0.00038	-0.00268	-0.00131
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00067	0.00001	0.00012	0.00006
61	C4	DYY	-0.00001	0.00025	0.00001	0.00003	0.00008
62	C4	DZZ	0.00004	0.00006	0.00001	-0.00007	-0.00007
63	C4	DXY	0.00000	0.00002	0.00000	0.00003	-0.00005
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00014	-0.98859	-0.00008	-0.11796	0.00004
67	C5	S	-0.00014	-0.02735	-0.00001	-0.00346	0.00003
68	C5	PX	-0.00002	-0.00029	0.00001	0.00004	-0.00004
69	C5	PY	0.00005	0.00001	0.00001	0.00018	0.00003
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00160	0.01017	0.00029	0.00455	-0.00095

72	C5	PX	0.00073	0.00075	0.00002	-0.00013	-0.00026
73	C5	PY	-0.00113	0.00058	-0.00020	-0.00038	0.00058
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.00177	0.00000	-0.00019	-0.00005
76	C5	DYY	-0.00002	0.00140	0.00000	-0.00025	-0.00004
77	C5	DZZ	-0.00006	0.00246	0.00000	0.00025	-0.00002
78	C5	DXY	-0.00001	-0.00007	0.00000	0.00005	0.00001
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00046	0.00136	-0.00006	-0.01430	-0.01185
82	C6	S	-0.00039	0.00028	-0.00006	-0.00024	-0.00022
83	C6	PX	-0.00005	-0.00001	-0.00004	0.00008	-0.00007
84	C6	PY	-0.00008	0.00009	0.00004	0.00003	0.00002
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00492	-0.00025	-0.00007	0.00468	0.00478
87	C6	PX	0.00336	0.00005	0.00043	0.00014	0.00194
88	C6	PY	-0.00061	-0.00310	-0.00001	-0.00259	-0.00091
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00008	0.00005	-0.00001	-0.00041	-0.00057
91	C6	DYY	0.00015	-0.00004	-0.00001	-0.00039	-0.00024
92	C6	DZZ	-0.00010	0.00007	-0.00003	-0.00006	-0.00010
93	C6	DXY	-0.00004	0.00004	0.00003	0.00020	-0.00004
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01480	-0.00004	0.00235	-0.00009	0.11103
97	C7	S	0.00054	-0.00009	0.00008	-0.00020	0.00281
98	C7	PX	0.00005	0.00000	0.00004	-0.00004	0.00015
99	C7	PY	0.00007	0.00003	-0.00005	0.00009	-0.00016
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00392	0.00270	0.00149	0.00542	0.00391
102	C7	PX	-0.00076	-0.00124	-0.00096	-0.00256	-0.00115
103	C7	PY	-0.00278	0.00045	0.00045	0.00076	0.00108
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00062	0.00001	-0.00005	0.00005	-0.00074
106	C7	DYY	-0.00041	0.00001	-0.00009	0.00002	-0.00049
107	C7	DZZ	-0.00014	-0.00003	-0.00002	-0.00005	-0.00037
108	C7	DXY	-0.00023	0.00001	-0.00007	-0.00001	0.00008
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00005	0.00001	-0.00005	-0.00003
112	O1	S	0.00000	-0.00010	0.00003	-0.00021	-0.00013
113	O1	PX	-0.00001	-0.00001	0.00000	0.00003	0.00000
114	O1	PY	0.00001	0.00001	0.00000	0.00001	0.00002
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.00015	0.00130	-0.00025	0.00160	0.00086
117	O1	PX	0.00009	-0.00005	0.00001	-0.00033	-0.00004
118	O1	PY	-0.00003	-0.00029	0.00007	-0.00043	-0.00027
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.00020	0.00002	-0.00015	-0.00010
121	O1	DYY	0.00002	-0.00018	0.00002	-0.00013	-0.00008
122	O1	DZZ	-0.00001	-0.00006	0.00002	-0.00010	-0.00008
123	O1	DXY	-0.00001	-0.00007	0.00000	0.00004	-0.00001
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

126	H4	S	0.00006	0.00021	0.00000	0.00002	-0.00001
127	H4	S	0.00042	-0.00187	0.00004	-0.00042	-0.00012
128	H4	PX	0.00000	0.00017	0.00000	0.00010	0.00001
129	H4	PY	0.00000	-0.00014	0.00000	-0.00016	-0.00002
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00011	0.00004	-0.00004	0.00007	0.00009
132	N1	S	0.00073	0.00017	0.00001	0.00016	0.00025
133	N1	PX	0.00005	-0.00001	-0.00001	0.00005	0.00006
134	N1	PY	-0.00010	0.00000	-0.00004	-0.00001	0.00002
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.00348	-0.00217	0.00092	-0.00301	-0.00300
137	N1	PX	-0.00214	0.00016	0.00018	-0.00010	-0.00081
138	N1	PY	-0.00012	-0.00084	0.00014	-0.00087	-0.00048
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00050	0.00011	-0.00014	0.00019	0.00020
141	N1	DYY	-0.00003	0.00003	-0.00012	0.00017	0.00021
142	N1	DZZ	0.00041	0.00008	-0.00002	0.00007	0.00018
143	N1	DXY	0.00011	0.00003	0.00009	0.00001	0.00003
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.00004	0.00001	-0.00001	-0.00030	0.00002
147	H6	S	-0.00034	0.00004	-0.00003	0.00177	0.00031
148	H6	PX	0.00000	-0.00010	0.00000	-0.00026	0.00000
149	H6	PY	-0.00001	-0.00008	0.00001	-0.00007	-0.00002
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.99379	-0.00007	0.05930	-0.00027	-0.00132
152	C8	S	0.02729	0.00007	0.00197	0.00013	-0.00008
153	C8	PX	-0.00029	-0.00003	0.00000	-0.00007	-0.00002
154	C8	PY	0.00028	0.00001	-0.00020	0.00005	0.00006
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.01057	-0.00080	-0.00566	-0.00118	0.00029
157	C8	PX	-0.00396	-0.00008	-0.00014	-0.00048	-0.00103
158	C8	PY	-0.00032	-0.00072	0.00107	-0.00160	-0.00039
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00159	0.00000	0.00027	-0.00001	0.00002
161	C8	DYY	-0.00110	0.00001	0.00023	0.00004	0.00014
162	C8	DZZ	-0.00236	0.00003	-0.00003	0.00006	0.00003
163	C8	DXY	-0.00028	-0.00001	0.00000	-0.00004	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00007	0.00001	0.00004	0.00002	-0.00003
167	H8	S	-0.00030	0.00031	0.00033	0.00060	0.00017
168	H8	PX	-0.00009	0.00000	-0.00001	0.00002	-0.00011
169	H8	PY	0.00011	0.00000	-0.00003	-0.00001	0.00001
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.05863	-0.00006	-0.99390	0.00105	0.00061
172	C10	S	0.00135	0.00000	-0.02744	0.00004	0.00001
173	C10	PX	0.00004	-0.00002	-0.00010	-0.00002	-0.00002
174	C10	PY	-0.00025	-0.00001	-0.00004	-0.00004	-0.00005
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00315	-0.00028	0.01163	-0.00076	-0.00023
177	C10	PX	0.00125	0.00025	-0.00017	0.00053	0.00066
178	C10	PY	0.00174	-0.00008	0.00101	-0.00018	0.00009
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

180	C10	DXX	-0.00058	-0.00001	0.00167	-0.00002	-0.00001
181	C10	DYY	-0.00050	0.00000	0.00145	-0.00002	-0.00002
182	C10	DZZ	-0.00023	0.00000	0.00256	0.00000	-0.00001
183	C10	DXY	0.00008	0.00001	0.00008	0.00002	0.00005
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.00010	-0.00002	0.00027	-0.00004	-0.00006
187	H16	S	-0.00052	-0.00010	-0.00197	-0.00017	-0.00019
188	H16	PX	-0.00012	0.00000	-0.00028	0.00000	-0.00001
189	H16	PY	0.00009	0.00000	0.00003	0.00000	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00012	0.00003	0.00022	0.00006	0.00006
192	H18	S	0.00066	0.00006	-0.00194	0.00016	0.00027
193	H18	PX	0.00006	0.00000	0.00020	0.00000	-0.00001
194	H18	PY	0.00013	0.00000	0.00011	0.00000	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00005	0.00000	0.00001	0.00000
197	C9	S	0.00000	0.00002	0.00000	0.00005	-0.00004
198	C9	PX	0.00001	-0.00001	0.00000	-0.00001	0.00000
199	C9	PY	-0.00001	-0.00001	0.00000	-0.00003	0.00002
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.00001	-0.00025	0.00001	-0.00014	0.00014
202	C9	PX	-0.00001	-0.00009	0.00002	-0.00010	-0.00002
203	C9	PY	0.00011	0.00020	-0.00003	0.00021	-0.00017
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	0.00006	0.00000	0.00004	0.00000
206	C9	DYY	0.00000	0.00001	0.00000	0.00002	-0.00001
207	C9	DZZ	0.00000	0.00000	0.00000	0.00002	-0.00002
208	C9	DXY	-0.00001	0.00002	0.00000	0.00001	0.00001
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.00001	0.00000	0.00000	-0.00001	0.00001
212	H3	S	-0.00006	-0.00009	0.00002	-0.00011	0.00007
213	H3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
214	H3	PY	0.00000	0.00000	0.00000	0.00001	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00002	0.00002	0.00000	0.00002	-0.00001
217	H5	S	-0.00003	0.00011	-0.00001	0.00010	0.00000
218	H5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
219	H5	PY	0.00000	0.00000	0.00000	-0.00001	0.00000
220	H5	PZ	0.00000	0.00001	0.00000	0.00001	0.00000
221	H7	S	0.00002	0.00002	0.00000	0.00002	-0.00001
222	H7	S	-0.00003	0.00011	-0.00001	0.00010	0.00000
223	H7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
224	H7	PY	0.00000	0.00000	0.00000	-0.00001	0.00000
225	H7	PZ	0.00000	-0.00001	0.00000	-0.00001	0.00000

MO: 11 12 13 14 15
Eigenvalues: -11.23182 -11.22847 -1.43013 -1.27321 -1.13071
(ev): -305.63346 -305.54247 -38.91592 -34.64594 -30.76832

			A	A	A	A	A
1	H1	S	0.00004	0.00025	-0.00620	0.00452	0.03571
2	H1	S	0.00044	-0.00209	0.00026	-0.00754	0.00369

3	H1	PX	0.00000	-0.00024	0.00118	-0.00045	-0.00376
4	H1	PY	-0.00001	-0.00011	0.00036	-0.00001	-0.00122
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01493	-0.99466	0.01629	-0.01587	-0.09051
7	C1	S	0.00030	-0.02771	-0.02953	0.03274	0.17011
8	C1	PX	0.00004	0.00027	0.01457	-0.00998	-0.06321
9	C1	PY	0.00002	0.00013	-0.01860	-0.01397	-0.00228
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00308	0.00839	-0.02690	-0.00274	0.09795
12	C1	PX	-0.00160	0.00032	0.00492	0.01936	-0.00169
13	C1	PY	-0.00057	0.00105	-0.01783	-0.00115	0.00566
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00007	0.00150	0.00002	0.00012	0.00462
16	C1	DYY	-0.00021	0.00163	-0.00312	0.00256	0.00524
17	C1	DZZ	-0.00010	0.00249	0.00146	-0.00087	-0.00738
18	C1	DXY	-0.00004	0.00009	0.00393	0.00058	-0.00291
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00031	-0.00033	0.00256	-0.02948	-0.08909
22	C2	S	0.00012	-0.00029	-0.00706	0.05458	0.17204
23	C2	PX	-0.00001	0.00005	-0.00277	0.02450	0.04652
24	C2	PY	0.00003	-0.00002	-0.00338	-0.01624	0.05474
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.00244	0.00483	0.00008	0.03863	0.08974
27	C2	PX	-0.00140	0.00247	0.01110	0.00772	-0.01030
28	C2	PY	-0.00106	-0.00004	-0.00488	-0.01343	-0.00243
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00004	0.00008	-0.00007	0.00156	0.00155
31	C2	DYY	0.00003	0.00005	-0.00005	0.00376	0.00721
32	C2	DZZ	0.00003	-0.00007	-0.00031	-0.00322	-0.00693
33	C2	DXY	-0.00003	0.00000	-0.00047	-0.00380	0.00224
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.11120	0.04025	0.00262	-0.06081	-0.06079
37	C3	S	0.00351	0.00113	-0.00583	0.11327	0.11797
38	C3	PX	0.00001	0.00004	0.00150	-0.02790	-0.01432
39	C3	PY	-0.00020	0.00001	-0.00420	-0.04467	0.05041
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00954	-0.00620	-0.01975	0.05279	0.06226
42	C3	PX	0.00027	-0.00058	-0.01921	-0.01945	0.00744
43	C3	PY	0.00106	0.00426	0.01976	0.00554	0.01982
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00009	0.00021	0.00003	0.00621	0.00201
46	C3	DYY	0.00034	0.00062	-0.00099	0.00544	0.00821
47	C3	DZZ	-0.00013	0.00005	0.00004	-0.00594	-0.00520
48	C3	DXY	0.00003	0.00010	0.00034	0.00283	0.00006
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00010	0.00979	0.07671	-0.00875	-0.09414
52	C4	S	0.00013	0.00030	-0.14337	0.01608	0.18693
53	C4	PX	-0.00002	0.00016	-0.01128	-0.00036	-0.01194
54	C4	PY	0.00001	-0.00012	-0.10579	-0.01437	-0.08564
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.00204	-0.00203	-0.00534	0.03740	0.10198

57	C4	PX	-0.00040	-0.00140	0.01211	0.00012	0.00151
58	C4	PY	0.00162	-0.00055	0.03856	-0.01100	-0.03074
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00003	0.00039	0.00849	0.00163	0.01181
61	C4	DYY	0.00000	0.00039	-0.02244	0.00001	-0.00152
62	C4	DZZ	0.00004	0.00000	0.01138	-0.00082	-0.00812
63	C4	DXY	0.00002	-0.00005	-0.00331	-0.00037	-0.00328
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00004	-0.00133	0.01436	-0.01301	-0.10698
67	C5	S	-0.00005	0.00027	-0.02680	0.02757	0.20249
68	C5	PX	0.00000	0.00008	-0.01793	0.00457	0.03794
69	C5	PY	-0.00001	0.00000	-0.01060	-0.01386	-0.05080
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00202	-0.00240	-0.00784	0.00593	0.15158
72	C5	PX	0.00032	-0.00137	-0.00575	-0.01547	0.01217
73	C5	PY	-0.00118	0.00156	-0.01311	0.00578	-0.01329
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00001	-0.00012	-0.00409	-0.00003	0.00572
76	C5	DYY	0.00000	-0.00004	-0.00071	0.00136	0.00726
77	C5	DZZ	-0.00001	0.00009	0.00146	-0.00051	-0.00943
78	C5	DXY	-0.00001	0.00001	-0.00365	0.00022	0.00413
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00267	-0.00050	0.00171	-0.11298	-0.02907
82	C6	S	-0.00013	0.00015	-0.00276	0.21798	0.05602
83	C6	PX	-0.00004	-0.00001	-0.00060	0.02423	-0.00469
84	C6	PY	0.00001	0.00014	-0.00137	-0.10599	0.10320
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00150	0.00047	-0.01626	0.04154	0.05675
87	C6	PX	0.00097	0.00268	0.00330	0.00929	0.00983
88	C6	PY	0.00274	-0.00412	-0.00979	0.02919	0.03149
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00024	-0.00004	-0.00030	-0.00093	0.00938
91	C6	DYY	-0.00012	-0.00003	-0.00066	0.01852	-0.00252
92	C6	DZZ	-0.00007	0.00004	0.00020	-0.01225	-0.00267
93	C6	DXY	0.00001	0.00000	-0.00006	-0.00149	-0.00214
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.98929	-0.01065	0.00025	-0.05284	-0.00585
97	C7	S	-0.02771	-0.00053	-0.00260	0.09704	0.00965
98	C7	PX	0.00026	0.00004	0.00025	-0.05402	0.00238
99	C7	PY	-0.00001	0.00008	0.00009	0.00090	0.03699
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.01463	0.00635	0.03172	0.06360	0.02502
102	C7	PX	-0.00326	-0.00311	-0.01214	-0.01692	-0.01040
103	C7	PY	0.00031	0.00055	0.00919	0.01369	-0.00322
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00121	-0.00007	0.00014	0.00522	-0.00156
106	C7	DYY	0.00169	-0.00002	0.00045	0.00391	0.00025
107	C7	DZZ	0.00232	-0.00004	-0.00033	-0.00547	-0.00026
108	C7	DXY	0.00024	0.00007	-0.00012	0.00088	-0.00416
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

111	O1	S	0.00001	-0.00005	0.19869	0.00610	0.03367
112	O1	S	0.00007	-0.00013	-0.43672	-0.01326	-0.07932
113	O1	PX	-0.00001	-0.00001	-0.05646	-0.00299	-0.04093
114	O1	PY	-0.00001	0.00001	0.05701	-0.00238	-0.06206
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.00060	0.00126	-0.45294	-0.01548	-0.07702
117	O1	PX	0.00007	0.00023	-0.03808	-0.00205	-0.02420
118	O1	PY	0.00012	-0.00008	0.04337	0.00032	-0.03702
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00004	-0.00012	-0.00896	-0.00038	-0.00789
121	O1	DYY	0.00005	-0.00026	-0.01538	-0.00006	0.00450
122	O1	DZZ	0.00003	-0.00007	0.00485	0.00019	-0.00161
123	O1	DXY	-0.00001	0.00005	-0.00400	-0.00025	-0.00312
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00002	-0.00009	-0.00615	0.00287	0.04607
127	H4	S	0.00020	-0.00069	-0.00063	-0.00699	0.00907
128	H4	PX	0.00000	-0.00001	-0.00097	0.00033	0.00345
129	H4	PY	0.00002	-0.00003	0.00046	-0.00018	-0.00369
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00008	0.00006	0.00049	-0.14549	0.05153
132	N1	S	-0.00023	0.00021	-0.00168	0.28830	-0.10701
133	N1	PX	0.00001	0.00002	-0.00032	0.08535	-0.04046
134	N1	PY	-0.00003	-0.00006	-0.00059	0.08472	0.00234
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00327	-0.00292	0.00139	0.33063	-0.10288
137	N1	PX	0.00044	-0.00049	0.00147	0.05264	-0.02143
138	N1	PY	0.00095	-0.00055	0.00072	0.03942	0.00698
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00022	0.00013	-0.00005	0.00447	-0.00525
141	N1	DYY	-0.00011	0.00008	-0.00005	0.00748	-0.00007
142	N1	DZZ	-0.00015	0.00010	-0.00022	-0.01361	0.00365
143	N1	DXY	-0.00001	-0.00002	-0.00001	0.00218	0.00139
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.00005	0.00000	-0.00002	0.01078	0.03504
147	H6	S	-0.00043	0.00055	0.00450	0.00123	-0.00140
148	H6	PX	0.00001	-0.00003	0.00003	0.00127	0.00362
149	H6	PY	0.00002	0.00001	0.00018	0.00060	0.00163
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.01523	0.00019	0.00037	-0.08657	0.04650
152	C8	S	0.00033	0.00018	-0.00010	0.16516	-0.09069
153	C8	PX	0.00006	-0.00007	0.00006	-0.06111	0.03221
154	C8	PY	0.00006	0.00003	-0.00020	0.05161	0.00531
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.00503	-0.00176	-0.00653	0.04241	-0.05469
157	C8	PX	-0.00077	-0.00095	0.00048	0.02983	-0.01517
158	C8	PY	-0.00239	-0.00232	-0.00929	0.00402	-0.00435
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00033	0.00003	-0.00015	0.01251	-0.00509
161	C8	DYY	0.00057	0.00002	-0.00020	0.00756	-0.00204
162	C8	DZZ	0.00011	0.00006	0.00013	-0.00981	0.00444
163	C8	DXY	0.00018	-0.00004	-0.00006	-0.00913	0.00457
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00049	0.00007	-0.00026	0.01424	0.00347
167	H8	S	-0.00110	0.00077	0.00245	0.00462	0.00370
168	H8	PX	-0.00036	-0.00003	0.00009	-0.00138	-0.00046
169	H8	PY	0.00000	0.00001	-0.00017	-0.00018	0.00056
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00143	-0.00002	0.00003	-0.02468	0.02710
172	C10	S	0.00003	0.00000	-0.00018	0.04663	-0.05226
173	C10	PX	0.00006	-0.00003	-0.00009	-0.01004	0.00901
174	C10	PY	-0.00002	-0.00004	-0.00026	0.02935	-0.02506
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.00028	-0.00098	-0.00477	0.03307	-0.03464
177	C10	PX	-0.00002	0.00079	0.00194	-0.01486	0.00625
178	C10	PY	-0.00018	-0.00022	-0.00076	0.00286	0.00008
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.00006	-0.00002	-0.00007	-0.00126	0.00081
181	C10	DYY	-0.00013	-0.00001	0.00001	0.00197	-0.00249
182	C10	DZZ	0.00005	-0.00001	-0.00005	-0.00183	0.00207
183	C10	DXY	0.00006	0.00003	-0.00001	-0.00274	0.00181
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00006	-0.00005	-0.00016	0.00850	-0.01175
187	H16	S	0.00001	-0.00027	-0.00027	0.00476	-0.00310
188	H16	PX	-0.00002	0.00000	-0.00003	-0.00078	0.00114
189	H16	PY	0.00002	0.00000	-0.00002	0.00028	-0.00063
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.00002	0.00008	0.00017	0.00916	-0.01342
192	H18	S	-0.00014	0.00023	0.00102	-0.00391	0.00033
193	H18	PX	0.00001	0.00000	0.00003	0.00107	-0.00102
194	H18	PY	-0.00001	0.00000	0.00003	0.00109	-0.00138
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	-0.00003	0.06057	0.00287	0.03593
197	C9	S	-0.00001	0.00002	-0.11069	-0.00537	-0.06957
198	C9	PX	0.00000	0.00003	0.07509	0.00328	0.03080
199	C9	PY	0.00001	-0.00001	0.04254	0.00138	0.00749
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00004	-0.00022	-0.02784	-0.00226	-0.03599
202	C9	PX	0.00004	0.00017	-0.00235	0.00007	-0.00330
203	C9	PY	-0.00004	0.00017	-0.00033	-0.00076	0.00027
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.00001	-0.00001	-0.01393	-0.00062	-0.00515
206	C9	DYY	0.00000	0.00001	0.00142	0.00009	0.00097
207	C9	DZZ	0.00000	0.00002	0.00915	0.00038	0.00296
208	C9	DXY	0.00000	-0.00002	-0.01446	-0.00049	-0.00386
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.00000	-0.02125	-0.00125	-0.02164
212	H3	S	0.00002	-0.00005	-0.00603	0.00011	-0.00638
213	H3	PX	0.00000	-0.00001	0.00019	-0.00001	-0.00031
214	H3	PY	0.00000	0.00000	0.00400	0.00017	0.00229
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00000	0.00004	-0.02188	-0.00118	-0.01661
217	H5	S	-0.00004	-0.00001	-0.00422	0.00004	-0.00287
218	H5	PX	0.00000	0.00000	0.00241	0.00011	0.00152

219	H5	PY	0.00000	-0.00002	-0.00055	-0.00003	-0.00060
220	H5	PZ	0.00000	0.00000	-0.00304	-0.00013	-0.00166
221	H7	S	0.00000	0.00004	-0.02188	-0.00118	-0.01661
222	H7	S	-0.00004	-0.00001	-0.00422	0.00004	-0.00287
223	H7	PX	0.00000	0.00000	0.00241	0.00011	0.00152
224	H7	PY	0.00000	-0.00002	-0.00055	-0.00003	-0.00060
225	H7	PZ	0.00000	0.00000	0.00304	0.00013	0.00166

MO:		16	17	18	19	20
Eigenvalues:		-1.06874	-1.03349	-1.00471	-0.96765	-0.89142
(ev):		-29.08200	-28.12281	-27.33952	-26.33104	-24.25674

		A	A	A	A	A	
1	H1	S	-0.04210	0.01786	-0.04039	-0.06499	-0.00852
2	H1	S	-0.01383	0.00887	-0.00197	-0.01493	-0.00424
3	H1	PX	0.00398	-0.00135	0.00444	0.00585	0.00065
4	H1	PY	0.00158	-0.00071	0.00072	0.00116	0.00080
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.07406	-0.02515	0.07305	0.09554	0.01529
7	C1	S	-0.13894	0.04709	-0.14070	-0.18394	-0.03015
8	C1	PX	0.01375	0.01260	0.04749	0.03366	-0.01256
9	C1	PY	0.03033	-0.04594	-0.06411	-0.03314	0.05262
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.10548	0.04857	-0.07061	-0.11440	-0.02504
12	C1	PX	0.00868	-0.00658	-0.01914	-0.01788	0.00119
13	C1	PY	0.00295	-0.00908	-0.01871	-0.02534	0.01669
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00087	-0.00111	-0.00387	-0.00633	0.00248
16	C1	DYY	-0.00823	0.00563	-0.00039	-0.00062	-0.00588
17	C1	DZZ	0.00647	-0.00258	0.00474	0.00678	0.00153
18	C1	DXY	0.00069	0.00336	0.00638	0.00214	-0.00466
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08246	0.02774	-0.09790	0.00232	0.04365
22	C2	S	0.15676	-0.05306	0.18836	-0.00284	-0.08880
23	C2	PX	0.02391	0.00966	0.02017	-0.00768	-0.04680
24	C2	PY	0.00839	-0.06620	0.04172	0.01446	0.14008
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.12242	-0.03097	0.13035	-0.02274	-0.06017
27	C2	PX	0.00801	0.00359	-0.00838	-0.01270	0.00605
28	C2	PY	0.00275	-0.01357	0.00664	-0.00316	0.02929
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00128	0.00307	0.00186	-0.00083	-0.00993
31	C2	DYY	0.00842	-0.00340	0.00601	-0.00019	0.00270
32	C2	DZZ	-0.00691	0.00165	-0.00767	0.00079	0.00380
33	C2	DXY	-0.00190	-0.00558	0.00075	0.00087	0.01084
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.10009	-0.07534	-0.03584	-0.02340	0.03607
37	C3	S	-0.19116	0.14579	0.06960	0.04539	-0.07381
38	C3	PX	-0.06446	-0.01048	0.00687	0.02385	0.07246
39	C3	PY	0.02480	-0.01744	-0.08078	-0.13091	-0.05911
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.13955	0.08624	0.04585	0.03588	-0.04157

42	C3	PX	-0.00474	-0.00050	0.01066	0.01765	0.01209
43	C3	PY	-0.00201	0.00225	-0.03767	-0.07364	-0.01970
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00319	0.00490	0.00389	0.00233	-0.00786
46	C3	DYY	-0.01407	0.00479	-0.00257	-0.00365	0.00230
47	C3	DZZ	0.00777	-0.00603	-0.00234	-0.00109	0.00267
48	C3	DXY	0.00606	0.00143	-0.00489	-0.00611	-0.00516
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01915	0.04241	0.09287	0.01058	-0.04032
52	C4	S	-0.03924	-0.08424	-0.18426	-0.02082	0.08445
53	C4	PX	-0.06425	0.05901	-0.06431	-0.11439	-0.08331
54	C4	PY	0.02846	-0.01373	-0.00175	0.14497	-0.05958
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.01231	-0.05705	-0.14550	-0.04625	0.07676
57	C4	PX	-0.00858	0.00443	-0.01657	-0.00839	-0.02950
58	C4	PY	-0.00505	0.02019	0.03417	0.02762	-0.02442
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00149	-0.00505	-0.00060	-0.00740	0.01418
61	C4	DYY	-0.00035	-0.00171	-0.00758	0.01285	-0.01064
62	C4	DZZ	0.00092	0.00469	0.00873	-0.00205	-0.00220
63	C4	DXY	0.00628	-0.00210	0.00988	0.00503	0.00403
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.05449	0.07105	-0.04742	-0.02129	-0.09399
67	C5	S	0.10618	-0.13717	0.08843	0.04100	0.18596
68	C5	PX	-0.02075	-0.01317	-0.07005	-0.00444	0.01754
69	C5	PY	-0.04882	0.00589	-0.09736	0.02996	0.05515
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.06178	-0.10294	0.07806	0.06084	0.14998
72	C5	PX	-0.00868	-0.00217	-0.00144	0.00623	-0.01152
73	C5	PY	0.00568	-0.00409	-0.01902	-0.00023	0.02319
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00295	-0.00383	-0.00947	0.00045	0.00858
76	C5	DYY	0.00677	-0.00387	0.01009	0.00201	-0.00020
77	C5	DZZ	-0.00374	0.00580	-0.00339	-0.00188	-0.00720
78	C5	DXY	0.00138	-0.00328	-0.00065	0.00205	0.00149
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.05846	-0.05665	-0.01611	0.00017	0.08238
82	C6	S	0.11672	0.11208	0.03037	-0.00213	-0.16801
83	C6	PX	-0.10105	0.04247	-0.00888	0.03609	0.04351
84	C6	PY	-0.05468	-0.02278	0.12031	0.00382	-0.10466
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.05427	0.07607	0.04038	0.00952	-0.15586
87	C6	PX	-0.00989	0.02773	-0.00307	0.00614	0.00376
88	C6	PY	0.01425	0.00081	0.03840	0.01213	-0.04409
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00950	0.00538	0.01190	0.00519	-0.00949
91	C6	DYY	0.01352	0.00131	-0.00637	-0.00347	0.00187
92	C6	DZZ	-0.00549	-0.00541	-0.00112	-0.00019	0.00574
93	C6	DXY	-0.00533	0.00539	-0.00673	-0.00106	-0.00014
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

96	C7	S	0.10899	-0.01574	-0.06771	-0.07718	-0.04742
97	C7	S	-0.20858	0.02800	0.12946	0.15018	0.09490
98	C7	PX	0.04975	-0.01677	-0.02469	-0.03633	-0.01753
99	C7	PY	-0.03090	0.08636	0.01157	0.02668	-0.02715
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.14186	0.04091	0.07915	0.07371	0.06056
102	C7	PX	-0.00078	-0.00750	0.00987	0.02125	0.00901
103	C7	PY	-0.00169	0.01019	-0.00508	-0.00640	-0.00450
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00351	0.00044	0.00293	0.00501	0.00471
106	C7	DYY	-0.00810	-0.00168	0.00368	0.00166	0.00027
107	C7	DZZ	0.00854	-0.00113	-0.00535	-0.00583	-0.00360
108	C7	DXY	0.00232	-0.00946	-0.00242	-0.00366	0.00391
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00797	-0.00234	-0.00686	-0.04673	0.04112
112	O1	S	0.01796	0.00772	0.01881	0.10638	-0.09460
113	O1	PX	-0.00868	0.05693	0.07601	-0.13342	0.02023
114	O1	PY	0.01052	0.06591	0.14423	-0.09973	0.00248
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.02469	-0.00402	0.00769	0.14318	-0.13116
117	O1	PX	-0.00243	0.03086	0.04507	-0.07107	0.01175
118	O1	PY	0.00579	0.03772	0.07919	-0.05112	-0.00212
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00035	0.00729	0.01271	-0.01248	0.00306
121	O1	DYY	-0.00086	-0.00486	-0.01019	0.00779	0.00021
122	O1	DZZ	0.00042	0.00066	0.00150	0.00184	-0.00141
123	O1	DXY	0.00173	0.00153	0.00728	-0.00076	0.00214
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.02906	-0.04457	0.02521	0.02729	0.08672
127	H4	S	0.00241	-0.00994	0.01067	0.01194	0.02585
128	H4	PX	0.00183	-0.00322	0.00083	0.00224	0.00532
129	H4	PY	-0.00252	0.00303	-0.00309	-0.00097	-0.00524
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.06702	-0.00328	0.06555	0.02414	-0.03575
132	N1	S	0.13832	0.00596	-0.13818	-0.05106	0.07607
133	N1	PX	-0.02349	-0.03238	-0.01885	0.00495	0.07469
134	N1	PY	0.07420	0.08935	-0.02218	0.01545	-0.05274
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.16746	0.00156	-0.14612	-0.06134	0.08604
137	N1	PX	0.00039	-0.01893	-0.01302	-0.00285	0.03419
138	N1	PY	0.03087	0.03535	-0.00426	0.00495	-0.02637
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00761	-0.00893	-0.00016	0.00055	0.01050
141	N1	DYY	0.00750	0.00658	-0.00235	-0.00059	-0.00728
142	N1	DZZ	-0.00315	-0.00020	0.00329	0.00064	-0.00290
143	N1	DXY	0.00098	0.00835	-0.00050	0.00364	-0.00058
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.04633	-0.01489	0.05690	-0.00062	-0.03520
147	H6	S	0.01240	-0.00417	0.01188	-0.00387	-0.00777
148	H6	PX	0.00469	-0.00134	0.00534	-0.00021	-0.00326
149	H6	PY	0.00139	-0.00115	0.00226	0.00024	0.00074

150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.05973	0.10478	-0.01926	0.01109	-0.02550
152	C8	S	-0.11672	-0.20539	0.03641	-0.02222	0.05363
153	C8	PX	-0.07948	-0.01887	0.08573	0.04075	-0.04871
154	C8	PY	0.00525	0.12952	-0.01034	0.09575	0.13389
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.08468	-0.13950	0.03957	-0.00105	0.03907
157	C8	PX	-0.00881	-0.01790	0.00793	0.00678	0.00446
158	C8	PY	-0.01597	0.00308	0.01253	0.03017	0.03801
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00492	0.00294	-0.00696	0.00099	0.01245
161	C8	DYY	-0.01086	-0.00793	0.00722	0.00223	-0.00402
162	C8	DZZ	0.00463	0.00764	-0.00094	0.00035	-0.00341
163	C8	DXY	-0.00916	0.00292	0.00844	0.00765	0.00234
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.05559	0.00114	0.03915	0.04244	0.03237
167	H8	S	-0.01066	-0.00105	0.00736	0.00452	0.00864
168	H8	PX	0.00555	-0.00013	-0.00361	-0.00376	-0.00267
169	H8	PY	-0.00071	0.00103	0.00042	0.00073	-0.00004
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.04977	0.13180	-0.02938	0.05405	0.08586
172	C10	S	-0.09534	-0.25340	0.05621	-0.10445	-0.16694
173	C10	PX	-0.00260	0.01903	0.01004	0.01497	-0.00764
174	C10	PY	-0.04046	-0.08618	0.01815	-0.01754	0.01281
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.07753	-0.19722	0.05074	-0.07824	-0.14095
177	C10	PX	0.00018	0.00367	0.00118	-0.00318	-0.01098
178	C10	PY	-0.00530	-0.00781	0.00394	0.00082	0.00971
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00191	0.00226	-0.00078	-0.00046	-0.00317
181	C10	DYY	-0.00490	-0.01141	0.00261	-0.00354	-0.00292
182	C10	DZZ	0.00404	0.01095	-0.00248	0.00465	0.00737
183	C10	DXY	-0.00035	0.00357	0.00105	0.00202	-0.00036
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.02971	-0.07442	0.02251	-0.03185	-0.07407
187	H16	S	-0.00679	-0.01773	0.00739	-0.00737	-0.02687
188	H16	PX	0.00307	0.00723	-0.00218	0.00296	0.00624
189	H16	PY	-0.00157	-0.00354	0.00108	-0.00121	-0.00228
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.02219	-0.07399	0.01282	-0.03976	-0.06985
192	H18	S	-0.00166	-0.01477	0.00181	-0.01426	-0.02854
193	H18	PX	-0.00159	-0.00532	0.00099	-0.00275	-0.00488
194	H18	PY	-0.00165	-0.00608	0.00077	-0.00303	-0.00409
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.00118	-0.04517	-0.08845	0.12012	-0.06968
197	C9	S	0.00234	0.08810	0.17312	-0.23432	0.13590
198	C9	PX	-0.00501	-0.01422	-0.02448	-0.02404	0.06104
199	C9	PY	0.00266	-0.00259	0.01003	-0.00903	0.02942
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.00068	0.06283	0.12898	-0.20316	0.14302
202	C9	PX	-0.00068	0.00555	0.00903	-0.02062	0.01919
203	C9	PY	0.00106	-0.00085	0.00358	0.00222	0.00355

204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00058	0.00285	0.00472	0.00109	-0.00698
206	C9	DYY	-0.00023	-0.00083	-0.00202	0.00059	0.00053
207	C9	DZZ	-0.00043	-0.00170	-0.00309	0.00005	0.00316
208	C9	DXY	0.00027	0.00162	0.00153	0.00197	-0.00610
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00205	0.03072	0.06738	-0.08951	0.06349
212	H3	S	0.00067	0.00995	0.02200	-0.03100	0.02471
213	H3	PX	0.00000	0.00060	0.00130	-0.00211	0.00171
214	H3	PY	-0.00015	-0.00297	-0.00616	0.00806	-0.00511
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00108	0.02810	0.05452	-0.09218	0.06522
217	H5	S	0.00009	0.00627	0.01354	-0.02619	0.02274
218	H5	PX	-0.00012	-0.00171	-0.00338	0.00418	-0.00220
219	H5	PY	0.00009	0.00076	0.00173	-0.00222	0.00178
220	H5	PZ	0.00004	0.00228	0.00454	-0.00688	0.00460
221	H7	S	-0.00108	0.02810	0.05452	-0.09218	0.06522
222	H7	S	0.00009	0.00627	0.01354	-0.02619	0.02274
223	H7	PX	-0.00012	-0.00171	-0.00338	0.00418	-0.00220
224	H7	PY	0.00009	0.00076	0.00173	-0.00222	0.00178
225	H7	PZ	-0.00004	-0.00228	-0.00454	0.00688	-0.00460

MO:	21	22	23	24	25
Eigenvalues:	-0.80914	-0.78893	-0.75398	-0.71283	-0.69053
(ev):	-22.01776	-21.46801	-20.51684	-19.39700	-18.79033

		A	A	A	A	A	
1	H1	S	0.08957	-0.05558	0.07055	-0.04284	-0.00203
2	H1	S	0.04411	-0.02156	0.04148	-0.02747	-0.00689
3	H1	PX	-0.00692	0.00301	-0.00388	0.00241	-0.00103
4	H1	PY	-0.00120	0.00339	-0.00259	0.00033	0.00274
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.05475	0.04801	-0.01669	-0.01564	-0.00206
7	C1	S	0.10543	-0.09677	0.03415	0.02966	0.00110
8	C1	PX	0.05386	-0.07982	0.11873	-0.09988	-0.06175
9	C1	PY	0.10514	0.15356	-0.04132	-0.01112	0.17702
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.11926	-0.06094	0.03315	0.03347	0.01070
12	C1	PX	0.01633	-0.04176	0.04066	-0.03564	-0.01654
13	C1	PY	0.03258	0.03364	-0.00567	-0.01127	0.06613
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00437	0.00142	-0.00080	0.00462	0.00494
16	C1	DYY	-0.00178	-0.00825	0.00314	-0.00438	-0.00786
17	C1	DZZ	-0.00363	0.00350	-0.00093	-0.00080	-0.00035
18	C1	DXY	-0.00543	-0.01001	0.00294	-0.00336	-0.00905
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08677	0.00552	0.01176	0.03219	0.01285
22	C2	S	0.17335	-0.00641	-0.02397	-0.06559	-0.02867
23	C2	PX	-0.08573	0.06374	-0.08517	0.10132	-0.03896
24	C2	PY	-0.02692	-0.14145	-0.00890	-0.02329	0.15879
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.14700	-0.03489	0.00329	-0.06238	-0.01868

27	C2	PX	-0.04706	0.00282	-0.01539	0.05109	-0.00232
28	C2	PY	-0.00619	-0.03559	0.00434	0.00754	0.04006
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00310	0.00641	-0.00306	-0.00264	-0.00819
31	C2	DYY	0.00183	-0.00347	0.00365	0.00262	0.00465
32	C2	DZZ	-0.00583	0.00041	0.00104	0.00152	0.00086
33	C2	DXY	0.00195	-0.00792	0.00017	-0.00297	0.00615
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.06495	0.05277	-0.00785	0.04330	0.01990
37	C3	S	-0.13054	-0.10537	0.01616	-0.08859	-0.04169
38	C3	PX	0.11679	-0.06392	0.17277	0.01088	-0.06959
39	C3	PY	0.01272	-0.12025	-0.00358	0.09313	-0.14481
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.10078	-0.09288	0.03403	-0.07563	-0.05787
42	C3	PX	0.03608	-0.00105	0.06218	-0.00631	-0.02028
43	C3	PY	-0.01317	-0.07611	-0.00745	0.02362	-0.03704
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00900	0.00559	-0.00449	-0.00187	0.00071
46	C3	DYY	0.00316	-0.00850	0.00196	0.00138	-0.00022
47	C3	DZZ	0.00481	0.00352	0.00067	0.00243	0.00047
48	C3	DXY	-0.00529	-0.00419	-0.00412	-0.00196	0.00095
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00925	-0.08006	0.01292	-0.00553	-0.00382
52	C4	S	-0.01960	0.17103	-0.02669	0.01005	0.00766
53	C4	PX	0.18642	0.01816	-0.05263	-0.06064	0.16597
54	C4	PY	0.01598	0.03798	0.07079	-0.22342	-0.09874
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.03915	0.10340	-0.01725	0.04564	0.00743
57	C4	PX	0.04726	0.00254	-0.01340	-0.02839	0.03589
58	C4	PY	0.01664	0.00290	0.00728	-0.03596	-0.01443
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.00605	0.00042	0.00217	0.01233	0.00604
61	C4	DYY	0.00315	0.00401	0.00046	-0.01830	-0.00934
62	C4	DZZ	0.00088	-0.00653	0.00032	0.00326	0.00138
63	C4	DXY	-0.00418	0.00082	-0.00031	-0.00251	0.00290
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.04337	0.04204	-0.02829	-0.01478	-0.03001
67	C5	S	-0.08825	-0.08315	0.05896	0.03039	0.05897
68	C5	PX	-0.09147	0.11815	-0.06156	0.11508	-0.10411
69	C5	PY	-0.12087	0.04637	0.09576	0.02166	-0.07418
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.07723	-0.06213	0.04892	0.00785	0.05566
72	C5	PX	-0.00871	0.04251	-0.03190	0.03758	-0.04391
73	C5	PY	-0.04097	-0.00713	0.04805	0.00764	-0.02159
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00975	0.00682	0.00182	0.00702	-0.00351
76	C5	DYY	0.00429	-0.00572	-0.00016	-0.00497	0.00247
77	C5	DZZ	0.00379	0.00251	-0.00160	-0.00120	-0.00152
78	C5	DXY	0.00204	0.00282	-0.00153	-0.00259	-0.00301
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

81	C6	S	0.04005	-0.06350	0.00675	-0.01563	-0.00295
82	C6	S	-0.08214	0.13213	-0.01212	0.03434	0.00679
83	C6	PX	-0.15669	-0.06580	-0.09797	-0.09750	0.12714
84	C6	PY	-0.01206	0.01108	-0.18498	-0.05396	-0.11850
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.06085	0.13298	-0.01740	0.01348	-0.01426
87	C6	PX	-0.05989	-0.02020	-0.02049	-0.03847	0.06205
88	C6	PY	-0.00008	0.02213	-0.06419	-0.01505	-0.03838
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00534	0.00236	-0.01119	-0.01153	-0.00134
91	C6	DYY	0.00252	-0.00004	0.00633	0.00733	0.00217
92	C6	DZZ	0.00294	-0.00448	-0.00040	-0.00145	-0.00154
93	C6	DXY	-0.01156	-0.00323	0.00766	0.00336	0.00276
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.05975	-0.04770	-0.04055	-0.03791	-0.00135
97	C7	S	0.12092	0.09513	0.08175	0.07494	0.00146
98	C7	PX	0.05970	0.01987	0.11954	0.14927	-0.10850
99	C7	PY	-0.07849	-0.08329	0.12687	-0.10779	-0.01879
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.08796	0.05525	0.06831	0.09473	0.00882
102	C7	PX	0.03556	0.03066	0.05591	0.06012	-0.04932
103	C7	PY	-0.02341	-0.03746	0.02237	-0.03399	-0.00892
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00371	0.00590	-0.00092	0.00503	0.00258
106	C7	DYY	0.00121	-0.00202	-0.00065	-0.00228	-0.00197
107	C7	DZZ	-0.00401	-0.00340	-0.00176	-0.00261	-0.00069
108	C7	DXY	0.00813	0.00333	-0.01065	0.00645	-0.00009
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00541	0.04426	0.00584	-0.02226	0.00513
112	O1	S	0.01188	-0.10397	-0.01222	0.05353	-0.01420
113	O1	PX	0.06890	0.00467	-0.05016	-0.00042	0.21744
114	O1	PY	-0.02850	-0.19951	-0.04677	0.29547	0.08164
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.01818	-0.15403	-0.02418	0.07983	-0.01290
117	O1	PX	0.04114	0.00203	-0.03197	0.00150	0.14548
118	O1	PY	-0.01433	-0.12203	-0.02600	0.18172	0.05038
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00119	-0.00452	-0.00221	0.00575	0.01171
121	O1	DYY	-0.00049	0.01087	0.00249	-0.00987	-0.00837
122	O1	DZZ	-0.00132	-0.00399	0.00071	0.00385	-0.00357
123	O1	DXY	-0.00756	-0.00832	0.00058	0.01379	-0.00643
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.04954	-0.06252	0.08480	-0.01972	0.03901
127	H4	S	-0.01702	-0.02932	0.03826	-0.00679	0.01855
128	H4	PX	-0.00394	-0.00252	0.00412	-0.00007	0.00027
129	H4	PY	0.00118	0.00464	-0.00375	0.00160	-0.00414
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01439	0.03597	-0.04039	-0.01554	0.01599
132	N1	S	0.03282	-0.07719	0.09163	0.03367	-0.03699
133	N1	PX	-0.00625	-0.06884	-0.13401	-0.08359	0.03669
134	N1	PY	-0.03887	0.12500	0.13249	0.08354	0.12583

135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.03989	-0.11124	0.08277	0.04434	-0.06203
137	N1	PX	0.00397	-0.03214	-0.06974	-0.03831	0.01673
138	N1	PY	-0.02651	0.04992	0.04588	0.03391	0.06315
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00390	-0.00955	-0.01764	-0.00992	-0.00170
141	N1	DYY	-0.00366	0.00924	0.01311	0.00686	0.00398
142	N1	DZZ	0.00036	0.00153	0.00161	0.00069	-0.00252
143	N1	DXY	-0.00649	0.00592	0.00319	0.00066	0.01396
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.11992	-0.01204	0.03260	-0.07956	-0.02152
147	H6	S	0.04952	-0.01087	0.02257	-0.03823	-0.01236
148	H6	PX	0.00886	-0.00057	0.00194	-0.00454	-0.00174
149	H6	PY	0.00299	-0.00244	0.00028	-0.00291	0.00202
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.03640	0.00944	0.08766	0.00605	0.03379
152	C8	S	0.07441	-0.02089	-0.18051	-0.01317	-0.06862
153	C8	PX	0.03213	0.14963	0.01922	0.10082	0.04747
154	C8	PY	0.06173	0.02944	-0.03744	-0.00111	0.12865
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.06839	-0.00284	-0.15129	-0.00691	-0.07104
157	C8	PX	0.01900	0.03259	-0.00919	0.02725	0.00967
158	C8	PY	0.03559	0.02045	-0.01817	0.00076	0.02575
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00683	-0.00707	-0.00244	0.00107	-0.00193
161	C8	DYY	-0.00332	0.00628	-0.00082	-0.00283	0.00626
162	C8	DZZ	-0.00266	0.00170	0.00665	0.00127	0.00174
163	C8	DXY	0.00667	0.00750	-0.00135	0.00350	-0.00082
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.08653	0.05824	0.09587	0.12486	-0.05693
167	H8	S	0.03852	0.02286	0.04879	0.07261	-0.03202
168	H8	PX	-0.00667	-0.00413	-0.00695	-0.00819	0.00382
169	H8	PY	-0.00018	-0.00067	0.00255	-0.00091	-0.00080
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.05192	-0.01064	-0.05708	0.00604	-0.02713
172	C10	S	-0.10200	0.01987	0.11249	-0.01285	0.05210
173	C10	PX	0.00208	0.06116	0.04399	0.06295	0.09375
174	C10	PY	0.06241	-0.00790	-0.15352	0.02728	-0.16326
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.08971	0.02822	0.11725	-0.01580	0.06940
177	C10	PX	-0.00741	0.01659	0.01818	0.02292	0.03725
178	C10	PY	0.02447	0.00099	-0.05084	0.01391	-0.05476
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.00513	0.00128	0.01152	-0.00048	0.01134
181	C10	DYY	0.00164	-0.00044	-0.00572	0.00058	-0.00806
182	C10	DZZ	0.00447	-0.00095	-0.00508	0.00033	-0.00275
183	C10	DXY	-0.00110	0.00189	0.00366	-0.00100	0.00361
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.05446	0.03989	0.10396	0.02270	0.10798
187	H16	S	-0.02343	0.02356	0.05900	0.01768	0.06922
188	H16	PX	0.00428	-0.00247	-0.00687	-0.00088	-0.00630

189	H16	PY	-0.00069	0.00122	0.00105	0.00126	0.00027
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.06636	-0.01030	0.09104	-0.04051	0.05047
192	H18	S	-0.03287	-0.00614	0.05154	-0.02072	0.03195
193	H18	PX	-0.00431	0.00011	0.00595	-0.00160	0.00414
194	H18	PY	-0.00296	-0.00113	0.00284	-0.00178	-0.00030
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.02926	-0.03874	-0.00927	0.01533	0.01918
197	C9	S	-0.05871	0.07420	0.01713	-0.02633	-0.03735
198	C9	PX	-0.03235	0.13325	0.05313	-0.17538	-0.12929
199	C9	PY	-0.05540	0.00220	0.01202	0.07437	-0.11180
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.06870	0.10817	0.03389	-0.06400	-0.08003
202	C9	PX	-0.00637	0.03780	0.01404	-0.05771	-0.03032
203	C9	PY	-0.02072	-0.00694	-0.00011	0.04212	-0.04303
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00438	-0.01421	-0.00535	0.01404	0.01436
206	C9	DYY	-0.00043	0.00262	0.00042	0.00007	-0.00332
207	C9	DZZ	-0.00169	0.00838	0.00336	-0.01199	-0.00728
208	C9	DXY	0.00595	-0.00714	-0.00433	0.00437	0.01453
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.04945	0.02519	0.01046	0.04028	-0.07055
212	H3	S	-0.02146	0.00978	0.00501	0.02649	-0.03946
213	H3	PX	-0.00103	0.00167	0.00066	-0.00138	-0.00209
214	H3	PY	0.00317	-0.00211	-0.00063	-0.00172	0.00346
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.02453	0.06819	0.02233	-0.07585	-0.04082
217	H5	S	-0.01074	0.03130	0.01166	-0.04388	-0.02506
218	H5	PX	0.00085	-0.00085	-0.00008	0.00020	-0.00021
219	H5	PY	-0.00131	0.00132	0.00045	-0.00031	-0.00208
220	H5	PZ	-0.00183	0.00428	0.00130	-0.00447	-0.00243
221	H7	S	-0.02453	0.06819	0.02233	-0.07585	-0.04082
222	H7	S	-0.01074	0.03130	0.01166	-0.04388	-0.02506
223	H7	PX	0.00085	-0.00085	-0.00008	0.00020	-0.00021
224	H7	PY	-0.00131	0.00132	0.00045	-0.00031	-0.00208
225	H7	PZ	0.00183	-0.00428	-0.00130	0.00447	0.00243

MO:	26	27	28	29	30
Eigenvalues:	-0.66680	-0.66574	-0.63677	-0.61061	-0.59333
(ev):	-18.14466	-18.11570	-17.32740	-16.61563	-16.14528

		A	A	A	A	A	
1	H1	S	0.00000	0.13519	0.06131	0.16822	0.09789
2	H1	S	0.00000	0.08301	0.04297	0.12321	0.07031
3	H1	PX	0.00000	-0.00715	-0.00233	-0.00856	-0.00547
4	H1	PY	0.00000	-0.00302	-0.00140	-0.00269	0.00038
5	H1	PZ	-0.00145	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	-0.04170	0.01101	-0.02142	-0.00632
7	C1	S	0.00000	0.08374	-0.02000	0.03999	0.00888
8	C1	PX	0.00000	0.16674	0.12658	0.21386	0.08818
9	C1	PY	0.00000	-0.01534	-0.04094	0.08491	0.19323
10	C1	PZ	-0.05881	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	0.07304	-0.04885	0.06053	0.02433

12	C1	PX	0.00000	0.08496	0.06698	0.09687	0.04890
13	C1	PY	0.00000	0.01004	0.00426	0.03108	0.08471
14	C1	PZ	-0.03466	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.00447	0.00025	0.01035	0.01028
16	C1	DYY	0.00000	-0.00242	0.00115	-0.00872	-0.01192
17	C1	DZZ	0.00000	-0.00242	0.00024	-0.00153	-0.00056
18	C1	DXY	0.00000	0.01134	0.00836	0.00611	-0.00346
19	C1	DXZ	0.00515	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00387	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.02483	0.02784	-0.01871	0.01434
22	C2	S	0.00000	-0.05255	-0.05625	0.03853	-0.02919
23	C2	PX	0.00000	-0.02340	0.24902	0.17614	0.04900
24	C2	PY	0.00000	-0.04401	0.11732	0.10838	-0.15818
25	C2	PZ	-0.01899	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.00956	-0.06198	0.04061	-0.01048
27	C2	PX	0.00000	0.01845	0.13053	0.07601	0.03636
28	C2	PY	0.00000	-0.00076	0.05073	0.03111	-0.04679
29	C2	PZ	-0.00761	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.00025	-0.01116	-0.00614	0.00445
31	C2	DYY	0.00000	0.00125	0.00887	0.00495	-0.00162
32	C2	DZZ	0.00000	0.00107	0.00205	-0.00051	0.00058
33	C2	DXY	0.00000	-0.00676	-0.00735	0.00157	-0.01135
34	C2	DXZ	-0.00106	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	-0.00157	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.01524	0.00693	0.03949	0.02437
37	C3	S	0.00000	-0.03105	-0.01414	-0.08142	-0.05195
38	C3	PX	0.00000	-0.09255	-0.02838	0.01088	-0.01001
39	C3	PY	0.00000	0.06981	0.04774	-0.06355	-0.18005
40	C3	PZ	-0.02055	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	-0.02589	0.02313	-0.10820	-0.04050
42	C3	PX	0.00000	-0.03488	-0.01707	-0.00244	-0.01752
43	C3	PY	0.00000	0.04573	0.02619	-0.02309	-0.06511
44	C3	PZ	-0.00619	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00076	0.00832	0.00053	0.00632
46	C3	DYY	0.00000	0.00206	-0.00783	-0.00275	-0.00741
47	C3	DZZ	0.00000	0.00017	0.00047	0.00136	0.00103
48	C3	DXY	0.00000	0.01448	0.00358	0.00296	-0.00337
49	C3	DXZ	0.00014	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00123	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.03909	0.03787	0.01496	-0.00783
52	C4	S	0.00000	-0.08616	-0.08146	-0.03314	0.01776
53	C4	PX	0.00000	-0.02548	-0.02913	-0.05564	0.01922
54	C4	PY	0.00000	0.06051	0.08757	0.04116	-0.06621
55	C4	PZ	-0.14054	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.04797	-0.06978	-0.01869	0.03370
57	C4	PX	0.00000	-0.00960	-0.00873	-0.01469	-0.00347
58	C4	PY	0.00000	-0.00222	-0.00947	0.01352	-0.01020
59	C4	PZ	-0.06533	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00372	-0.00016	0.00074	0.01488
61	C4	DYY	0.00000	-0.00266	0.00532	-0.00010	-0.01804
62	C4	DZZ	0.00000	0.00193	0.00033	0.00060	0.00163
63	C4	DXY	0.00000	-0.00566	0.01529	-0.00019	-0.00279
64	C4	DXZ	-0.00273	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.01386	0.00000	0.00000	0.00000	0.00000

66	C5	S	0.00000	-0.02036	-0.03819	0.00153	-0.00927
67	C5	S	0.00000	0.04320	0.07866	-0.00158	0.01766
68	C5	PX	0.00000	-0.11545	-0.02276	0.09343	-0.01734
69	C5	PY	0.00000	0.14895	-0.07374	-0.19609	0.18518
70	C5	PZ	-0.03835	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.02123	0.05903	-0.02064	0.02221
72	C5	PX	0.00000	-0.06628	-0.03035	0.04806	-0.02201
73	C5	PY	0.00000	0.08495	0.00055	-0.07576	0.07919
74	C5	PZ	-0.02128	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	-0.00057	-0.00840	-0.00898	0.00592
76	C5	DYY	0.00000	0.00112	0.00762	0.00522	-0.00255
77	C5	DZZ	0.00000	-0.00130	-0.00183	0.00062	-0.00105
78	C5	DXY	0.00000	-0.00884	-0.00556	0.00726	-0.01062
79	C5	DXZ	-0.00358	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00042	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.04351	-0.02974	0.00329	-0.04001
82	C6	S	0.00000	0.09570	0.06321	-0.00804	0.08713
83	C6	PX	0.00000	0.02407	-0.00947	-0.01638	-0.04887
84	C6	PY	0.00000	-0.05608	0.05784	0.05462	0.06813
85	C6	PZ	-0.01278	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	0.07597	0.04900	-0.02451	0.08668
87	C6	PX	0.00000	0.01651	-0.00829	0.00400	-0.02435
88	C6	PY	0.00000	-0.02847	0.01162	0.01299	0.00720
89	C6	PZ	-0.00787	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.00066	-0.00685	-0.00291	0.00750
91	C6	DYY	0.00000	-0.00011	0.00641	0.00556	-0.00803
92	C6	DZZ	0.00000	-0.00285	-0.00098	0.00001	-0.00113
93	C6	DXY	0.00000	0.00447	0.00206	-0.01299	-0.00685
94	C6	DXZ	-0.00030	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.00030	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.03415	-0.00399	-0.00791	-0.01884
97	C7	S	0.00000	-0.06875	0.00725	0.01652	0.03988
98	C7	PX	0.00000	-0.08398	0.14560	-0.05993	-0.03999
99	C7	PY	0.00000	-0.16399	-0.00943	-0.04447	0.05441
100	C7	PZ	-0.00764	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	-0.05357	0.01357	0.02305	0.01352
102	C7	PX	0.00000	-0.05195	0.06623	-0.03156	0.00282
103	C7	PY	0.00000	-0.05271	-0.00241	-0.00941	0.03247
104	C7	PZ	-0.00432	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00300	0.00386	0.00310	0.00132
106	C7	DYY	0.00000	0.00550	-0.00339	-0.00155	-0.00185
107	C7	DZZ	0.00000	0.00133	-0.00025	-0.00094	-0.00070
108	C7	DXY	0.00000	0.01187	-0.00176	0.00432	-0.00506
109	C7	DXZ	0.00074	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.00074	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00756	0.00643	-0.01749	0.00779
112	O1	S	0.00000	0.01892	-0.01958	0.04467	-0.01633
113	O1	PX	0.00000	-0.09240	0.18061	-0.21438	0.03483
114	O1	PY	0.00000	0.02412	-0.08231	0.02150	0.10904
115	O1	PZ	-0.40066	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	0.02772	-0.00779	0.05747	-0.03823
117	O1	PX	0.00000	-0.06477	0.12437	-0.15219	0.02360
118	O1	PY	0.00000	0.01820	-0.05386	0.01879	0.07307
119	O1	PZ	-0.26458	0.00000	0.00000	0.00000	0.00000

120	O1	DXX	0.00000	-0.00295	0.00939	-0.01144	0.00424
121	O1	DYY	0.00000	-0.00030	-0.00746	0.00604	-0.00188
122	O1	DZZ	0.00000	0.00250	-0.00474	0.00546	0.00043
123	O1	DXY	0.00000	0.00365	-0.00887	0.00698	0.00362
124	O1	DXZ	-0.01809	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.01235	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	0.13156	0.01793	-0.12666	0.10417
127	H4	S	0.00000	0.07609	-0.00697	-0.08246	0.07454
128	H4	PX	0.00000	0.00569	0.00006	-0.00436	0.00437
129	H4	PY	0.00000	-0.00489	-0.00219	0.00466	-0.00239
130	H4	PZ	-0.00090	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	0.03760	-0.01122	0.00350	0.03446
132	N1	S	0.00000	-0.08240	0.02469	-0.00945	-0.07499
133	N1	PX	0.00000	-0.01417	-0.03453	0.08633	-0.01322
134	N1	PY	0.00000	0.16044	-0.01297	-0.03641	0.01407
135	N1	PZ	-0.00802	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	-0.13827	0.03907	-0.00074	-0.12222
137	N1	PX	0.00000	-0.00337	-0.01888	0.05132	-0.00277
138	N1	PY	0.00000	0.07456	-0.00609	-0.01214	0.00163
139	N1	PZ	-0.00394	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.00493	-0.00449	0.00887	-0.00089
141	N1	DYY	0.00000	0.00909	0.00187	-0.00752	0.00504
142	N1	DZZ	0.00000	-0.00071	0.00119	-0.00186	0.00055
143	N1	DXY	0.00000	0.00939	-0.00324	0.00145	-0.00174
144	N1	DXZ	-0.00051	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	-0.00072	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00000	-0.00642	-0.19416	-0.10381	-0.01513
147	H6	S	0.00000	0.00360	-0.11850	-0.07692	-0.00542
148	H6	PX	0.00000	-0.00060	-0.01016	-0.00520	-0.00053
149	H6	PY	0.00000	-0.00072	-0.00314	-0.00073	-0.00263
150	H6	PZ	-0.00042	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.04177	0.00160	0.00538	-0.00529
152	C8	S	0.00000	0.08657	-0.00444	-0.00936	0.00937
153	C8	PX	0.00000	0.18515	-0.00806	-0.04445	-0.00859
154	C8	PY	0.00000	-0.00779	-0.09522	0.17134	-0.06158
155	C8	PZ	-0.00458	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	0.07050	-0.00373	-0.00003	0.02351
157	C8	PX	0.00000	0.05415	-0.00534	-0.00432	0.02303
158	C8	PY	0.00000	0.00093	-0.02199	0.03904	0.00259
159	C8	PZ	-0.00212	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.00946	0.00021	0.00821	-0.01125
161	C8	DYY	0.00000	0.00784	-0.00346	-0.00259	0.00995
162	C8	DZZ	0.00000	-0.00113	0.00037	-0.00075	0.00012
163	C8	DXY	0.00000	-0.00136	-0.00119	0.00239	0.01080
164	C8	DXZ	0.00018	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	-0.00028	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	-0.07637	0.09307	-0.02312	-0.00696
167	H8	S	0.00000	-0.04162	0.06353	-0.01120	-0.01302
168	H8	PX	0.00000	0.00483	-0.00519	0.00155	0.00020
169	H8	PY	0.00000	-0.00262	0.00054	-0.00061	0.00109
170	H8	PZ	-0.00012	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	0.01053	0.00420	0.00059	-0.00487
172	C10	S	0.00000	-0.02199	-0.00787	-0.00230	0.01124
173	C10	PX	0.00000	0.13466	-0.03838	0.03337	-0.30449

174	C10	PY	0.00000	0.16030	0.07629	-0.17309	-0.00037
175	C10	PZ	-0.00175	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	-0.02631	-0.01314	0.00075	0.01931
177	C10	PX	0.00000	0.05809	-0.01576	0.01162	-0.15249
178	C10	PY	0.00000	0.06366	0.03014	-0.07018	-0.01334
179	C10	PZ	-0.00081	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.00640	-0.00471	0.00959	-0.00932
181	C10	DYY	0.00000	0.00344	0.00374	-0.00698	0.00777
182	C10	DZZ	0.00000	0.00122	0.00052	-0.00066	0.00024
183	C10	DXY	0.00000	-0.00628	-0.00158	0.00394	0.01363
184	C10	DXZ	0.00005	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	-0.00022	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.02940	-0.04099	0.05634	-0.18132
187	H16	S	0.00000	0.01771	-0.02779	0.04442	-0.13822
188	H16	PX	0.00000	-0.00087	0.00227	-0.00294	0.00770
189	H16	PY	0.00000	0.00295	0.00034	-0.00139	-0.00388
190	H16	PZ	-0.00004	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	-0.13134	-0.01873	0.05740	0.14597
192	H18	S	0.00000	-0.08414	-0.01246	0.04162	0.09397
193	H18	PX	0.00000	-0.00548	-0.00145	0.00339	0.00413
194	H18	PY	0.00000	-0.00465	0.00046	-0.00008	0.00646
195	H18	PZ	-0.00004	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00245	0.00335	0.00561	0.00515
197	C9	S	0.00000	-0.00663	-0.00854	-0.01329	-0.00970
198	C9	PX	0.00000	0.03067	0.02408	0.04930	-0.08657
199	C9	PY	0.00000	0.02472	-0.23187	0.14276	0.03471
200	C9	PZ	-0.31445	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	0.00704	-0.02188	0.01224	-0.02238
202	C9	PX	0.00000	0.00553	0.02415	0.00381	-0.03306
203	C9	PY	0.00000	0.00290	-0.10782	0.05543	0.01463
204	C9	PZ	-0.12903	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	-0.00249	0.00726	-0.00848	0.00461
206	C9	DYY	0.00000	-0.00038	-0.01059	0.00530	0.00232
207	C9	DZZ	0.00000	0.00170	0.00480	0.00096	-0.00614
208	C9	DXY	0.00000	-0.00466	0.01104	-0.01184	0.00200
209	C9	DXZ	-0.00428	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.01540	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.00879	-0.14637	0.07842	0.02524
212	H3	S	0.00000	0.00782	-0.10136	0.06080	0.02305
213	H3	PX	0.00000	0.00039	-0.00122	0.00119	-0.00077
214	H3	PY	0.00000	-0.00024	0.00652	-0.00314	-0.00106
215	H3	PZ	-0.00480	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.14889	0.00619	0.03925	-0.00724	-0.03672
217	H5	S	0.11158	0.00611	0.02785	-0.00212	-0.02704
218	H5	PX	-0.00577	0.00040	-0.00090	0.00125	0.00019
219	H5	PY	0.00255	0.00017	-0.00244	0.00138	-0.00041
220	H5	PZ	0.00469	0.00020	0.00240	-0.00075	-0.00227
221	H7	S	-0.14889	0.00619	0.03925	-0.00724	-0.03672
222	H7	S	-0.11158	0.00611	0.02785	-0.00212	-0.02704
223	H7	PX	0.00577	0.00040	-0.00090	0.00125	0.00019
224	H7	PY	-0.00255	0.00017	-0.00244	0.00138	-0.00041
225	H7	PZ	0.00469	-0.00020	-0.00240	0.00075	0.00227

MO:

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Eigenvalues: -0.57233 -0.56064 -0.55923 -0.53266 -0.51654
 (ev): -15.57390 -15.25578 -15.21754 -14.49451 -14.05566

		A	A	A	A	A	
1	H1	S	0.04066	0.02166	0.00000	0.01612	0.00000
2	H1	S	0.03337	0.02542	0.00000	0.00751	0.00000
3	H1	PX	-0.00136	0.00013	0.00000	-0.00138	0.00000
4	H1	PY	-0.00070	-0.00078	0.00000	0.00018	0.00000
5	H1	PZ	0.00000	0.00000	0.00224	0.00000	0.00123
6	C1	S	0.01459	-0.00550	0.00000	0.00864	0.00000
7	C1	S	-0.03071	0.00835	0.00000	-0.01836	0.00000
8	C1	PX	0.08661	0.03933	0.00000	0.02380	0.00000
9	C1	PY	0.00860	-0.09128	0.00000	0.08984	0.00000
10	C1	PZ	0.00000	0.00000	0.11241	0.00000	0.08591
11	C1	S	-0.03155	0.04429	0.00000	-0.04476	0.00000
12	C1	PX	0.03014	0.00546	0.00000	0.01952	0.00000
13	C1	PY	0.01873	-0.04365	0.00000	0.06011	0.00000
14	C1	PZ	0.00000	0.00000	0.06295	0.00000	0.05449
15	C1	DXX	0.00449	0.00273	0.00000	0.00046	0.00000
16	C1	DYY	-0.00431	-0.00134	0.00000	-0.00149	0.00000
17	C1	DZZ	0.00050	-0.00068	0.00000	-0.00010	0.00000
18	C1	DXY	-0.00297	0.00811	0.00000	-0.00398	0.00000
19	C1	DXZ	0.00000	0.00000	-0.00728	0.00000	-0.00831
20	C1	DYZ	0.00000	0.00000	-0.00255	0.00000	0.00653
21	C2	S	-0.00651	-0.00326	0.00000	0.00112	0.00000
22	C2	S	0.01665	0.00398	0.00000	0.00149	0.00000
23	C2	PX	0.03659	-0.03078	0.00000	0.12026	0.00000
24	C2	PY	-0.05283	-0.22527	0.00000	-0.13517	0.00000
25	C2	PZ	0.00000	0.00000	0.12140	0.00000	0.01884
26	C2	S	-0.00409	0.03703	0.00000	-0.01399	0.00000
27	C2	PX	-0.00288	-0.00748	0.00000	0.05935	0.00000
28	C2	PY	-0.02948	-0.08480	0.00000	-0.05696	0.00000
29	C2	PZ	0.00000	0.00000	0.06650	0.00000	0.01421
30	C2	DXX	0.00008	0.01252	0.00000	0.00307	0.00000
31	C2	DYY	0.00075	-0.00921	0.00000	-0.00209	0.00000
32	C2	DZZ	0.00033	-0.00112	0.00000	0.00061	0.00000
33	C2	DXY	0.00396	-0.00428	0.00000	-0.01425	0.00000
34	C2	DXZ	0.00000	0.00000	0.00814	0.00000	-0.00036
35	C2	DYZ	0.00000	0.00000	0.00129	0.00000	0.00595
36	C3	S	-0.01603	0.01705	0.00000	-0.00527	0.00000
37	C3	S	0.03403	-0.03629	0.00000	0.01069	0.00000
38	C3	PX	0.23169	-0.02858	0.00000	0.01230	0.00000
39	C3	PY	-0.14982	0.11103	0.00000	-0.09141	0.00000
40	C3	PZ	0.00000	0.00000	0.18426	0.00000	-0.03999
41	C3	S	0.00533	-0.06184	0.00000	0.02838	0.00000
42	C3	PX	0.10726	-0.02247	0.00000	0.01124	0.00000
43	C3	PY	-0.02204	0.03115	0.00000	-0.00909	0.00000
44	C3	PZ	0.00000	0.00000	0.10895	0.00000	-0.02610
45	C3	DXX	-0.01131	-0.00328	0.00000	0.00651	0.00000
46	C3	DYY	0.00578	0.00404	0.00000	-0.00749	0.00000
47	C3	DZZ	0.00005	0.00009	0.00000	0.00011	0.00000
48	C3	DXY	-0.01069	0.00320	0.00000	-0.00722	0.00000
49	C3	DXZ	0.00000	0.00000	-0.00302	0.00000	0.00117
50	C3	DYZ	0.00000	0.00000	-0.00712	0.00000	0.00822

51	C4	S	-0.01829	0.01035	0.00000	-0.00822	0.00000
52	C4	S	0.04460	-0.02068	0.00000	0.01936	0.00000
53	C4	PX	-0.16130	-0.16175	0.00000	0.08116	0.00000
54	C4	PY	-0.07228	-0.06828	0.00000	0.06201	0.00000
55	C4	PZ	0.00000	0.00000	0.10870	0.00000	0.19874
56	C4	S	0.04197	-0.00872	0.00000	-0.00379	0.00000
57	C4	PX	-0.06314	-0.07348	0.00000	0.04058	0.00000
58	C4	PY	-0.00641	-0.01219	0.00000	0.00964	0.00000
59	C4	PZ	0.00000	0.00000	0.06189	0.00000	0.11993
60	C4	DXX	0.01233	0.01055	0.00000	0.00137	0.00000
61	C4	DYY	-0.01171	-0.00995	0.00000	-0.00253	0.00000
62	C4	DZZ	0.00098	0.00187	0.00000	-0.00103	0.00000
63	C4	DXY	0.01355	0.00369	0.00000	0.00137	0.00000
64	C4	DXZ	0.00000	0.00000	0.00135	0.00000	0.00154
65	C4	DYZ	0.00000	0.00000	-0.00484	0.00000	0.00936
66	C5	S	-0.01223	0.00577	0.00000	-0.00035	0.00000
67	C5	S	0.02552	-0.01204	0.00000	-0.00481	0.00000
68	C5	PX	0.21234	0.11376	0.00000	-0.08685	0.00000
69	C5	PY	-0.01547	0.19828	0.00000	0.14101	0.00000
70	C5	PZ	0.00000	0.00000	0.10056	0.00000	0.07776
71	C5	S	0.05167	-0.00920	0.00000	0.03710	0.00000
72	C5	PX	0.09896	0.03868	0.00000	-0.04960	0.00000
73	C5	PY	-0.03274	0.07049	0.00000	0.06010	0.00000
74	C5	PZ	0.00000	0.00000	0.06193	0.00000	0.05099
75	C5	DXX	0.00747	0.01091	0.00000	-0.00008	0.00000
76	C5	DYY	-0.00532	-0.00714	0.00000	0.00365	0.00000
77	C5	DZZ	-0.00037	-0.00035	0.00000	-0.00110	0.00000
78	C5	DXY	0.00873	-0.00294	0.00000	-0.01280	0.00000
79	C5	DXZ	0.00000	0.00000	0.00304	0.00000	0.00591
80	C5	DYZ	0.00000	0.00000	-0.00664	0.00000	0.00071
81	C6	S	0.02335	0.01064	0.00000	-0.00294	0.00000
82	C6	S	-0.05049	-0.02494	0.00000	0.00055	0.00000
83	C6	PX	-0.15797	-0.06450	0.00000	-0.06108	0.00000
84	C6	PY	-0.06518	0.14022	0.00000	0.23011	0.00000
85	C6	PZ	0.00000	0.00000	0.23109	0.00000	-0.09462
86	C6	S	-0.02883	-0.03142	0.00000	0.04742	0.00000
87	C6	PX	-0.05509	-0.02183	0.00000	-0.02895	0.00000
88	C6	PY	-0.03155	0.04223	0.00000	0.06963	0.00000
89	C6	PZ	0.00000	0.00000	0.13526	0.00000	-0.05806
90	C6	DXX	-0.00140	0.00664	0.00000	0.01048	0.00000
91	C6	DYY	0.00035	-0.00543	0.00000	-0.00745	0.00000
92	C6	DZZ	0.00062	0.00102	0.00000	0.00183	0.00000
93	C6	DXY	-0.00547	-0.01106	0.00000	-0.00980	0.00000
94	C6	DXZ	0.00000	0.00000	0.00405	0.00000	-0.00217
95	C6	DYZ	0.00000	0.00000	-0.01115	0.00000	0.01007
96	C7	S	0.00216	-0.00513	0.00000	-0.00188	0.00000
97	C7	S	-0.00176	0.01073	0.00000	0.00321	0.00000
98	C7	PX	-0.23428	-0.02754	0.00000	0.01257	0.00000
99	C7	PY	0.18743	-0.14480	0.00000	0.10914	0.00000
100	C7	PZ	0.00000	0.00000	0.14676	0.00000	-0.06559
101	C7	S	-0.00762	0.03647	0.00000	0.02433	0.00000
102	C7	PX	-0.11571	-0.02435	0.00000	0.00151	0.00000
103	C7	PY	0.06761	-0.04735	0.00000	0.03407	0.00000
104	C7	PZ	0.00000	0.00000	0.08504	0.00000	-0.04196

105	C7	DXX	-0.01737	0.00436	0.00000	0.00107	0.00000
106	C7	DYY	0.01502	-0.00241	0.00000	-0.00167	0.00000
107	C7	DZZ	0.00103	-0.00072	0.00000	0.00022	0.00000
108	C7	DXY	-0.00694	0.01202	0.00000	-0.00697	0.00000
109	C7	DXZ	0.00000	0.00000	-0.01161	0.00000	0.00517
110	C7	DYZ	0.00000	0.00000	0.00410	0.00000	0.00074
111	O1	S	0.00879	-0.00154	0.00000	0.02192	0.00000
112	O1	S	-0.01860	0.00361	0.00000	-0.05224	0.00000
113	O1	PX	0.11260	0.04803	0.00000	0.14085	0.00000
114	O1	PY	0.07338	0.11186	0.00000	-0.08666	0.00000
115	O1	PZ	0.00000	0.00000	0.03953	0.00000	0.32398
116	O1	S	-0.04372	0.00352	0.00000	-0.08718	0.00000
117	O1	PX	0.08256	0.03338	0.00000	0.10492	0.00000
118	O1	PY	0.05250	0.08318	0.00000	-0.07372	0.00000
119	O1	PZ	0.00000	0.00000	0.02839	0.00000	0.25348
120	O1	DXX	0.00974	0.00977	0.00000	0.00235	0.00000
121	O1	DYY	-0.00551	-0.01150	0.00000	0.00695	0.00000
122	O1	DZZ	-0.00060	0.00071	0.00000	-0.00493	0.00000
123	O1	DXY	0.00348	0.00489	0.00000	-0.00518	0.00000
124	O1	DXZ	0.00000	0.00000	-0.00157	0.00000	0.00353
125	O1	DYZ	0.00000	0.00000	-0.00479	0.00000	-0.01659
126	H4	S	-0.09283	0.03431	0.00000	0.11186	0.00000
127	H4	S	-0.07059	0.02911	0.00000	0.08315	0.00000
128	H4	PX	-0.00219	0.00292	0.00000	0.00326	0.00000
129	H4	PY	0.00433	0.00138	0.00000	-0.00314	0.00000
130	H4	PZ	0.00000	0.00000	0.00189	0.00000	0.00180
131	N1	S	-0.00766	0.00315	0.00000	-0.02493	0.00000
132	N1	S	0.01924	-0.00879	0.00000	0.05666	0.00000
133	N1	PX	-0.10779	0.10458	0.00000	0.01363	0.00000
134	N1	PY	0.03147	-0.13595	0.00000	-0.25312	0.00000
135	N1	PZ	0.00000	0.00000	0.23856	0.00000	-0.13762
136	N1	S	0.00387	0.01388	0.00000	0.09168	0.00000
137	N1	PX	-0.06260	0.06300	0.00000	-0.00413	0.00000
138	N1	PY	0.00436	-0.06446	0.00000	-0.13757	0.00000
139	N1	PZ	0.00000	0.00000	0.15075	0.00000	-0.09338
140	N1	DXX	-0.00706	0.01522	0.00000	0.00864	0.00000
141	N1	DYY	0.00540	-0.01426	0.00000	-0.01423	0.00000
142	N1	DZZ	0.00191	-0.00132	0.00000	0.00283	0.00000
143	N1	DXY	-0.00547	-0.00407	0.00000	-0.01431	0.00000
144	N1	DXZ	0.00000	0.00000	0.01594	0.00000	-0.00966
145	N1	DYZ	0.00000	0.00000	0.01698	0.00000	-0.00806
146	H6	S	-0.00209	0.07041	0.00000	-0.05128	0.00000
147	H6	S	-0.00742	0.05763	0.00000	-0.03642	0.00000
148	H6	PX	0.00007	0.00358	0.00000	-0.00164	0.00000
149	H6	PY	-0.00154	-0.00158	0.00000	-0.00276	0.00000
150	H6	PZ	0.00000	0.00000	0.00253	0.00000	0.00031
151	C8	S	-0.00921	-0.01004	0.00000	0.00733	0.00000
152	C8	S	0.01765	0.02352	0.00000	-0.01555	0.00000
153	C8	PX	0.06034	-0.06236	0.00000	-0.13646	0.00000
154	C8	PY	-0.08868	0.25146	0.00000	0.01034	0.00000
155	C8	PZ	0.00000	0.00000	0.17383	0.00000	-0.11704
156	C8	S	0.00400	0.05138	0.00000	-0.01885	0.00000
157	C8	PX	0.00683	-0.00820	0.00000	-0.08929	0.00000
158	C8	PY	-0.02742	0.05587	0.00000	-0.00779	0.00000

159	C8	PZ	0.00000	0.00000	0.10041	0.00000	-0.07198
160	C8	DXX	-0.01127	0.01652	0.00000	0.01423	0.00000
161	C8	DYY	0.00879	-0.01064	0.00000	-0.01385	0.00000
162	C8	DZZ	0.00057	-0.00183	0.00000	-0.00099	0.00000
163	C8	DXY	-0.00184	0.00677	0.00000	-0.00689	0.00000
164	C8	DXZ	0.00000	0.00000	-0.00511	0.00000	0.00305
165	C8	DYZ	0.00000	0.00000	0.00415	0.00000	-0.00065
166	H8	S	-0.16984	-0.00207	0.00000	0.00787	0.00000
167	H8	S	-0.13204	0.00377	0.00000	0.01032	0.00000
168	H8	PX	0.00800	0.00038	0.00000	-0.00005	0.00000
169	H8	PY	0.00219	-0.00235	0.00000	0.00156	0.00000
170	H8	PZ	0.00000	0.00000	0.00307	0.00000	-0.00135
171	C10	S	-0.00731	0.01534	0.00000	0.00810	0.00000
172	C10	S	0.01532	-0.03248	0.00000	-0.01709	0.00000
173	C10	PX	0.07475	0.05110	0.00000	0.21538	0.00000
174	C10	PY	0.13040	-0.22192	0.00000	-0.00968	0.00000
175	C10	PZ	0.00000	0.00000	0.08709	0.00000	-0.06724
176	C10	S	0.01645	-0.04722	0.00000	-0.02362	0.00000
177	C10	PX	0.03884	0.02205	0.00000	0.12001	0.00000
178	C10	PY	0.05516	-0.09712	0.00000	0.01015	0.00000
179	C10	PZ	0.00000	0.00000	0.05071	0.00000	-0.04299
180	C10	DXX	-0.00442	0.01177	0.00000	0.00880	0.00000
181	C10	DYY	0.00208	-0.00808	0.00000	-0.00712	0.00000
182	C10	DZZ	0.00006	-0.00001	0.00000	-0.00014	0.00000
183	C10	DXY	-0.00684	0.00441	0.00000	-0.01439	0.00000
184	C10	DXZ	0.00000	0.00000	-0.00196	0.00000	0.00143
185	C10	DYZ	0.00000	0.00000	0.00938	0.00000	-0.00665
186	H16	S	0.02297	0.06613	0.00000	0.13848	0.00000
187	H16	S	0.01098	0.05923	0.00000	0.11797	0.00000
188	H16	PX	-0.00113	-0.00304	0.00000	-0.00550	0.00000
189	H16	PY	0.00216	-0.00201	0.00000	0.00232	0.00000
190	H16	PZ	0.00000	0.00000	0.00185	0.00000	-0.00143
191	H18	S	-0.08520	0.05870	0.00000	-0.11287	0.00000
192	H18	S	-0.06447	0.05088	0.00000	-0.07810	0.00000
193	H18	PX	-0.00358	0.00333	0.00000	-0.00349	0.00000
194	H18	PY	-0.00177	-0.00084	0.00000	-0.00420	0.00000
195	H18	PZ	0.00000	0.00000	0.00190	0.00000	-0.00146
196	C9	S	-0.00163	-0.00289	0.00000	-0.00125	0.00000
197	C9	S	0.00514	0.00473	0.00000	0.00553	0.00000
198	C9	PX	-0.05583	0.02765	0.00000	-0.12200	0.00000
199	C9	PY	-0.10152	-0.21429	0.00000	0.13169	0.00000
200	C9	PZ	0.00000	0.00000	-0.12387	0.00000	-0.28302
201	C9	S	-0.01335	-0.00125	0.00000	-0.00775	0.00000
202	C9	PX	-0.01244	0.02102	0.00000	-0.04919	0.00000
203	C9	PY	-0.04501	-0.10844	0.00000	0.07342	0.00000
204	C9	PZ	0.00000	0.00000	-0.05825	0.00000	-0.13154
205	C9	DXX	0.00860	0.01085	0.00000	-0.00302	0.00000
206	C9	DYY	-0.00613	-0.01752	0.00000	0.01614	0.00000
207	C9	DZZ	-0.00138	0.00623	0.00000	-0.01088	0.00000
208	C9	DXY	0.00673	0.00480	0.00000	0.00516	0.00000
209	C9	DXZ	0.00000	0.00000	-0.00906	0.00000	-0.03027
210	C9	DYZ	0.00000	0.00000	0.00305	0.00000	0.00408
211	H3	S	-0.05990	-0.14589	0.00000	0.10972	0.00000
212	H3	S	-0.04805	-0.11726	0.00000	0.09249	0.00000

213	H3	PX	-0.00132	-0.00122	0.00000	-0.00016	0.00000
214	H3	PY	0.00236	0.00591	0.00000	-0.00457	0.00000
215	H3	PZ	0.00000	0.00000	-0.00206	0.00000	-0.00492
216	H5	S	-0.00023	0.04886	0.06856	-0.06616	0.17248
217	H5	S	-0.00051	0.04198	0.05712	-0.06193	0.16182
218	H5	PX	-0.00075	-0.00106	-0.00214	0.00016	-0.00480
219	H5	PY	-0.00149	-0.00217	0.00136	0.00078	0.00324
220	H5	PZ	0.00005	0.00290	0.00190	-0.00375	0.00457
221	H7	S	-0.00023	0.04886	-0.06856	-0.06616	-0.17248
222	H7	S	-0.00051	0.04198	-0.05712	-0.06193	-0.16182
223	H7	PX	-0.00075	-0.00106	0.00214	0.00016	0.00480
224	H7	PY	-0.00149	-0.00217	-0.00136	0.00078	-0.00324
225	H7	PZ	-0.00005	-0.00290	0.00190	0.00375	0.00457

MO:	36	37	38	39	40
Eigenvalues:	-0.50639	-0.49379	-0.42839	-0.41333	-0.39930
(ev):	-13.77952	-13.43683	-11.65714	-11.24742	-10.86560

		A	A	A	A	A	
1	H1	S	-0.02589	-0.11153	0.00000	0.06460	0.00000
2	H1	S	-0.03694	-0.09881	0.00000	0.06995	0.00000
3	H1	PX	0.00198	0.00337	0.00000	-0.00208	0.00000
4	H1	PY	-0.00312	0.00209	0.00000	-0.00037	0.00000
5	H1	PZ	0.00000	0.00000	-0.00331	0.00000	-0.00580
6	C1	S	-0.00310	-0.01853	0.00000	0.00878	0.00000
7	C1	S	0.00972	0.03815	0.00000	-0.01944	0.00000
8	C1	PX	0.04148	-0.18460	0.00000	0.07912	0.00000
9	C1	PY	-0.21580	-0.01188	0.00000	0.04487	0.00000
10	C1	PZ	0.00000	0.00000	-0.13795	0.00000	-0.23812
11	C1	S	-0.01783	0.06703	0.00000	-0.05137	0.00000
12	C1	PX	0.02876	-0.11732	0.00000	0.04597	0.00000
13	C1	PY	-0.06753	-0.02635	0.00000	0.05947	0.00000
14	C1	PZ	0.00000	0.00000	-0.10950	0.00000	-0.18530
15	C1	DXX	-0.00763	-0.01040	0.00000	0.00658	0.00000
16	C1	DYY	0.00996	0.00798	0.00000	-0.00712	0.00000
17	C1	DZZ	-0.00059	-0.00034	0.00000	-0.00024	0.00000
18	C1	DXY	0.00549	-0.01021	0.00000	0.00841	0.00000
19	C1	DXZ	0.00000	0.00000	0.00830	0.00000	0.00889
20	C1	DYZ	0.00000	0.00000	-0.00166	0.00000	0.00446
21	C2	S	-0.00056	-0.00202	0.00000	0.01898	0.00000
22	C2	S	0.00414	0.00590	0.00000	-0.03822	0.00000
23	C2	PX	0.04536	0.18199	0.00000	-0.11150	0.00000
24	C2	PY	0.00123	0.00542	0.00000	0.07809	0.00000
25	C2	PZ	0.00000	0.00000	-0.22060	0.00000	0.19298
26	C2	S	-0.00963	0.01018	0.00000	-0.10901	0.00000
27	C2	PX	0.01685	0.12395	0.00000	-0.06783	0.00000
28	C2	PY	-0.00483	0.00585	0.00000	0.02450	0.00000
29	C2	PZ	0.00000	0.00000	-0.16704	0.00000	0.14320
30	C2	DXX	-0.00368	-0.01093	0.00000	0.00546	0.00000
31	C2	DYY	0.00289	0.01039	0.00000	-0.00616	0.00000
32	C2	DZZ	0.00058	0.00001	0.00000	0.00068	0.00000
33	C2	DXY	-0.00124	-0.01475	0.00000	0.00892	0.00000
34	C2	DXZ	0.00000	0.00000	-0.00846	0.00000	0.00697
35	C2	DYZ	0.00000	0.00000	-0.01369	0.00000	0.00447

36	C3	S	-0.00120	-0.00233	0.00000	-0.02013	0.00000
37	C3	S	0.00119	0.00448	0.00000	0.04055	0.00000
38	C3	PX	0.07399	0.14134	0.00000	-0.21264	0.00000
39	C3	PY	0.19322	0.03215	0.00000	-0.05395	0.00000
40	C3	PZ	0.00000	0.00000	-0.05267	0.00000	-0.24781
41	C3	S	0.01587	-0.03082	0.00000	0.11885	0.00000
42	C3	PX	0.05592	0.06233	0.00000	-0.11493	0.00000
43	C3	PY	0.08986	0.02228	0.00000	0.02323	0.00000
44	C3	PZ	0.00000	0.00000	-0.04530	0.00000	-0.18030
45	C3	DXX	-0.01285	-0.01426	0.00000	0.00758	0.00000
46	C3	DYY	0.01406	0.01336	0.00000	-0.00457	0.00000
47	C3	DZZ	-0.00018	0.00046	0.00000	-0.00023	0.00000
48	C3	DXY	0.00571	-0.01227	0.00000	0.00546	0.00000
49	C3	DXZ	0.00000	0.00000	0.00284	0.00000	-0.01220
50	C3	DYZ	0.00000	0.00000	-0.00780	0.00000	0.00127
51	C4	S	-0.00087	0.01738	0.00000	0.00147	0.00000
52	C4	S	0.00270	-0.03919	0.00000	-0.00227	0.00000
53	C4	PX	-0.07401	0.20849	0.00000	-0.06244	0.00000
54	C4	PY	0.15577	-0.03219	0.00000	0.01568	0.00000
55	C4	PZ	0.00000	0.00000	-0.10133	0.00000	-0.09542
56	C4	S	-0.02465	-0.05831	0.00000	-0.02101	0.00000
57	C4	PX	-0.00572	0.07100	0.00000	-0.03715	0.00000
58	C4	PY	0.00113	0.02807	0.00000	-0.00014	0.00000
59	C4	PZ	0.00000	0.00000	-0.06501	0.00000	-0.06861
60	C4	DXX	-0.00849	-0.01052	0.00000	0.00309	0.00000
61	C4	DYY	0.01304	0.00871	0.00000	-0.00317	0.00000
62	C4	DZZ	-0.00307	0.00099	0.00000	-0.00002	0.00000
63	C4	DXY	0.01691	-0.01861	0.00000	0.00470	0.00000
64	C4	DXZ	0.00000	0.00000	0.00196	0.00000	-0.01495
65	C4	DYZ	0.00000	0.00000	0.02356	0.00000	0.01326
66	C5	S	-0.01104	0.00529	0.00000	-0.00507	0.00000
67	C5	S	0.02223	-0.01290	0.00000	0.00676	0.00000
68	C5	PX	0.02062	-0.20312	0.00000	0.04669	0.00000
69	C5	PY	-0.00461	-0.02000	0.00000	-0.02053	0.00000
70	C5	PZ	0.00000	0.00000	-0.23534	0.00000	0.13043
71	C5	S	0.05499	-0.03530	0.00000	0.04164	0.00000
72	C5	PX	-0.00060	-0.10627	0.00000	0.03840	0.00000
73	C5	PY	0.00380	0.00580	0.00000	-0.04131	0.00000
74	C5	PZ	0.00000	0.00000	-0.17241	0.00000	0.10373
75	C5	DXX	-0.00091	-0.00966	0.00000	0.00221	0.00000
76	C5	DYY	0.00210	0.00857	0.00000	-0.00226	0.00000
77	C5	DZZ	-0.00043	-0.00012	0.00000	-0.00109	0.00000
78	C5	DXY	0.00308	-0.01677	0.00000	0.00776	0.00000
79	C5	DXZ	0.00000	0.00000	-0.00291	0.00000	-0.00509
80	C5	DYZ	0.00000	0.00000	0.01519	0.00000	-0.01151
81	C6	S	0.00920	0.01605	0.00000	0.01984	0.00000
82	C6	S	-0.01972	-0.03737	0.00000	-0.05634	0.00000
83	C6	PX	-0.11097	-0.21494	0.00000	0.16778	0.00000
84	C6	PY	-0.05438	0.05338	0.00000	0.09514	0.00000
85	C6	PZ	0.00000	0.00000	-0.04713	0.00000	0.15686
86	C6	S	-0.02215	-0.03596	0.00000	0.03956	0.00000
87	C6	PX	-0.04009	-0.09489	0.00000	0.06261	0.00000
88	C6	PY	-0.01190	-0.01770	0.00000	-0.02026	0.00000
89	C6	PZ	0.00000	0.00000	-0.02859	0.00000	0.11016

90	C6	DXX	-0.00768	-0.00440	0.00000	0.01137	0.00000
91	C6	DYY	0.00690	0.00360	0.00000	-0.01043	0.00000
92	C6	DZZ	-0.00065	0.00084	0.00000	0.00181	0.00000
93	C6	DXY	-0.00172	-0.00280	0.00000	0.03310	0.00000
94	C6	DXZ	0.00000	0.00000	0.00412	0.00000	-0.01541
95	C6	DYZ	0.00000	0.00000	-0.01423	0.00000	-0.01149
96	C7	S	-0.00043	-0.02306	0.00000	-0.01279	0.00000
97	C7	S	0.00540	0.05016	0.00000	0.02577	0.00000
98	C7	PX	-0.09658	-0.18438	0.00000	-0.06143	0.00000
99	C7	PY	-0.15961	-0.02947	0.00000	-0.14457	0.00000
100	C7	PZ	0.00000	0.00000	0.04953	0.00000	-0.21888
101	C7	S	-0.00514	0.09121	0.00000	0.09684	0.00000
102	C7	PX	-0.05858	-0.10228	0.00000	-0.03381	0.00000
103	C7	PY	-0.06707	-0.01611	0.00000	-0.09782	0.00000
104	C7	PZ	0.00000	0.00000	0.03997	0.00000	-0.17271
105	C7	DXX	-0.00628	-0.01194	0.00000	0.00280	0.00000
106	C7	DYY	0.00655	0.01070	0.00000	0.00053	0.00000
107	C7	DZZ	0.00038	-0.00009	0.00000	0.00025	0.00000
108	C7	DXY	0.01496	0.00761	0.00000	0.00143	0.00000
109	C7	DXZ	0.00000	0.00000	-0.00362	0.00000	0.01005
110	C7	DYZ	0.00000	0.00000	-0.00734	0.00000	-0.01124
111	O1	S	0.02868	-0.02215	0.00000	0.00250	0.00000
112	O1	S	-0.07026	0.05219	0.00000	-0.00685	0.00000
113	O1	PX	0.27489	-0.18061	0.00000	0.01936	0.00000
114	O1	PY	-0.22849	0.03889	0.00000	-0.00249	0.00000
115	O1	PZ	0.00000	0.00000	0.29100	0.00000	0.11367
116	O1	S	-0.10269	0.08847	0.00000	-0.00686	0.00000
117	O1	PX	0.21289	-0.13929	0.00000	0.01551	0.00000
118	O1	PY	-0.18687	0.04229	0.00000	-0.00741	0.00000
119	O1	PZ	0.00000	0.00000	0.24980	0.00000	0.10141
120	O1	DXX	0.00581	-0.00785	0.00000	0.00042	0.00000
121	O1	DYY	0.00904	-0.00239	0.00000	0.00057	0.00000
122	O1	DZZ	-0.00909	0.00448	0.00000	-0.00092	0.00000
123	O1	DXY	-0.00832	-0.00194	0.00000	0.00128	0.00000
124	O1	DXZ	0.00000	0.00000	0.00746	0.00000	0.00246
125	O1	DYZ	0.00000	0.00000	-0.00584	0.00000	-0.00052
126	H4	S	-0.00602	0.09612	0.00000	-0.03681	0.00000
127	H4	S	-0.03225	0.09644	0.00000	-0.03133	0.00000
128	H4	PX	-0.00083	0.00188	0.00000	-0.00052	0.00000
129	H4	PY	-0.00069	-0.00343	0.00000	0.00073	0.00000
130	H4	PZ	0.00000	0.00000	-0.00467	0.00000	0.00299
131	N1	S	0.00764	-0.02227	0.00000	-0.06294	0.00000
132	N1	S	-0.01804	0.04936	0.00000	0.13584	0.00000
133	N1	PX	-0.01908	-0.16375	0.00000	-0.40913	0.00000
134	N1	PY	0.08491	-0.05837	0.00000	-0.22161	0.00000
135	N1	PZ	0.00000	0.00000	0.09663	0.00000	0.21210
136	N1	S	-0.01938	0.07957	0.00000	0.24386	0.00000
137	N1	PX	-0.00211	-0.10387	0.00000	-0.32214	0.00000
138	N1	PY	0.04379	-0.05054	0.00000	-0.18013	0.00000
139	N1	PZ	0.00000	0.00000	0.07260	0.00000	0.17022
140	N1	DXX	-0.00060	-0.00620	0.00000	-0.02185	0.00000
141	N1	DYY	0.00160	-0.00242	0.00000	-0.00646	0.00000
142	N1	DZZ	-0.00089	0.00379	0.00000	0.01056	0.00000
143	N1	DXY	0.00234	-0.01035	0.00000	-0.00989	0.00000

144	N1	DXZ	0.00000	0.00000	0.01029	0.00000	0.00820
145	N1	DYZ	0.00000	0.00000	-0.00135	0.00000	0.01531
146	H6	S	-0.03105	-0.12763	0.00000	0.04963	0.00000
147	H6	S	-0.02997	-0.09725	0.00000	0.07588	0.00000
148	H6	PX	-0.00118	-0.00428	0.00000	0.00145	0.00000
149	H6	PY	-0.00073	-0.00252	0.00000	0.00113	0.00000
150	H6	PZ	0.00000	0.00000	-0.00447	0.00000	0.00441
151	C8	S	-0.02017	-0.00814	0.00000	0.02728	0.00000
152	C8	S	0.04202	0.01508	0.00000	-0.06687	0.00000
153	C8	PX	0.10740	0.10309	0.00000	0.18952	0.00000
154	C8	PY	0.14664	0.09950	0.00000	0.00175	0.00000
155	C8	PZ	0.00000	0.00000	0.20478	0.00000	-0.01817
156	C8	S	0.06965	0.04263	0.00000	-0.05179	0.00000
157	C8	PX	0.07069	0.04120	0.00000	0.02986	0.00000
158	C8	PY	0.05245	0.00741	0.00000	-0.02319	0.00000
159	C8	PZ	0.00000	0.00000	0.14212	0.00000	-0.00699
160	C8	DXX	-0.00133	-0.00062	0.00000	0.00252	0.00000
161	C8	DYY	0.00291	-0.00013	0.00000	-0.00712	0.00000
162	C8	DZZ	-0.00032	0.00060	0.00000	0.00183	0.00000
163	C8	DXY	0.01244	0.01602	0.00000	0.02389	0.00000
164	C8	DXZ	0.00000	0.00000	-0.00024	0.00000	-0.01443
165	C8	DYZ	0.00000	0.00000	-0.00719	0.00000	-0.00194
166	H8	S	-0.06280	-0.10831	0.00000	-0.01887	0.00000
167	H8	S	-0.05322	-0.10528	0.00000	-0.02476	0.00000
168	H8	PX	0.00231	0.00400	0.00000	0.00144	0.00000
169	H8	PY	-0.00238	-0.00103	0.00000	-0.00251	0.00000
170	H8	PZ	0.00000	0.00000	0.00101	0.00000	-0.00511
171	C10	S	0.00692	0.00711	0.00000	0.00836	0.00000
172	C10	S	-0.01491	-0.01490	0.00000	-0.01930	0.00000
173	C10	PX	-0.09582	-0.02588	0.00000	-0.01723	0.00000
174	C10	PY	-0.10031	-0.06729	0.00000	-0.02924	0.00000
175	C10	PZ	0.00000	0.00000	0.16060	0.00000	-0.01725
176	C10	S	-0.01748	-0.04217	0.00000	-0.05445	0.00000
177	C10	PX	-0.06122	-0.01516	0.00000	-0.00022	0.00000
178	C10	PY	-0.05487	-0.03967	0.00000	-0.00078	0.00000
179	C10	PZ	0.00000	0.00000	0.12153	0.00000	-0.01554
180	C10	DXX	-0.00052	0.00028	0.00000	-0.00165	0.00000
181	C10	DYY	0.00151	0.00059	0.00000	0.00329	0.00000
182	C10	DZZ	0.00030	0.00018	0.00000	-0.00045	0.00000
183	C10	DXY	0.01215	0.00705	0.00000	0.00837	0.00000
184	C10	DXZ	0.00000	0.00000	-0.00259	0.00000	-0.00119
185	C10	DYZ	0.00000	0.00000	0.01315	0.00000	-0.00168
186	H16	S	-0.05338	-0.01414	0.00000	-0.02113	0.00000
187	H16	S	-0.04549	-0.01374	0.00000	-0.01911	0.00000
188	H16	PX	0.00184	0.00001	0.00000	-0.00002	0.00000
189	H16	PY	-0.00241	-0.00121	0.00000	-0.00032	0.00000
190	H16	PZ	0.00000	0.00000	0.00354	0.00000	-0.00059
191	H18	S	0.09160	0.04198	0.00000	0.02638	0.00000
192	H18	S	0.07419	0.04471	0.00000	0.06381	0.00000
193	H18	PX	0.00330	0.00121	0.00000	-0.00015	0.00000
194	H18	PY	0.00162	0.00068	0.00000	0.00120	0.00000
195	H18	PZ	0.00000	0.00000	0.00347	0.00000	-0.00008
196	C9	S	-0.00985	0.00514	0.00000	0.00052	0.00000
197	C9	S	0.02521	-0.01368	0.00000	-0.00037	0.00000

198	C9	PX	-0.15200	0.12712	0.00000	-0.02082	0.00000
199	C9	PY	0.11852	-0.02805	0.00000	0.00633	0.00000
200	C9	PZ	0.00000	0.00000	-0.08512	0.00000	-0.01142
201	C9	S	0.00800	0.00112	0.00000	-0.00306	0.00000
202	C9	PX	-0.05535	0.04860	0.00000	-0.01054	0.00000
203	C9	PY	0.07529	-0.01766	0.00000	0.00356	0.00000
204	C9	PZ	0.00000	0.00000	-0.02852	0.00000	0.00720
205	C9	DXX	-0.00461	-0.00236	0.00000	0.00036	0.00000
206	C9	DYY	0.02049	-0.00804	0.00000	0.00164	0.00000
207	C9	DZZ	-0.01288	0.00876	0.00000	-0.00145	0.00000
208	C9	DXY	0.01160	-0.00791	0.00000	0.00062	0.00000
209	C9	DXZ	0.00000	0.00000	-0.01782	0.00000	-0.00573
210	C9	DYZ	0.00000	0.00000	-0.00080	0.00000	-0.00043
211	H3	S	0.11986	-0.04371	0.00000	0.00787	0.00000
212	H3	S	0.10113	-0.03898	0.00000	0.00798	0.00000
213	H3	PX	-0.00020	0.00103	0.00000	-0.00024	0.00000
214	H3	PY	-0.00519	0.00206	0.00000	-0.00025	0.00000
215	H3	PZ	0.00000	0.00000	-0.00170	0.00000	-0.00032
216	H5	S	-0.07307	0.04665	0.06815	-0.00830	0.01620
217	H5	S	-0.07698	0.04645	0.08774	-0.00746	0.03569
218	H5	PX	-0.00059	0.00051	-0.00141	0.00004	-0.00044
219	H5	PY	0.00095	0.00052	0.00096	-0.00035	-0.00020
220	H5	PZ	-0.00381	0.00252	0.00165	-0.00046	0.00044
221	H7	S	-0.07307	0.04665	-0.06815	-0.00830	-0.01620
222	H7	S	-0.07698	0.04645	-0.08774	-0.00746	-0.03569
223	H7	PX	-0.00059	0.00051	0.00141	0.00004	0.00044
224	H7	PY	0.00095	0.00052	-0.00096	-0.00035	0.00020
225	H7	PZ	0.00381	-0.00252	0.00165	0.00046	0.00044

MO:	41	42	43	44	45
Eigenvalues:	-0.32668	-0.28259	0.04162	0.17416	0.20872
(ev):	-8.88935	-7.68968	1.13250	4.73911	5.67969

		A	A	A	A	A
1	H1	S	0.00000	0.00000	0.00000	0.00000
2	H1	S	0.00000	0.00000	0.00000	0.00000
3	H1	PX	0.00000	0.00000	0.00000	0.00000
4	H1	PY	0.00000	0.00000	0.00000	0.00000
5	H1	PZ	0.00027	-0.00692	0.00366	0.01010
6	C1	S	0.00000	0.00000	0.00000	0.00000
7	C1	S	0.00000	0.00000	0.00000	0.00000
8	C1	PX	0.00000	0.00000	0.00000	0.00000
9	C1	PY	0.00000	0.00000	0.00000	0.00000
10	C1	PZ	0.00513	-0.26612	0.11129	0.21402
11	C1	S	0.00000	0.00000	0.00000	0.00000
12	C1	PX	0.00000	0.00000	0.00000	0.00000
13	C1	PY	0.00000	0.00000	0.00000	0.00000
14	C1	PZ	-0.00684	-0.25860	0.15890	0.42522
15	C1	DXX	0.00000	0.00000	0.00000	0.00000
16	C1	DYY	0.00000	0.00000	0.00000	0.00000
17	C1	DZZ	0.00000	0.00000	0.00000	0.00000
18	C1	DXY	0.00000	0.00000	0.00000	0.00000
19	C1	DXZ	0.00263	0.01395	0.00334	0.00782
20	C1	DYZ	-0.00741	-0.01552	-0.01204	0.01153

21	C2	S	0.00000	0.00000	0.00000	0.00000	0.00000
22	C2	S	0.00000	0.00000	0.00000	0.00000	0.00000
23	C2	PX	0.00000	0.00000	0.00000	0.00000	0.00000
24	C2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
25	C2	PZ	-0.11942	0.17099	0.14818	0.29353	0.02086
26	C2	S	0.00000	0.00000	0.00000	0.00000	0.00000
27	C2	PX	0.00000	0.00000	0.00000	0.00000	0.00000
28	C2	PY	0.00000	0.00000	0.00000	0.00000	0.00000
29	C2	PZ	-0.10910	0.14903	0.22670	0.54919	0.04792
30	C2	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
31	C2	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
32	C2	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
33	C2	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
34	C2	DXZ	0.00070	0.00344	0.00713	-0.00840	0.01159
35	C2	DYZ	-0.01817	0.00847	-0.01507	-0.00783	-0.02714
36	C3	S	0.00000	0.00000	0.00000	0.00000	0.00000
37	C3	S	0.00000	0.00000	0.00000	0.00000	0.00000
38	C3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
39	C3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
40	C3	PZ	0.13961	0.16922	0.12553	-0.21038	-0.18417
41	C3	S	0.00000	0.00000	0.00000	0.00000	0.00000
42	C3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
43	C3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
44	C3	PZ	0.11812	0.16547	0.15524	-0.38075	-0.36087
45	C3	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
46	C3	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
47	C3	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
48	C3	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
49	C3	DXZ	-0.00581	0.00727	-0.01383	0.01423	-0.01313
50	C3	DYZ	-0.00461	-0.02533	0.01634	0.00929	-0.02113
51	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
52	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
53	C4	PX	0.00000	0.00000	0.00000	0.00000	0.00000
54	C4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
55	C4	PZ	-0.08024	-0.22400	-0.16130	-0.08844	0.34258
56	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
57	C4	PX	0.00000	0.00000	0.00000	0.00000	0.00000
58	C4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
59	C4	PZ	-0.05219	-0.19200	-0.17043	-0.16732	0.58402
60	C4	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
61	C4	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
62	C4	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
63	C4	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
64	C4	DXZ	0.00756	-0.01753	0.01479	0.02904	0.00401
65	C4	DYZ	0.00778	0.01829	0.00149	-0.00121	0.00332
66	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
67	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
68	C5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
69	C5	PY	0.00000	0.00000	0.00000	0.00000	0.00000
70	C5	PZ	-0.20954	0.09769	-0.18409	-0.19910	-0.20184
71	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
72	C5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
73	C5	PY	0.00000	0.00000	0.00000	0.00000	0.00000
74	C5	PZ	-0.17959	0.10648	-0.25284	-0.41246	-0.40746

75	C5	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
76	C5	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
77	C5	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
78	C5	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
79	C5	DXZ	-0.00191	-0.01026	-0.00887	-0.01403	0.02083
80	C5	DYZ	0.00848	-0.01222	-0.01149	-0.02125	0.00585
81	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
82	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
83	C6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
84	C6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
85	C6	PZ	0.21093	-0.01530	0.17335	-0.12048	0.25817
86	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
87	C6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
88	C6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
89	C6	PZ	0.17581	-0.02564	0.17898	-0.18729	0.46859
90	C6	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
91	C6	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
92	C6	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
93	C6	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
94	C6	DXZ	0.00706	0.00432	-0.00204	-0.02435	-0.00940
95	C6	DYZ	-0.01503	0.02087	0.02387	0.00433	0.00987
96	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
97	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
98	C7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
99	C7	PY	0.00000	0.00000	0.00000	0.00000	0.00000
100	C7	PZ	-0.00309	0.27311	-0.21089	0.09618	0.15049
101	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
102	C7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
103	C7	PY	0.00000	0.00000	0.00000	0.00000	0.00000
104	C7	PZ	-0.00479	0.25381	-0.26918	0.21400	0.31348
105	C7	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
106	C7	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
107	C7	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
108	C7	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
109	C7	DXZ	-0.00125	-0.00977	0.00279	0.00355	0.00334
110	C7	DYZ	0.01474	0.01023	0.00682	-0.01767	-0.01250
111	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
112	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
113	O1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
114	O1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
115	O1	PZ	0.09876	0.16033	0.08997	0.06019	-0.11936
116	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
117	O1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
118	O1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
119	O1	PZ	0.08931	0.15819	0.09326	0.08020	-0.16892
120	O1	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
121	O1	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
122	O1	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
123	O1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
124	O1	DXZ	0.00345	0.00396	0.00526	0.00748	-0.00390
125	O1	DYZ	-0.00001	0.00293	0.00572	0.00300	-0.01615
126	H4	S	0.00000	0.00000	0.00000	0.00000	0.00000
127	H4	S	0.00000	0.00000	0.00000	0.00000	0.00000
128	H4	PX	0.00000	0.00000	0.00000	0.00000	0.00000

129	H4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
130	H4	PZ	-0.00478	0.00240	-0.00617	-0.00811	-0.00938
131	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
132	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
133	N1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
134	N1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	PZ	0.16889	-0.22253	-0.19390	0.00111	-0.18178
136	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
137	N1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
138	N1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
139	N1	PZ	0.15004	-0.20173	-0.21764	0.01862	-0.30439
140	N1	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
141	N1	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
142	N1	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
143	N1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
144	N1	DXZ	0.00175	-0.01066	-0.01315	0.00351	-0.01200
145	N1	DYZ	0.02184	-0.00769	0.00163	-0.00817	0.01206
146	H6	S	0.00000	0.00000	0.00000	0.00000	0.00000
147	H6	S	0.00000	0.00000	0.00000	0.00000	0.00000
148	H6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
149	H6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
150	H6	PZ	-0.00259	0.00424	0.00436	0.01246	0.00053
151	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
152	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
153	C8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
154	C8	PY	0.00000	0.00000	0.00000	0.00000	0.00000
155	C8	PZ	-0.24885	-0.03916	-0.08851	0.17224	-0.04798
156	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
157	C8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
158	C8	PY	0.00000	0.00000	0.00000	0.00000	0.00000
159	C8	PZ	-0.19579	-0.04032	-0.13599	0.23399	-0.07956
160	C8	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
161	C8	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
162	C8	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
163	C8	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
164	C8	DXZ	-0.01301	0.01692	0.00655	0.00418	0.02098
165	C8	DYZ	0.02377	0.00932	-0.02649	0.01025	0.00357
166	H8	S	0.00000	0.00000	0.00000	0.00000	0.00000
167	H8	S	0.00000	0.00000	0.00000	0.00000	0.00000
168	H8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
169	H8	PY	0.00000	0.00000	0.00000	0.00000	0.00000
170	H8	PZ	-0.00036	0.00699	-0.00733	0.00449	0.00718
171	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
172	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
173	C10	PX	0.00000	0.00000	0.00000	0.00000	0.00000
174	C10	PY	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	PZ	-0.29828	-0.05634	0.26317	-0.16804	0.03159
176	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
177	C10	PX	0.00000	0.00000	0.00000	0.00000	0.00000
178	C10	PY	0.00000	0.00000	0.00000	0.00000	0.00000
179	C10	PZ	-0.26390	-0.05066	0.37306	-0.30374	0.07443
180	C10	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
181	C10	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
182	C10	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000

183	C10	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
184	C10	DXZ	0.00259	0.00281	0.00098	-0.00145	0.00575
185	C10	DYZ	-0.01893	-0.00256	-0.00244	0.01199	-0.00231
186	H16	S	0.00000	0.00000	0.00000	0.00000	0.00000
187	H16	S	0.00000	0.00000	0.00000	0.00000	0.00000
188	H16	PX	0.00000	0.00000	0.00000	0.00000	0.00000
189	H16	PY	0.00000	0.00000	0.00000	0.00000	0.00000
190	H16	PZ	-0.00710	-0.00102	0.00867	-0.00722	0.00243
191	H18	S	0.00000	0.00000	0.00000	0.00000	0.00000
192	H18	S	0.00000	0.00000	0.00000	0.00000	0.00000
193	H18	PX	0.00000	0.00000	0.00000	0.00000	0.00000
194	H18	PY	0.00000	0.00000	0.00000	0.00000	0.00000
195	H18	PZ	-0.00657	-0.00174	0.00831	-0.00738	0.00055
196	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
197	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
198	C9	PX	0.00000	0.00000	0.00000	0.00000	0.00000
199	C9	PY	0.00000	0.00000	0.00000	0.00000	0.00000
200	C9	PZ	-0.01648	0.00190	-0.00200	-0.02571	-0.04464
201	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
202	C9	PX	0.00000	0.00000	0.00000	0.00000	0.00000
203	C9	PY	0.00000	0.00000	0.00000	0.00000	0.00000
204	C9	PZ	-0.00055	0.03193	0.02738	-0.04912	-0.17572
205	C9	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
206	C9	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
207	C9	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
208	C9	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
209	C9	DXZ	-0.00576	-0.00774	-0.00645	-0.00633	0.00945
210	C9	DYZ	-0.00071	-0.00067	-0.00116	-0.00186	-0.00122
211	H3	S	0.00000	0.00000	0.00000	0.00000	0.00000
212	H3	S	0.00000	0.00000	0.00000	0.00000	0.00000
213	H3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
214	H3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
215	H3	PZ	-0.00042	-0.00017	-0.00028	-0.00055	-0.00123
216	H5	S	0.01770	0.01653	0.01498	0.01802	-0.02033
217	H5	S	0.02831	0.06204	0.04534	-0.04716	-0.21259
218	H5	PX	-0.00021	-0.00045	0.00015	0.00114	-0.00006
219	H5	PY	0.00030	-0.00061	0.00063	0.00191	0.00027
220	H5	PZ	0.00037	0.00051	0.00015	-0.00062	-0.00042
221	H7	S	-0.01770	-0.01653	-0.01498	-0.01802	0.02033
222	H7	S	-0.02831	-0.06204	-0.04534	0.04716	0.21259
223	H7	PX	0.00021	0.00045	-0.00015	-0.00114	0.00006
224	H7	PY	-0.00030	0.00061	-0.00063	-0.00191	-0.00027
225	H7	PZ	0.00037	0.00051	0.00015	-0.00062	-0.00042

MO:	46	47	48	49	50
Eigenvalues:	0.24034	0.26187	0.27027	0.28712	0.28819
(ev):	6.53990	7.12597	7.35443	7.81290	7.84201

		A	A	A	A	A	
1	H1	S	-0.00619	0.03893	0.02832	0.00000	-0.03004
2	H1	S	1.08684	0.20809	0.66057	0.00000	-0.85845
3	H1	PX	-0.00260	0.00192	-0.00132	0.00000	0.00245
4	H1	PY	0.00254	-0.00148	-0.00673	0.00000	0.00480
5	H1	PZ	0.00000	0.00000	0.00000	0.00401	0.00000

6	C1	S	0.05094	0.01548	0.01412	0.00000	-0.01494
7	C1	S	-0.09647	-0.02132	0.01187	0.00000	-0.01147
8	C1	PX	-0.11575	-0.00380	-0.06031	0.00000	0.09776
9	C1	PY	-0.05439	0.00687	-0.03961	0.00000	0.03417
10	C1	PZ	0.00000	0.00000	0.00000	0.03752	0.00000
11	C1	S	-0.57641	-0.10038	-0.51255	0.00000	0.59910
12	C1	PX	-0.68766	0.03191	-0.27120	0.00000	0.29158
13	C1	PY	-0.20704	-0.17457	-0.28345	0.00000	0.50676
14	C1	PZ	0.00000	0.00000	0.00000	0.20662	0.00000
15	C1	DXX	-0.00170	0.01614	0.01332	0.00000	-0.01069
16	C1	DYY	-0.00101	-0.00600	-0.01096	0.00000	0.00874
17	C1	DZZ	0.00082	-0.00324	0.00234	0.00000	-0.00267
18	C1	DXY	0.00190	0.00092	-0.00032	0.00000	-0.00140
19	C1	DXZ	0.00000	0.00000	0.00000	0.00830	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00573	0.00000
21	C2	S	0.01054	0.04900	0.01417	0.00000	0.01593
22	C2	S	-0.02742	-0.06174	-0.01166	0.00000	-0.01555
23	C2	PX	0.01756	0.13624	0.04484	0.00000	0.09234
24	C2	PY	-0.00273	0.03270	-0.00946	0.00000	0.03848
25	C2	PZ	0.00000	0.00000	0.00000	0.04340	0.00000
26	C2	S	-0.19832	-0.90900	-0.36237	0.00000	-0.32974
27	C2	PX	0.12896	0.53309	0.05994	0.00000	0.40415
28	C2	PY	-0.01499	0.41024	-0.06562	0.00000	0.29295
29	C2	PZ	0.00000	0.00000	0.00000	0.14642	0.00000
30	C2	DXX	0.00150	0.01467	-0.00216	0.00000	0.00623
31	C2	DYY	-0.00118	-0.01093	0.00084	0.00000	-0.00457
32	C2	DZZ	-0.00258	-0.00003	0.00021	0.00000	0.00090
33	C2	DXY	0.00127	0.01071	0.00380	0.00000	0.00547
34	C2	DXZ	0.00000	0.00000	0.00000	-0.00932	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00260	0.00000
36	C3	S	-0.00308	0.02750	0.00517	0.00000	-0.01280
37	C3	S	0.01417	-0.06468	0.00531	0.00000	-0.00644
38	C3	PX	-0.00424	0.02618	-0.01320	0.00000	0.09111
39	C3	PY	0.03231	0.00581	-0.07439	0.00000	0.02315
40	C3	PZ	0.00000	0.00000	0.00000	-0.08611	0.00000
41	C3	S	-0.28257	-0.11029	-0.55799	0.00000	0.79586
42	C3	PX	0.05252	-0.28012	0.17599	0.00000	0.21015
43	C3	PY	0.10233	-0.10052	0.14321	0.00000	-0.02272
44	C3	PZ	0.00000	0.00000	0.00000	-0.30890	0.00000
45	C3	DXX	-0.00139	0.01128	-0.01130	0.00000	0.00919
46	C3	DYY	-0.00402	-0.00749	0.00683	0.00000	-0.00404
47	C3	DZZ	0.00119	-0.00352	-0.00166	0.00000	-0.00170
48	C3	DXY	-0.00875	-0.00978	-0.00137	0.00000	-0.00064
49	C3	DXZ	0.00000	0.00000	0.00000	0.02664	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.00417	0.00000
51	C4	S	-0.00321	0.01247	0.00197	0.00000	0.00625
52	C4	S	-0.02486	-0.01750	0.00909	0.00000	-0.03073
53	C4	PX	-0.00618	0.01113	-0.00306	0.00000	0.02019
54	C4	PY	-0.03216	-0.08070	-0.09100	0.00000	0.06727
55	C4	PZ	0.00000	0.00000	0.00000	-0.01878	0.00000
56	C4	S	0.01515	0.06311	0.04453	0.00000	-0.11309
57	C4	PX	-0.02026	-0.04517	0.07317	0.00000	-0.28361
58	C4	PY	0.30425	-0.08013	-0.10468	0.00000	0.19724
59	C4	PZ	0.00000	0.00000	0.00000	-0.11812	0.00000

60	C4	DXX	-0.01474	-0.00938	-0.01108	0.00000	0.00934
61	C4	DYY	0.01511	0.02505	0.02022	0.00000	-0.00988
62	C4	DZZ	-0.00253	-0.00586	-0.00427	0.00000	0.00139
63	C4	DXY	0.00924	0.01180	0.00252	0.00000	0.00850
64	C4	DXZ	0.00000	0.00000	0.00000	0.00409	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00287	0.00000
66	C5	S	0.01515	0.04388	0.01875	0.00000	0.01638
67	C5	S	-0.02142	-0.04567	-0.02363	0.00000	0.00073
68	C5	PX	0.00917	0.11400	0.02734	0.00000	0.09577
69	C5	PY	-0.02867	-0.09987	-0.06392	0.00000	-0.04198
70	C5	PZ	0.00000	0.00000	0.00000	0.01654	0.00000
71	C5	S	-0.17293	-1.00320	-0.20067	0.00000	-0.69296
72	C5	PX	0.04067	0.30822	0.09382	0.00000	0.20899
73	C5	PY	-0.24188	-0.44948	-0.29734	0.00000	-0.20524
74	C5	PZ	0.00000	0.00000	0.00000	-0.02684	0.00000
75	C5	DXX	0.00621	0.00432	0.00769	0.00000	-0.01111
76	C5	DYY	-0.00471	-0.00177	-0.00140	0.00000	0.00290
77	C5	DZZ	0.00111	0.00031	-0.00084	0.00000	0.00392
78	C5	DXY	-0.00911	-0.01916	-0.00988	0.00000	-0.00115
79	C5	DXZ	0.00000	0.00000	0.00000	-0.00585	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.00170	0.00000
81	C6	S	0.00971	0.00361	0.00870	0.00000	-0.00991
82	C6	S	-0.02500	-0.00510	-0.03215	0.00000	0.03227
83	C6	PX	-0.03025	0.03576	-0.03611	0.00000	0.03921
84	C6	PY	-0.00328	0.03687	-0.03602	0.00000	-0.00720
85	C6	PZ	0.00000	0.00000	0.00000	-0.09263	0.00000
86	C6	S	0.02000	-0.03886	0.15318	0.00000	0.10525
87	C6	PX	0.04187	-0.25476	0.03621	0.00000	-0.03187
88	C6	PY	-0.09139	-0.11285	-0.00845	0.00000	-0.14376
89	C6	PZ	0.00000	0.00000	0.00000	-0.26219	0.00000
90	C6	DXX	-0.00279	-0.01897	0.00864	0.00000	-0.01259
91	C6	DYY	0.00744	0.02347	-0.00077	0.00000	0.01290
92	C6	DZZ	-0.00213	-0.00172	-0.00414	0.00000	0.00200
93	C6	DXY	0.00555	-0.00015	-0.00057	0.00000	-0.00521
94	C6	DXZ	0.00000	0.00000	0.00000	-0.01943	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.02113	0.00000
96	C7	S	-0.00025	-0.02390	0.04688	0.00000	-0.00671
97	C7	S	-0.00581	0.04419	-0.06732	0.00000	0.00865
98	C7	PX	-0.01761	0.05800	-0.18041	0.00000	0.07349
99	C7	PY	0.01734	0.02943	0.02840	0.00000	0.01052
100	C7	PZ	0.00000	0.00000	0.00000	0.21306	0.00000
101	C7	S	0.05476	0.26039	-0.70134	0.00000	0.07176
102	C7	PX	-0.15135	0.49960	-1.07502	0.00000	0.42282
103	C7	PY	0.15457	0.31217	0.12646	0.00000	-0.43524
104	C7	PZ	0.00000	0.00000	0.00000	0.62851	0.00000
105	C7	DXX	-0.00207	-0.00375	0.00321	0.00000	-0.01455
106	C7	DYY	0.00087	0.00053	-0.00004	0.00000	0.00978
107	C7	DZZ	-0.00044	0.00051	-0.00032	0.00000	0.00062
108	C7	DXY	0.00186	0.00469	-0.00258	0.00000	-0.00187
109	C7	DXZ	0.00000	0.00000	0.00000	0.02366	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.01682	0.00000
111	O1	S	-0.00429	-0.02637	-0.03259	0.00000	0.03394
112	O1	S	0.00399	0.04905	0.05186	0.00000	-0.04810
113	O1	PX	0.04676	0.03350	0.05065	0.00000	-0.06171

114	O1	PY	-0.02972	-0.06217	-0.04713	0.00000	0.01427
115	O1	PZ	0.00000	0.00000	0.00000	0.01926	0.00000
116	O1	S	-0.00273	0.27781	0.39420	0.00000	-0.47112
117	O1	PX	0.15852	0.07491	0.12333	0.00000	-0.15826
118	O1	PY	0.09908	-0.03163	-0.03626	0.00000	0.04233
119	O1	PZ	0.00000	0.00000	0.00000	0.06273	0.00000
120	O1	DXX	-0.00217	0.00333	-0.00079	0.00000	0.00550
121	O1	DYY	-0.01146	-0.01183	-0.01108	0.00000	0.00523
122	O1	DZZ	0.00134	-0.00646	-0.00975	0.00000	0.01049
123	O1	DXY	-0.00596	-0.00477	0.00132	0.00000	-0.01016
124	O1	DXZ	0.00000	0.00000	0.00000	0.00178	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.00172	0.00000
126	H4	S	0.02096	0.04489	0.02851	0.00000	-0.00783
127	H4	S	0.33185	1.18998	0.52532	0.00000	0.60583
128	H4	PX	-0.00087	0.00049	-0.00219	0.00000	0.00585
129	H4	PY	-0.00111	-0.00283	-0.00144	0.00000	0.00047
130	H4	PZ	0.00000	0.00000	0.00000	0.00116	0.00000
131	N1	S	-0.00046	-0.01114	0.01356	0.00000	-0.00210
132	N1	S	0.01018	0.04777	-0.05357	0.00000	0.02579
133	N1	PX	-0.00043	0.01307	-0.03989	0.00000	0.07087
134	N1	PY	0.02334	0.02993	0.03395	0.00000	0.02181
135	N1	PZ	0.00000	0.00000	0.00000	0.24798	0.00000
136	N1	S	-0.04520	-0.10487	0.08509	0.00000	-0.17155
137	N1	PX	-0.00809	0.00664	0.01086	0.00000	0.04287
138	N1	PY	0.00191	-0.04749	-0.01644	0.00000	-0.05721
139	N1	PZ	0.00000	0.00000	0.00000	0.50593	0.00000
140	N1	DXX	0.00441	0.00517	0.00071	0.00000	-0.00356
141	N1	DYY	-0.00218	-0.00750	-0.00241	0.00000	0.00386
142	N1	DZZ	0.00215	0.00661	-0.00728	0.00000	0.00439
143	N1	DXY	-0.00225	0.00508	-0.00421	0.00000	0.00798
144	N1	DXZ	0.00000	0.00000	0.00000	-0.01260	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.01121	0.00000
146	H6	S	0.00610	0.04324	-0.00559	0.00000	0.02550
147	H6	S	0.22392	1.22351	0.24505	0.00000	0.74365
148	H6	PX	0.00081	0.00260	0.00089	0.00000	0.00162
149	H6	PY	0.00096	0.00003	-0.00013	0.00000	0.00066
150	H6	PZ	0.00000	0.00000	0.00000	0.00306	0.00000
151	C8	S	-0.00745	-0.00367	-0.01191	0.00000	0.01143
152	C8	S	0.01386	-0.01272	0.03365	0.00000	-0.01122
153	C8	PX	-0.00159	0.02899	-0.02810	0.00000	0.03565
154	C8	PY	0.01770	0.01968	0.00538	0.00000	-0.05602
155	C8	PZ	0.00000	0.00000	0.00000	-0.39579	0.00000
156	C8	S	0.13811	0.39890	-0.28415	0.00000	-0.34031
157	C8	PX	0.06333	0.08820	0.21986	0.00000	-0.17930
158	C8	PY	-0.08972	0.24413	-0.21555	0.00000	0.07315
159	C8	PZ	0.00000	0.00000	0.00000	-0.87698	0.00000
160	C8	DXX	-0.00168	0.00249	-0.01443	0.00000	0.01473
161	C8	DYY	0.00157	0.00330	0.00655	0.00000	-0.01119
162	C8	DZZ	0.00061	-0.00142	0.00087	0.00000	-0.00134
163	C8	DXY	-0.00082	-0.00445	0.00515	0.00000	-0.00779
164	C8	DXZ	0.00000	0.00000	0.00000	-0.00292	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	-0.00217	0.00000
166	H8	S	-0.00913	-0.00938	-0.00870	0.00000	-0.03141
167	H8	S	0.13767	-0.63734	1.55074	0.00000	-0.59359

168	H8	PX	-0.00115	0.00224	-0.00654	0.00000	-0.00023
169	H8	PY	0.00156	0.00261	-0.00141	0.00000	-0.00311
170	H8	PZ	0.00000	0.00000	0.00000	0.01426	0.00000
171	C10	S	-0.00350	-0.04121	0.05811	0.00000	0.07719
172	C10	S	0.00971	0.04891	-0.05729	0.00000	-0.09223
173	C10	PX	0.00321	0.06129	-0.10503	0.00000	0.00463
174	C10	PY	-0.00804	-0.05219	0.09314	0.00000	0.12911
175	C10	PZ	0.00000	0.00000	0.00000	0.15426	0.00000
176	C10	S	-0.04562	0.74536	-1.14521	0.00000	-1.11468
177	C10	PX	0.01985	0.20569	-0.47057	0.00000	0.14040
178	C10	PY	-0.09823	-0.25327	0.33936	0.00000	0.63849
179	C10	PZ	0.00000	0.00000	0.00000	0.60369	0.00000
180	C10	DXX	-0.00082	-0.00229	0.00197	0.00000	0.00447
181	C10	DYY	-0.00113	-0.00063	-0.00107	0.00000	0.00536
182	C10	DZZ	0.00077	-0.00217	0.00519	0.00000	0.00297
183	C10	DXY	-0.00045	0.00030	-0.00226	0.00000	0.00714
184	C10	DXZ	0.00000	0.00000	0.00000	0.00697	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	-0.02995	0.00000
186	H16	S	-0.00050	-0.00733	0.00825	0.00000	0.00102
187	H16	S	-0.06089	-0.71531	1.19181	0.00000	0.69927
188	H16	PX	-0.00011	0.00091	-0.00209	0.00000	0.00197
189	H16	PY	-0.00020	-0.00296	0.00482	0.00000	0.00340
190	H16	PZ	0.00000	0.00000	0.00000	0.01044	0.00000
191	H18	S	-0.00066	-0.01014	0.01453	0.00000	0.03636
192	H18	S	-0.05236	-0.31846	0.38882	0.00000	1.20170
193	H18	PX	0.00021	0.00054	-0.00034	0.00000	-0.00039
194	H18	PY	0.00017	-0.00159	0.00213	0.00000	0.00234
195	H18	PZ	0.00000	0.00000	0.00000	0.00941	0.00000
196	C9	S	0.12324	-0.02388	-0.01554	0.00000	0.00859
197	C9	S	-0.08691	0.01342	0.01833	0.00000	-0.01893
198	C9	PX	-0.11757	0.08721	0.07042	0.00000	-0.03007
199	C9	PY	-0.03064	0.01990	0.05310	0.00000	-0.11934
200	C9	PZ	0.00000	0.00000	0.00000	-0.04506	0.00000
201	C9	S	-2.21528	0.50303	0.37139	0.00000	-0.25642
202	C9	PX	-0.36198	0.39307	0.38058	0.00000	-0.28991
203	C9	PY	-0.06116	0.00045	0.22787	0.00000	-0.51874
204	C9	PZ	0.00000	0.00000	0.00000	-0.18214	0.00000
205	C9	DXX	0.00477	-0.00394	-0.00013	0.00000	-0.00374
206	C9	DYY	0.01537	0.00003	-0.00028	0.00000	0.00391
207	C9	DZZ	0.00676	-0.00654	-0.00563	0.00000	0.00495
208	C9	DXY	-0.00217	0.00457	0.00352	0.00000	-0.00256
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00129	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.00103	0.00000
211	H3	S	0.01559	0.01435	0.00409	0.00000	0.00932
212	H3	S	0.89048	-0.08429	-0.30514	0.00000	0.67073
213	H3	PX	-0.00236	0.00264	0.00213	0.00000	-0.00169
214	H3	PY	-0.00060	-0.00059	0.00112	0.00000	-0.00195
215	H3	PZ	0.00000	0.00000	0.00000	-0.00083	0.00000
216	H5	S	-0.00331	-0.01623	-0.01326	0.00154	0.01194
217	H5	S	1.05077	-0.42321	-0.29044	-0.19845	0.06697
218	H5	PX	-0.00182	0.00260	0.00292	0.00081	-0.00272
219	H5	PY	-0.00368	0.00107	0.00039	0.00103	-0.00101
220	H5	PZ	0.00269	-0.00005	0.00072	-0.00102	-0.00105
221	H7	S	-0.00331	-0.01623	-0.01326	-0.00154	0.01194

222	H7	S	1.05077	-0.42321	-0.29044	0.19845	0.06697
223	H7	PX	-0.00182	0.00260	0.00292	-0.00081	-0.00272
224	H7	PY	-0.00368	0.00107	0.00039	-0.00103	-0.00101
225	H7	PZ	-0.00269	0.00005	-0.00072	-0.00102	0.00105

MO:		51	52	53	54	55
Eigenvalues:		0.30343	0.31075	0.31495	0.32001	0.32750
(ev):		8.25679	8.45594	8.57019	8.70780	8.91174

		A	A	A	A	A	
1	H1	S	-0.00467	-0.02783	-0.03848	0.00000	-0.04848
2	H1	S	0.26537	-0.75614	0.07471	0.00000	-0.88657
3	H1	PX	-0.00169	0.00070	-0.00318	0.00000	-0.00135
4	H1	PY	-0.00693	-0.00008	0.00147	0.00000	-0.00127
5	H1	PZ	0.00000	0.00000	0.00000	-0.00586	0.00000
6	C1	S	0.00934	-0.02912	0.01226	0.00000	-0.03780
7	C1	S	-0.02252	0.01516	-0.02113	0.00000	0.03436
8	C1	PX	0.00409	0.08723	-0.00936	0.00000	0.08843
9	C1	PY	0.00966	-0.01104	-0.00592	0.00000	0.04089
10	C1	PZ	0.00000	0.00000	0.00000	0.07258	0.00000
11	C1	S	-0.23505	0.59110	-0.22465	0.00000	0.48640
12	C1	PX	-0.03381	0.40995	-0.04719	0.00000	0.45332
13	C1	PY	-0.32498	0.15931	-0.13183	0.00000	0.16536
14	C1	PZ	0.00000	0.00000	0.00000	-0.05990	0.00000
15	C1	DXX	0.00057	-0.00918	-0.01193	0.00000	-0.01437
16	C1	DYY	-0.00766	-0.00295	0.00292	0.00000	0.00662
17	C1	DZZ	0.00062	0.00178	0.00326	0.00000	-0.00262
18	C1	DXY	-0.01070	-0.00156	-0.00209	0.00000	-0.00717
19	C1	DXZ	0.00000	0.00000	0.00000	-0.01150	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00257	0.00000
21	C2	S	-0.00026	0.02448	-0.03172	0.00000	0.04951
22	C2	S	0.00736	-0.02237	0.06933	0.00000	-0.06261
23	C2	PX	-0.00153	0.08678	0.01159	0.00000	0.13473
24	C2	PY	-0.00393	0.05952	0.01382	0.00000	0.00780
25	C2	PZ	0.00000	0.00000	0.00000	0.01158	0.00000
26	C2	S	-0.05539	-0.53634	0.32967	0.00000	-0.71272
27	C2	PX	-0.09959	0.46174	-0.36177	0.00000	0.98315
28	C2	PY	0.08800	0.24381	0.01640	0.00000	-0.05734
29	C2	PZ	0.00000	0.00000	0.00000	0.06748	0.00000
30	C2	DXX	0.00340	-0.00090	0.00220	0.00000	-0.00244
31	C2	DYY	-0.00464	0.00163	-0.00515	0.00000	0.00528
32	C2	DZZ	0.00116	0.00095	0.00270	0.00000	0.00253
33	C2	DXY	-0.00362	-0.00032	0.00236	0.00000	0.00130
34	C2	DXZ	0.00000	0.00000	0.00000	0.00015	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	-0.00388	0.00000
36	C3	S	0.01435	-0.00064	-0.00750	0.00000	-0.00037
37	C3	S	-0.01617	-0.02716	0.05087	0.00000	0.00202
38	C3	PX	0.04178	-0.00554	0.01624	0.00000	0.04334
39	C3	PY	-0.01582	0.00047	-0.00541	0.00000	-0.02191
40	C3	PZ	0.00000	0.00000	0.00000	-0.05935	0.00000
41	C3	S	-0.30941	0.34857	-0.67024	0.00000	-0.02177
42	C3	PX	0.18064	-0.30051	0.14735	0.00000	0.08548
43	C3	PY	-0.17161	-0.01655	0.38559	0.00000	0.08671
44	C3	PZ	0.00000	0.00000	0.00000	-0.06076	0.00000

45	C3	DXX	0.00901	-0.00131	-0.00413	0.00000	0.00297
46	C3	DYY	-0.01219	0.00758	-0.00455	0.00000	-0.00208
47	C3	DZZ	0.00061	-0.00256	0.00288	0.00000	-0.00122
48	C3	DXY	0.00112	0.00646	0.00936	0.00000	0.00985
49	C3	DXZ	0.00000	0.00000	0.00000	0.00318	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00303	0.00000
51	C4	S	-0.03384	-0.01300	-0.02054	0.00000	0.02250
52	C4	S	0.03910	-0.02604	0.02652	0.00000	-0.05333
53	C4	PX	0.00642	-0.00674	-0.00297	0.00000	0.08417
54	C4	PY	0.00218	0.09694	0.06546	0.00000	0.02855
55	C4	PZ	0.00000	0.00000	0.00000	0.10029	0.00000
56	C4	S	0.43241	0.32887	0.12399	0.00000	0.07629
57	C4	PX	0.22837	-0.13579	0.21081	0.00000	0.04347
58	C4	PY	0.01798	0.20112	0.37996	0.00000	-0.12481
59	C4	PZ	0.00000	0.00000	0.00000	0.15399	0.00000
60	C4	DXX	-0.00989	-0.00237	-0.00138	0.00000	0.01684
61	C4	DYY	-0.00533	-0.01013	-0.00452	0.00000	-0.01172
62	C4	DZZ	0.00110	0.00153	0.00513	0.00000	-0.00217
63	C4	DXY	-0.00582	-0.00147	-0.00844	0.00000	0.00681
64	C4	DXZ	0.00000	0.00000	0.00000	0.00505	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.01407	0.00000
66	C5	S	0.01232	0.01145	0.04184	0.00000	-0.06736
67	C5	S	-0.03371	-0.00149	-0.06707	0.00000	0.09619
68	C5	PX	-0.03056	0.02801	0.03270	0.00000	-0.00781
69	C5	PY	0.01192	-0.05532	-0.06175	0.00000	0.07594
70	C5	PZ	0.00000	0.00000	0.00000	-0.03169	0.00000
71	C5	S	-0.03587	-0.45718	-0.42662	0.00000	0.88318
72	C5	PX	-0.00667	-0.01465	0.52124	0.00000	-0.58837
73	C5	PY	0.00485	-0.19843	-0.25667	0.00000	0.41663
74	C5	PZ	0.00000	0.00000	0.00000	-0.10713	0.00000
75	C5	DXX	0.00533	-0.00771	-0.00614	0.00000	-0.00815
76	C5	DYY	-0.00258	0.00277	0.00767	0.00000	0.00146
77	C5	DZZ	-0.00193	0.00227	0.00029	0.00000	0.00060
78	C5	DXY	0.00180	0.00445	0.00963	0.00000	-0.01144
79	C5	DXZ	0.00000	0.00000	0.00000	0.00580	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.00133	0.00000
81	C6	S	-0.01848	-0.00044	0.01543	0.00000	-0.00319
82	C6	S	0.02313	0.01973	-0.04779	0.00000	0.00813
83	C6	PX	0.04501	-0.01932	0.02959	0.00000	0.02071
84	C6	PY	0.03354	0.00360	0.01761	0.00000	0.05130
85	C6	PZ	0.00000	0.00000	0.00000	0.00305	0.00000
86	C6	S	0.38781	-0.19904	0.24991	0.00000	-0.23927
87	C6	PX	0.12346	-0.33843	0.17007	0.00000	0.10678
88	C6	PY	0.14168	-0.26389	0.08529	0.00000	-0.17563
89	C6	PZ	0.00000	0.00000	0.00000	-0.01107	0.00000
90	C6	DXX	-0.00408	-0.00355	0.00759	0.00000	-0.00101
91	C6	DYY	0.00699	0.00122	0.00640	0.00000	-0.00325
92	C6	DZZ	0.00086	0.00197	-0.00363	0.00000	0.00083
93	C6	DXY	-0.00596	0.00307	-0.00793	0.00000	-0.00394
94	C6	DXZ	0.00000	0.00000	0.00000	-0.00661	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.00243	0.00000
96	C7	S	0.00235	-0.00525	0.06047	0.00000	0.05456
97	C7	S	-0.02271	0.03303	-0.11854	0.00000	-0.07202
98	C7	PX	0.06397	-0.05109	-0.10726	0.00000	-0.08038

99	C7	PY	0.02991	-0.05293	0.03927	0.00000	0.03554
100	C7	PZ	0.00000	0.00000	0.00000	0.05195	0.00000
101	C7	S	0.08644	-0.18843	-0.48964	0.00000	-0.75765
102	C7	PX	0.30663	-0.09239	-0.99134	0.00000	-0.50232
103	C7	PY	-0.00570	0.02841	0.30980	0.00000	0.09398
104	C7	PZ	0.00000	0.00000	0.00000	0.10915	0.00000
105	C7	DXX	-0.01107	0.00750	0.00345	0.00000	0.00290
106	C7	DYY	0.01232	-0.01089	0.01158	0.00000	0.00665
107	C7	DZZ	-0.00315	0.00386	-0.00745	0.00000	-0.00216
108	C7	DXY	0.00211	-0.00134	0.00264	0.00000	0.00365
109	C7	DXZ	0.00000	0.00000	0.00000	0.00513	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.00230	0.00000
111	O1	S	-0.00086	0.04323	0.07180	0.00000	-0.03196
112	O1	S	0.00775	-0.03756	-0.06026	0.00000	0.02165
113	O1	PX	0.05660	-0.04120	-0.11936	0.00000	0.05243
114	O1	PY	0.01156	-0.00684	-0.01998	0.00000	0.06383
115	O1	PZ	0.00000	0.00000	0.00000	-0.11176	0.00000
116	O1	S	0.00016	-0.67365	-1.13329	0.00000	0.51144
117	O1	PX	0.13016	-0.14289	-0.43076	0.00000	0.21801
118	O1	PY	-0.03764	-0.06522	-0.02882	0.00000	0.10914
119	O1	PZ	0.00000	0.00000	0.00000	-0.29008	0.00000
120	O1	DXX	-0.00375	0.00701	0.02176	0.00000	-0.01341
121	O1	DYY	0.00915	0.02135	0.02772	0.00000	-0.01441
122	O1	DZZ	0.00600	0.02537	0.03568	0.00000	-0.01585
123	O1	DXY	0.00877	-0.00069	-0.00028	0.00000	-0.00535
124	O1	DXZ	0.00000	0.00000	0.00000	0.00169	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.01031	0.00000
126	H4	S	0.00808	-0.01497	-0.01429	0.00000	0.00047
127	H4	S	0.01583	0.33830	0.79367	0.00000	-1.12102
128	H4	PX	-0.00275	0.00349	0.00436	0.00000	-0.00059
129	H4	PY	-0.00229	-0.00017	0.00017	0.00000	0.00449
130	H4	PZ	0.00000	0.00000	0.00000	-0.00253	0.00000
131	N1	S	-0.00973	0.01555	-0.01570	0.00000	0.00294
132	N1	S	0.03566	-0.04092	0.02702	0.00000	-0.01034
133	N1	PX	0.05896	-0.06785	-0.01109	0.00000	0.00871
134	N1	PY	-0.02658	0.03072	-0.02390	0.00000	-0.02068
135	N1	PZ	0.00000	0.00000	0.00000	0.01752	0.00000
136	N1	S	-0.01286	-0.12631	0.19796	0.00000	-0.10162
137	N1	PX	0.00915	0.01884	0.01370	0.00000	-0.09563
138	N1	PY	-0.05007	-0.06565	-0.02393	0.00000	-0.01046
139	N1	PZ	0.00000	0.00000	0.00000	0.04109	0.00000
140	N1	DXX	-0.00286	0.00406	0.00561	0.00000	0.00276
141	N1	DYY	-0.00239	0.00007	-0.01382	0.00000	-0.01037
142	N1	DZZ	0.00557	-0.00271	0.00028	0.00000	-0.00055
143	N1	DXY	0.00880	-0.00788	0.00708	0.00000	0.00425
144	N1	DXZ	0.00000	0.00000	0.00000	-0.00284	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00254	0.00000
146	H6	S	0.00340	-0.00459	-0.00915	0.00000	0.01186
147	H6	S	-0.03265	0.79117	-0.43356	0.00000	1.36405
148	H6	PX	-0.00064	0.00277	-0.00202	0.00000	0.00460
149	H6	PY	0.00165	0.00091	-0.00055	0.00000	0.00001
150	H6	PZ	0.00000	0.00000	0.00000	0.00067	0.00000
151	C8	S	0.00182	-0.00246	-0.00834	0.00000	-0.01252
152	C8	S	-0.01423	0.01081	0.01809	0.00000	0.02019

153	C8	PX	0.08544	-0.08901	0.08547	0.00000	0.03502
154	C8	PY	-0.00543	-0.00168	0.07590	0.00000	0.06448
155	C8	PZ	0.00000	0.00000	0.00000	-0.04664	0.00000
156	C8	S	0.07929	-0.03710	-0.04664	0.00000	0.10893
157	C8	PX	-0.10378	0.23776	0.09784	0.00000	-0.04646
158	C8	PY	0.01019	0.12725	-0.22820	0.00000	0.02148
159	C8	PZ	0.00000	0.00000	0.00000	-0.10522	0.00000
160	C8	DXX	0.01542	-0.01720	-0.00304	0.00000	-0.00032
161	C8	DYY	-0.01049	0.01164	-0.00110	0.00000	-0.00004
162	C8	DZZ	-0.00277	0.00280	0.00085	0.00000	0.00091
163	C8	DXY	-0.01520	0.02117	-0.01865	0.00000	-0.01425
164	C8	DXZ	0.00000	0.00000	0.00000	0.00245	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00115	0.00000
166	H8	S	-0.03123	0.02199	0.01337	0.00000	0.02118
167	H8	S	-0.41093	0.22138	1.41897	0.00000	1.01991
168	H8	PX	0.00016	-0.00039	-0.00199	0.00000	-0.00045
169	H8	PY	0.00249	-0.00429	0.00359	0.00000	0.00224
170	H8	PZ	0.00000	0.00000	0.00000	0.00371	0.00000
171	C10	S	0.03012	-0.02285	-0.03237	0.00000	-0.02018
172	C10	S	-0.03611	0.02612	0.03770	0.00000	0.01914
173	C10	PX	0.13513	-0.18803	0.13826	0.00000	0.09905
174	C10	PY	0.07012	-0.07205	-0.02233	0.00000	-0.01424
175	C10	PZ	0.00000	0.00000	0.00000	0.01260	0.00000
176	C10	S	-0.47744	0.43288	0.34659	0.00000	0.31635
177	C10	PX	0.69617	-1.00561	0.69341	0.00000	0.50356
178	C10	PY	0.31519	-0.30749	-0.08371	0.00000	0.01305
179	C10	PZ	0.00000	0.00000	0.00000	0.06870	0.00000
180	C10	DXX	-0.00074	0.00219	-0.00757	0.00000	-0.00538
181	C10	DYY	0.00344	-0.00337	0.00022	0.00000	-0.00017
182	C10	DZZ	0.00084	-0.00066	-0.00067	0.00000	-0.00011
183	C10	DXY	0.00920	-0.01107	0.00919	0.00000	0.00604
184	C10	DXZ	0.00000	0.00000	0.00000	0.00146	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	-0.00368	0.00000
186	H16	S	-0.01216	0.01750	-0.03625	0.00000	-0.02501
187	H16	S	-0.44276	0.81765	-1.08089	0.00000	-0.74860
188	H16	PX	0.00277	-0.00346	0.00088	0.00000	0.00063
189	H16	PY	0.00122	-0.00128	0.00142	0.00000	0.00125
190	H16	PZ	0.00000	0.00000	0.00000	0.00119	0.00000
191	H18	S	0.02726	-0.02938	0.01932	0.00000	0.01237
192	H18	S	1.14026	-1.35200	0.36500	0.00000	0.30606
193	H18	PX	0.00183	-0.00289	0.00387	0.00000	0.00293
194	H18	PY	0.00172	-0.00196	0.00012	0.00000	-0.00029
195	H18	PZ	0.00000	0.00000	0.00000	0.00088	0.00000
196	C9	S	-0.00252	-0.01053	-0.04933	0.00000	0.05010
197	C9	S	0.01139	0.00573	0.04870	0.00000	-0.05856
198	C9	PX	-0.09592	-0.13991	-0.10398	0.00000	0.07226
199	C9	PY	0.25929	0.10619	-0.08105	0.00000	0.00093
200	C9	PZ	0.00000	0.00000	0.00000	0.35397	0.00000
201	C9	S	0.10505	0.11501	0.78685	0.00000	-0.85523
202	C9	PX	-0.37029	-0.81416	-0.69389	0.00000	0.30449
203	C9	PY	1.17120	0.49082	-0.34613	0.00000	0.11343
204	C9	PZ	0.00000	0.00000	0.00000	1.49800	0.00000
205	C9	DXX	0.00455	-0.00129	-0.00372	0.00000	0.00368
206	C9	DYY	-0.00809	-0.00284	0.00802	0.00000	-0.00863

207	C9	DZZ	0.00441	0.01198	0.00994	0.00000	-0.00130
208	C9	DXY	0.00431	0.00034	-0.00859	0.00000	0.00699
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00090	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00821	0.00000
211	H3	S	-0.04890	-0.03196	0.02027	0.00000	-0.03633
212	H3	S	-1.65992	-0.93690	-0.09336	0.00000	0.33069
213	H3	PX	0.00073	-0.00173	-0.00502	0.00000	0.00323
214	H3	PY	0.00587	0.00390	0.00150	0.00000	-0.00055
215	H3	PZ	0.00000	0.00000	0.00000	0.00886	0.00000
216	H5	S	0.01780	0.03698	0.02573	0.03442	0.00253
217	H5	S	0.64376	0.62127	-0.11680	1.65672	0.25596
218	H5	PX	-0.00230	-0.00594	-0.00329	-0.00149	0.00025
219	H5	PY	0.00471	0.00310	-0.00433	-0.00294	0.00463
220	H5	PZ	-0.00005	-0.00189	-0.00183	0.00625	0.00028
221	H7	S	0.01780	0.03698	0.02573	-0.03442	0.00253
222	H7	S	0.64376	0.62127	-0.11680	-1.65672	0.25596
223	H7	PX	-0.00230	-0.00594	-0.00329	0.00149	0.00025
224	H7	PY	0.00471	0.00310	-0.00433	0.00294	0.00463
225	H7	PZ	0.00005	0.00189	0.00183	0.00625	-0.00028

MO:	56	57	58	59	60
Eigenvalues:	0.34257	0.38340	0.40188	0.43117	0.43713
(ev):	9.32173	10.43278	10.93575	11.73272	11.89486

		A	A	A	A	A	
1	H1	S	0.00671	0.00000	-0.06753	0.05645	0.05346
2	H1	S	-1.28388	0.00000	-0.55255	-0.27599	-0.72249
3	H1	PX	0.00563	0.00000	-0.00152	0.00879	0.00623
4	H1	PY	-0.00244	0.00000	-0.00544	-0.00791	0.00193
5	H1	PZ	0.00000	-0.01587	0.00000	0.00000	0.00000
6	C1	S	-0.04912	0.00000	0.01491	-0.02798	-0.04996
7	C1	S	0.07957	0.00000	-0.05400	0.06888	0.01839
8	C1	PX	0.14604	0.00000	0.08031	0.00672	0.03089
9	C1	PY	-0.01368	0.00000	0.02674	-0.12945	-0.03671
10	C1	PZ	0.00000	-0.20358	0.00000	0.00000	0.00000
11	C1	S	0.76353	0.00000	-0.23067	0.46137	1.22731
12	C1	PX	0.73712	0.00000	0.96305	0.22601	0.39842
13	C1	PY	0.29545	0.00000	-1.15381	0.14930	-0.05196
14	C1	PZ	0.00000	-0.66158	0.00000	0.00000	0.00000
15	C1	DXX	0.01065	0.00000	-0.01233	0.02607	0.02156
16	C1	DYY	-0.01190	0.00000	0.00200	-0.02922	-0.02132
17	C1	DZZ	0.00329	0.00000	-0.00113	0.00767	-0.00294
18	C1	DXY	-0.00061	0.00000	-0.02379	0.00366	0.01742
19	C1	DXZ	0.00000	-0.02089	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.00947	0.00000	0.00000	0.00000
21	C2	S	-0.05195	0.00000	0.01755	0.03906	0.03134
22	C2	S	0.08340	0.00000	-0.01232	-0.00821	-0.04726
23	C2	PX	-0.06179	0.00000	-0.08988	-0.00287	-0.06792
24	C2	PY	-0.07166	0.00000	0.05338	-0.00449	0.01292
25	C2	PZ	0.00000	0.19839	0.00000	0.00000	0.00000
26	C2	S	0.62107	0.00000	-0.40399	-1.28135	-0.72267
27	C2	PX	-0.84029	0.00000	-0.68359	-0.11847	-0.07342
28	C2	PY	-0.28830	0.00000	0.78303	0.88753	-0.77940
29	C2	PZ	0.00000	0.63790	0.00000	0.00000	0.00000

30	C2	DXX	0.00294	0.00000	0.01108	-0.01007	-0.01895
31	C2	DYY	-0.00813	0.00000	-0.01263	0.00541	0.01622
32	C2	DZZ	0.00207	0.00000	0.00065	0.00197	-0.00161
33	C2	DXY	0.01297	0.00000	-0.01994	-0.02940	-0.00841
34	C2	DXZ	0.00000	-0.02006	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	-0.00041	0.00000	0.00000	0.00000
36	C3	S	0.00106	0.00000	0.05599	0.02933	0.03172
37	C3	S	0.00188	0.00000	-0.07774	-0.06614	-0.04750
38	C3	PX	-0.00519	0.00000	0.08758	0.04579	-0.18314
39	C3	PY	-0.09408	0.00000	0.03897	-0.13845	-0.04047
40	C3	PZ	0.00000	0.30802	0.00000	0.00000	0.00000
41	C3	S	0.11315	0.00000	-1.67746	0.77700	-0.95378
42	C3	PX	-0.01997	0.00000	-0.29406	0.39121	-1.12370
43	C3	PY	0.11382	0.00000	-0.25585	-0.62175	0.12388
44	C3	PZ	0.00000	0.74766	0.00000	0.00000	0.00000
45	C3	DXX	-0.00882	0.00000	0.02978	-0.01015	-0.01460
46	C3	DYY	0.01422	0.00000	-0.04311	0.03257	0.00523
47	C3	DZZ	-0.00154	0.00000	-0.00125	-0.00718	0.00127
48	C3	DXY	0.01567	0.00000	0.02250	-0.00607	-0.00376
49	C3	DXZ	0.00000	0.01119	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	-0.00559	0.00000	0.00000	0.00000
51	C4	S	0.00914	0.00000	-0.07733	-0.04883	0.01756
52	C4	S	-0.01604	0.00000	0.08618	0.05212	-0.02875
53	C4	PX	-0.03951	0.00000	-0.02449	-0.22215	-0.13135
54	C4	PY	-0.05360	0.00000	-0.04395	-0.09802	-0.06614
55	C4	PZ	0.00000	0.26738	0.00000	0.00000	0.00000
56	C4	S	-0.16725	0.00000	1.99205	1.21439	0.07907
57	C4	PX	-0.06087	0.00000	0.53103	-1.27733	-0.62829
58	C4	PY	-0.02999	0.00000	-0.25431	-0.91970	-0.11918
59	C4	PZ	0.00000	0.59937	0.00000	0.00000	0.00000
60	C4	DXX	-0.00461	0.00000	0.00746	-0.01099	-0.01549
61	C4	DYY	0.00267	0.00000	-0.00877	0.01029	0.02216
62	C4	DZZ	-0.00172	0.00000	0.00727	0.00077	-0.00181
63	C4	DXY	0.00688	0.00000	-0.00746	-0.01086	-0.00262
64	C4	DXZ	0.00000	-0.00226	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00637	0.00000	0.00000	0.00000
66	C5	S	0.03401	0.00000	0.03687	0.04961	-0.00701
67	C5	S	-0.03326	0.00000	-0.05860	-0.01115	0.00367
68	C5	PX	0.14521	0.00000	-0.04954	-0.14403	-0.05725
69	C5	PY	-0.06413	0.00000	0.03626	0.01079	-0.09407
70	C5	PZ	0.00000	-0.19154	0.00000	0.00000	0.00000
71	C5	S	-0.57219	0.00000	-0.67258	-1.64646	0.35518
72	C5	PX	0.80142	0.00000	-0.07837	-1.34242	-0.47419
73	C5	PY	-0.62623	0.00000	0.09741	-0.17276	-0.93968
74	C5	PZ	0.00000	-0.58587	0.00000	0.00000	0.00000
75	C5	DXX	0.00190	0.00000	0.01269	0.02130	0.01170
76	C5	DYY	0.00148	0.00000	-0.01571	-0.02055	-0.00644
77	C5	DZZ	0.00295	0.00000	-0.00182	-0.00112	-0.00431
78	C5	DXY	0.00142	0.00000	0.01732	0.01103	0.00505
79	C5	DXZ	0.00000	0.01055	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	-0.01070	0.00000	0.00000	0.00000
81	C6	S	0.01809	0.00000	-0.08186	-0.05079	0.00542
82	C6	S	-0.02540	0.00000	0.10008	0.09287	-0.05341
83	C6	PX	0.06516	0.00000	0.08743	-0.13896	-0.10589

84	C6	PY	-0.06050	0.00000	0.15878	0.03885	-0.02965
85	C6	PZ	0.00000	-0.32688	0.00000	0.00000	0.00000
86	C6	S	-0.04536	0.00000	1.45262	1.08715	-0.34145
87	C6	PX	0.11487	0.00000	-0.28276	-0.93680	-0.07443
88	C6	PY	0.11467	0.00000	0.53157	0.52225	-0.60720
89	C6	PZ	0.00000	-0.72723	0.00000	0.00000	0.00000
90	C6	DXX	0.01329	0.00000	-0.01263	0.00711	0.01046
91	C6	DYY	-0.00565	0.00000	0.00477	-0.00516	-0.02271
92	C6	DZZ	-0.00104	0.00000	0.00863	0.00780	-0.00148
93	C6	DXY	-0.01567	0.00000	-0.00110	-0.01700	0.01425
94	C6	DXZ	0.00000	0.00384	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00379	0.00000	0.00000	0.00000
96	C7	S	0.00326	0.00000	0.02851	-0.02471	-0.01947
97	C7	S	-0.02107	0.00000	-0.06004	0.06616	0.00674
98	C7	PX	-0.02851	0.00000	0.03834	-0.09123	0.02876
99	C7	PY	-0.02239	0.00000	-0.02232	-0.00335	0.06833
100	C7	PZ	0.00000	-0.05969	0.00000	0.00000	0.00000
101	C7	S	0.18263	0.00000	-0.52008	-0.28196	1.10671
102	C7	PX	-0.31697	0.00000	0.18825	0.02676	0.03522
103	C7	PY	-0.34842	0.00000	1.32622	-1.09910	0.87839
104	C7	PZ	0.00000	-0.40822	0.00000	0.00000	0.00000
105	C7	DXX	0.01254	0.00000	-0.01767	0.00133	0.03343
106	C7	DYY	-0.00138	0.00000	0.01871	-0.00615	-0.02646
107	C7	DZZ	-0.00486	0.00000	-0.00448	0.00257	0.00123
108	C7	DXY	-0.00920	0.00000	0.01925	-0.01009	0.00369
109	C7	DXZ	0.00000	-0.01291	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.02592	0.00000	0.00000	0.00000
111	O1	S	-0.04524	0.00000	0.01174	-0.00555	-0.00582
112	O1	S	0.01644	0.00000	-0.01792	0.00597	0.05016
113	O1	PX	0.14406	0.00000	0.02813	-0.04134	-0.03071
114	O1	PY	0.01949	0.00000	0.09940	-0.06224	-0.10969
115	O1	PZ	0.00000	-0.07103	0.00000	0.00000	0.00000
116	O1	S	0.77098	0.00000	-0.16646	0.17573	-0.09420
117	O1	PX	0.38082	0.00000	0.03091	0.01353	-0.07577
118	O1	PY	0.10125	0.00000	0.27858	-0.24517	-0.23644
119	O1	PZ	0.00000	-0.15183	0.00000	0.00000	0.00000
120	O1	DXX	-0.01385	0.00000	0.00102	-0.00569	0.00629
121	O1	DYY	-0.03491	0.00000	-0.00283	0.00887	0.00612
122	O1	DZZ	-0.02873	0.00000	0.00621	0.00006	0.01445
123	O1	DXY	-0.00291	0.00000	0.00560	0.00849	-0.00068
124	O1	DXZ	0.00000	-0.00313	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	-0.01517	0.00000	0.00000	0.00000
126	H4	S	0.01979	0.00000	-0.03718	-0.02317	-0.00355
127	H4	S	1.38695	0.00000	0.04545	-0.38728	0.23054
128	H4	PX	0.00284	0.00000	-0.00564	-0.00977	-0.00094
129	H4	PY	-0.00326	0.00000	-0.01005	-0.01152	-0.00251
130	H4	PZ	0.00000	-0.01287	0.00000	0.00000	0.00000
131	N1	S	-0.01102	0.00000	-0.00166	0.00739	0.07571
132	N1	S	0.01059	0.00000	-0.03733	-0.00941	-0.09495
133	N1	PX	-0.00351	0.00000	-0.09141	0.05364	-0.10242
134	N1	PY	-0.03362	0.00000	-0.04220	-0.06118	0.03703
135	N1	PZ	0.00000	0.13848	0.00000	0.00000	0.00000
136	N1	S	0.20157	0.00000	0.40943	-0.17547	-1.53284
137	N1	PX	0.06822	0.00000	0.14894	0.23102	-0.67484

138	N1	PY	-0.00410	0.00000	-0.22641	-0.26196	0.17441
139	N1	PZ	0.00000	0.36123	0.00000	0.00000	0.00000
140	N1	DXX	-0.00223	0.00000	-0.00489	-0.00549	0.00849
141	N1	DYY	0.00183	0.00000	-0.01437	0.00949	0.00282
142	N1	DZZ	-0.00404	0.00000	0.00037	0.00068	0.01678
143	N1	DXY	0.00696	0.00000	0.00240	-0.00174	-0.01156
144	N1	DXZ	0.00000	0.00559	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	-0.02108	0.00000	0.00000	0.00000
146	H6	S	0.00555	0.00000	-0.00226	-0.06253	-0.06302
147	H6	S	-1.20794	0.00000	-0.30437	0.39887	-0.18278
148	H6	PX	-0.00395	0.00000	-0.00339	0.00267	0.00425
149	H6	PY	-0.00411	0.00000	0.00925	0.01221	-0.00095
150	H6	PZ	0.00000	0.01433	0.00000	0.00000	0.00000
151	C8	S	0.03307	0.00000	-0.06385	0.07109	-0.08020
152	C8	S	-0.03017	0.00000	0.03498	-0.07064	0.05562
153	C8	PX	0.00612	0.00000	0.14223	-0.07633	-0.14756
154	C8	PY	-0.02278	0.00000	0.04779	-0.00746	-0.01862
155	C8	PZ	0.00000	0.00183	0.00000	0.00000	0.00000
156	C8	S	-0.84729	0.00000	1.80359	-2.42556	2.50362
157	C8	PX	-0.19895	0.00000	1.24924	-0.74681	-0.82917
158	C8	PY	-0.04479	0.00000	-0.09370	0.93923	-0.56754
159	C8	PZ	0.00000	0.01225	0.00000	0.00000	0.00000
160	C8	DXX	-0.00121	0.00000	-0.01094	0.00486	-0.01782
161	C8	DYY	-0.00040	0.00000	0.00450	-0.01902	0.02921
162	C8	DZZ	0.00022	0.00000	-0.00150	-0.00109	0.00438
163	C8	DXY	-0.00413	0.00000	0.01397	0.00771	-0.00370
164	C8	DXZ	0.00000	-0.02041	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	-0.00471	0.00000	0.00000	0.00000
166	H8	S	0.03269	0.00000	-0.05806	-0.00471	0.10550
167	H8	S	0.27638	0.00000	0.05962	0.03589	-0.22852
168	H8	PX	0.00256	0.00000	-0.00382	-0.00022	0.00897
169	H8	PY	-0.00361	0.00000	0.00536	-0.00411	0.00659
170	H8	PZ	0.00000	-0.00744	0.00000	0.00000	0.00000
171	C10	S	-0.02545	0.00000	0.02968	-0.04443	0.04449
172	C10	S	0.01653	0.00000	-0.00211	-0.03220	0.01769
173	C10	PX	0.00878	0.00000	-0.05248	0.04258	0.11738
174	C10	PY	-0.01191	0.00000	-0.02170	-0.02955	0.09225
175	C10	PZ	0.00000	0.00777	0.00000	0.00000	0.00000
176	C10	S	0.54677	0.00000	-0.98231	1.87753	-1.46032
177	C10	PX	0.10742	0.00000	-0.65684	0.14316	0.97466
178	C10	PY	0.17769	0.00000	-0.82302	1.30135	-0.75803
179	C10	PZ	0.00000	-0.00267	0.00000	0.00000	0.00000
180	C10	DXX	0.00100	0.00000	-0.00952	0.01535	-0.00282
181	C10	DYY	0.00031	0.00000	0.00398	-0.00082	-0.01286
182	C10	DZZ	-0.00364	0.00000	0.00568	-0.01297	0.01453
183	C10	DXY	0.00267	0.00000	0.00060	-0.00209	-0.03097
184	C10	DXZ	0.00000	-0.00718	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	-0.00160	0.00000	0.00000	0.00000
186	H16	S	-0.00833	0.00000	-0.01359	0.03327	0.05547
187	H16	S	-0.28533	0.00000	0.64343	-0.39870	-0.50793
188	H16	PX	0.00057	0.00000	-0.00465	0.00363	0.00170
189	H16	PY	0.00085	0.00000	-0.00196	0.00381	-0.01337
190	H16	PZ	0.00000	-0.00100	0.00000	0.00000	0.00000
191	H18	S	0.00538	0.00000	-0.01133	0.02033	-0.10435

192	H18	S	-0.07874	0.00000	-0.54740	0.25181	0.81432
193	H18	PX	0.00009	0.00000	0.00015	-0.00189	0.00088
194	H18	PY	0.00071	0.00000	-0.00484	0.00476	0.00495
195	H18	PZ	0.00000	0.00177	0.00000	0.00000	0.00000
196	C9	S	0.06629	0.00000	0.01687	-0.01121	-0.00426
197	C9	S	-0.04674	0.00000	-0.00452	0.02809	0.00447
198	C9	PX	0.06224	0.00000	0.05777	-0.02749	-0.01684
199	C9	PY	0.00726	0.00000	-0.11001	-0.09268	-0.05151
200	C9	PZ	0.00000	-0.00915	0.00000	0.00000	0.00000
201	C9	S	-1.23005	0.00000	-0.41039	-0.02981	-0.01542
202	C9	PX	0.43694	0.00000	0.17282	-0.24373	-0.34350
203	C9	PY	0.33875	0.00000	-0.16857	-0.31072	-0.13551
204	C9	PZ	0.00000	-0.03840	0.00000	0.00000	0.00000
205	C9	DXX	0.00452	0.00000	0.00826	-0.00103	-0.00335
206	C9	DYY	-0.00827	0.00000	-0.01684	-0.01076	-0.00509
207	C9	DZZ	0.00036	0.00000	0.00607	0.00946	0.01096
208	C9	DXY	0.01557	0.00000	0.00384	-0.00547	0.00396
209	C9	DXZ	0.00000	0.00978	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	-0.00135	0.00000	0.00000	0.00000
211	H3	S	-0.05470	0.00000	-0.05837	-0.01757	-0.01443
212	H3	S	0.26943	0.00000	0.49475	0.33937	0.12080
213	H3	PX	0.00488	0.00000	-0.00053	-0.00232	0.00082
214	H3	PY	0.00038	0.00000	-0.00109	-0.00185	0.00060
215	H3	PZ	0.00000	-0.00128	0.00000	0.00000	0.00000
216	H5	S	-0.00018	-0.02425	0.02426	0.03103	0.03121
217	H5	S	0.42355	-0.04936	-0.00432	0.04669	0.15230
218	H5	PX	-0.00119	-0.00174	0.00017	-0.00175	-0.00341
219	H5	PY	0.00677	-0.00140	0.00451	0.00206	0.00376
220	H5	PZ	0.00032	0.00117	0.00030	-0.00016	-0.00210
221	H7	S	-0.00018	0.02425	0.02426	0.03103	0.03121
222	H7	S	0.42355	0.04936	-0.00432	0.04669	0.15230
223	H7	PX	-0.00119	0.00174	0.00017	-0.00175	-0.00341
224	H7	PY	0.00677	0.00140	0.00451	0.00206	0.00376
225	H7	PZ	-0.00032	0.00117	-0.00030	0.00016	0.00210

MO:	61	62	63	64	65
Eigenvalues:	0.47510	0.48296	0.52777	0.54410	0.58615
(ev):	12.92810	13.14198	14.36134	14.80580	15.94991

		A	A	A	A	A	
1	H1	S	-0.01773	0.08117	-0.00474	0.04481	0.03253
2	H1	S	-0.07907	-0.68322	0.24568	-0.87928	-0.16288
3	H1	PX	0.00150	0.00787	0.00168	0.00657	0.00202
4	H1	PY	-0.00904	0.00954	-0.00871	0.00529	0.00188
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.05204	-0.03251	0.01795	0.07163	0.01020
7	C1	S	0.10016	0.06327	-0.02989	-0.07724	-0.10584
8	C1	PX	-0.07915	-0.01594	0.03310	0.11134	0.10067
9	C1	PY	-0.07970	0.06482	-0.07929	0.14171	-0.12170
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.22583	0.48532	-0.09553	-1.94114	0.58689
12	C1	PX	0.48549	0.42346	0.19227	1.38850	0.55527
13	C1	PY	-1.79880	0.61493	-1.10533	1.07466	-1.36977
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

15	C1	DXX	0.01855	0.02825	0.00166	0.00854	-0.00577
16	C1	DYY	-0.02328	-0.01246	-0.00047	0.00096	-0.01453
17	C1	DZZ	0.00364	-0.00204	0.00031	-0.01194	0.00437
18	C1	DXY	-0.01003	0.03256	-0.02318	0.01222	0.01576
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.03934	-0.00378	0.00249	0.05760	-0.02396
22	C2	S	0.02976	0.03759	-0.00712	-0.06923	0.11587
23	C2	PX	0.06595	0.00599	0.06534	-0.11388	0.13754
24	C2	PY	-0.06045	-0.03453	-0.10230	-0.15126	-0.07928
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	1.40739	0.09357	-0.34674	-2.02289	-0.66521
27	C2	PX	0.56950	-0.45794	0.72472	-0.85806	0.41589
28	C2	PY	-0.34751	0.62066	-1.49704	-1.62005	-1.03943
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01296	0.03857	-0.02451	0.00299	0.00291
31	C2	DYY	-0.01229	-0.01333	0.02460	-0.00642	0.01105
32	C2	DZZ	0.00210	-0.00445	-0.00088	-0.00659	0.00232
33	C2	DXY	0.02635	0.00236	0.00021	0.01397	-0.00255
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.09614	0.00694	-0.04060	-0.05095	0.00223
37	C3	S	-0.11078	0.02914	0.06789	0.03005	0.11898
38	C3	PX	-0.01848	-0.00388	0.03603	-0.00903	-0.26456
39	C3	PY	-0.13630	-0.04907	-0.17090	0.08226	-0.03397
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-2.02561	-0.35604	0.48163	1.59967	-0.96161
42	C3	PX	-0.52808	-0.32397	0.26707	0.09379	-1.65224
43	C3	PY	-0.94777	0.10141	-1.37569	1.06263	-0.79829
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00649	0.00591	0.00326	0.02069	0.00917
46	C3	DYY	0.00721	0.02196	-0.00411	-0.01899	0.02476
47	C3	DZZ	-0.01290	-0.00845	0.00264	0.00443	-0.00265
48	C3	DXY	0.01516	-0.02840	0.02581	-0.01510	0.00023
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.04553	0.05688	-0.04880	-0.00162	-0.09495
52	C4	S	-0.04705	-0.05954	0.05256	-0.00283	-0.10834
53	C4	PX	0.09696	-0.10546	0.05535	0.02322	-0.03016
54	C4	PY	-0.14437	-0.06721	-0.08143	-0.09447	0.20541
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.24763	-0.96676	1.56054	0.80795	3.08555
57	C4	PX	1.37729	-0.40272	0.16708	-0.02434	-0.01136
58	C4	PY	-0.91973	-1.10263	-0.26926	-1.45530	0.83883
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.02005	0.00059	-0.01027	0.01216	-0.03458
61	C4	DYY	0.02712	0.01235	0.00698	-0.00129	-0.00986
62	C4	DZZ	-0.01104	-0.01578	0.00626	-0.01108	0.02124
63	C4	DXY	-0.02201	-0.01073	0.01206	0.03468	-0.00029
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.01911	0.01967	-0.01635	-0.04706	0.02919
67	C5	S	-0.01412	0.00173	0.04316	0.05981	-0.11302
68	C5	PX	-0.03766	0.01068	-0.06133	0.04961	-0.17684

69	C5	PY	0.02570	0.11736	-0.12399	-0.05096	-0.04245
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.89835	-0.62503	0.89532	1.68451	0.31788
72	C5	PX	0.38251	-0.17501	-0.87524	-0.75173	-0.98379
73	C5	PY	1.02999	0.75608	-0.82989	-1.52085	-0.78148
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00080	0.00878	0.01060	0.02569	-0.01536
76	C5	DYY	0.01995	0.01108	-0.00681	-0.00993	-0.00546
77	C5	DZZ	-0.00813	-0.00533	0.00454	0.00163	-0.00107
78	C5	DXY	-0.02686	-0.01916	-0.01165	-0.02682	-0.00404
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.02002	0.02239	0.00467	0.02341	0.10547
82	C6	S	0.01502	0.04382	0.02275	-0.02782	0.09962
83	C6	PX	0.25979	-0.07575	0.07362	-0.00992	-0.01172
84	C6	PY	-0.05808	0.08923	-0.07377	0.04598	0.04203
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.81762	-1.23951	-1.19529	-0.65108	-3.76111
87	C6	PX	0.63036	-0.31984	0.65913	-0.04450	-0.35397
88	C6	PY	-0.32187	1.78064	-0.49941	0.91225	1.02233
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00683	-0.00154	0.02346	0.00612	0.04088
91	C6	DYY	0.01192	0.01326	-0.03976	-0.00892	0.01920
92	C6	DZZ	-0.00054	-0.01071	0.00126	-0.00414	-0.02311
93	C6	DXY	-0.02335	0.00082	-0.01049	0.02067	0.00076
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.01125	-0.02178	0.02257	0.03784	-0.03270
97	C7	S	0.04720	0.09531	-0.03054	-0.08724	0.10138
98	C7	PX	-0.01806	-0.06477	0.02921	0.07127	-0.05166
99	C7	PY	-0.00005	0.12170	-0.15330	0.08486	0.00081
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.26216	0.45077	-0.54215	-0.60806	0.57534
102	C7	PX	0.83536	-1.09257	0.03986	0.41070	0.17598
103	C7	PY	0.75655	0.39575	-1.01105	0.20403	0.91674
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.01185	0.00980	-0.00647	-0.02618	0.04544
106	C7	DYY	-0.00423	0.01103	0.00940	0.01661	-0.01266
107	C7	DZZ	-0.00197	-0.00047	-0.00363	-0.00591	-0.00580
108	C7	DXY	0.00330	0.00132	-0.03163	0.01658	-0.00189
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.01467	-0.03332	0.00637	-0.03129	0.04862
112	O1	S	0.04246	0.01967	0.03830	0.07527	-0.03978
113	O1	PX	-0.04343	-0.02748	-0.04231	-0.10796	0.05831
114	O1	PY	-0.18720	-0.13956	-0.01204	-0.05225	0.17749
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.18677	0.73843	-0.33207	0.42023	-1.02738
117	O1	PX	-0.39897	-0.08056	-0.15564	-0.31107	0.15489
118	O1	PY	-0.57329	-0.59439	0.00022	-0.49095	0.79043
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00265	-0.01222	-0.00441	-0.03151	0.00161
121	O1	DYY	-0.00409	-0.00424	0.01465	0.02509	0.01014
122	O1	DZZ	0.00663	-0.02027	0.02368	0.00830	0.03507

123	O1	DXY	0.00061	0.00552	-0.01023	-0.02932	0.00352
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.09377	0.04560	0.04104	0.06678	0.01637
127	H4	S	-0.53728	-0.49752	-0.06686	0.10485	-0.17318
128	H4	PX	-0.00185	-0.00518	-0.00606	-0.01290	-0.00155
129	H4	PY	0.00988	0.00366	0.00120	-0.00484	0.00031
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01475	-0.10286	-0.01821	-0.02094	-0.07347
132	N1	S	0.00189	0.07644	-0.00343	-0.02184	0.06399
133	N1	PX	0.00418	-0.01055	0.12268	0.04550	0.00111
134	N1	PY	-0.01105	0.04241	-0.15597	0.02021	0.09403
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.24538	2.95948	0.68862	0.95415	2.32000
137	N1	PX	-0.08617	0.79739	0.35084	0.09185	0.37483
138	N1	PY	-0.26076	0.91515	0.12906	0.26577	0.88851
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.01252	-0.00417	-0.00193	0.00617	0.02221
141	N1	DYY	-0.00919	0.00705	0.01144	-0.00851	0.00382
142	N1	DZZ	-0.00746	-0.04170	-0.01442	-0.01968	-0.04726
143	N1	DXY	0.02107	0.00383	0.00127	-0.01608	-0.00300
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.06036	0.08245	-0.05009	0.02392	-0.03419
147	H6	S	0.04501	-0.20473	0.28476	-0.72222	0.18775
148	H6	PX	-0.00109	-0.01195	0.00665	-0.00109	0.00096
149	H6	PY	-0.01214	0.00675	-0.00553	-0.00438	-0.00004
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.04062	-0.01025	0.01150	-0.01740	0.03269
152	C8	S	-0.07440	0.09966	-0.01382	0.06253	0.14759
153	C8	PX	0.10261	0.09616	0.00415	0.02044	-0.05769
154	C8	PY	0.04595	-0.11718	-0.23509	0.18176	0.05187
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.64914	0.61965	1.33618	-0.94051	-0.97053
157	C8	PX	0.51967	1.16203	0.62629	0.34893	0.59215
158	C8	PY	1.17588	-1.90945	-2.55456	1.59541	0.38489
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00230	-0.00226	0.02834	0.00967	0.00479
161	C8	DYY	0.01651	0.02475	0.01049	-0.03782	0.05032
162	C8	DZZ	-0.00821	-0.00618	-0.01401	0.01060	-0.00741
163	C8	DXY	0.00268	-0.00694	-0.00906	-0.00510	-0.00108
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.01358	-0.00025	-0.02129	-0.06346	0.05972
167	H8	S	-0.60637	0.76086	-0.00929	-0.12312	-0.28567
168	H8	PX	0.00437	-0.00308	-0.00263	-0.00330	0.00844
169	H8	PY	0.00316	-0.00161	-0.01983	0.00634	-0.00122
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.02620	0.03057	0.03852	-0.02054	-0.01809
172	C10	S	0.01744	0.08944	0.05217	-0.08434	0.12118
173	C10	PX	-0.01972	-0.04576	-0.05031	-0.04050	-0.00908
174	C10	PY	0.05236	0.07755	-0.00535	-0.10739	0.14191
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.97343	-2.03963	-2.37983	1.53269	0.21178

177	C10	PX	-0.68963	-0.06424	0.43201	-0.63449	-0.39663
178	C10	PY	0.85568	-1.46746	-2.13990	1.22162	0.59968
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00850	-0.01320	-0.02036	-0.00076	0.02065
181	C10	DYY	-0.00542	0.01529	0.00874	0.00988	-0.00186
182	C10	DZZ	-0.00343	0.00837	0.00586	-0.01084	0.00182
183	C10	DXY	0.00687	0.01541	0.01151	0.02494	0.00813
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.03144	-0.08488	-0.12873	-0.01860	0.04020
187	H16	S	0.53310	0.18387	-0.32839	0.44565	0.39406
188	H16	PX	-0.00147	-0.00235	-0.00207	-0.00051	0.00330
189	H16	PY	0.00446	0.00299	0.00065	0.00958	0.00705
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.01991	0.01856	-0.01808	0.11727	0.05559
192	H18	S	-0.13416	-0.26931	-0.42409	-0.14583	0.18722
193	H18	PX	-0.00425	0.00396	0.00718	0.00109	-0.00356
194	H18	PY	0.00150	-0.01252	-0.00840	-0.00553	-0.00586
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.00668	-0.00359	-0.00696	0.00029	0.00156
197	C9	S	0.03558	0.00617	-0.01155	-0.10849	-0.01571
198	C9	PX	-0.01194	-0.06174	0.07507	0.10599	0.09745
199	C9	PY	-0.12711	-0.00245	-0.04630	0.08182	-0.04781
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.09365	0.01643	0.17949	0.43624	-0.13494
202	C9	PX	-0.67083	-0.33838	-0.26582	-0.55480	0.30369
203	C9	PY	-0.12770	-0.04943	-0.16055	-0.12606	-0.02117
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00239	-0.00590	0.00514	-0.00255	0.01364
206	C9	DYY	-0.00294	0.00018	-0.01107	0.00291	-0.02674
207	C9	DZZ	0.02363	0.00705	0.00870	-0.00051	-0.00168
208	C9	DXY	0.00886	0.00231	0.00023	0.00065	0.00373
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.02758	0.01061	-0.02617	0.02779	-0.08731
212	H3	S	0.13379	-0.02145	0.12081	-0.14805	0.19663
213	H3	PX	0.00096	0.00193	-0.00071	0.00486	-0.00263
214	H3	PY	0.00539	0.00021	0.00073	0.00278	-0.00388
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.06696	0.01545	0.04034	0.03421	0.00744
217	H5	S	0.20436	0.20742	-0.03824	0.09237	-0.15246
218	H5	PX	-0.00484	-0.00305	0.00003	-0.00025	0.00175
219	H5	PY	0.00481	0.00251	0.00344	0.00142	0.00596
220	H5	PZ	-0.00295	-0.00352	0.00100	-0.00204	0.00450
221	H7	S	0.06696	0.01545	0.04034	0.03421	0.00744
222	H7	S	0.20436	0.20742	-0.03824	0.09237	-0.15246
223	H7	PX	-0.00484	-0.00305	0.00003	-0.00025	0.00175
224	H7	PY	0.00481	0.00251	0.00344	0.00142	0.00596
225	H7	PZ	0.00295	0.00352	-0.00100	0.00204	-0.00450

MO:	66	67	68	69	70
Eigenvalues:	0.62933	0.66412	0.69372	0.70634	0.72492
(ev):	17.12506	18.07154	18.87710	19.22061	19.72606

		A	A	A	A	A	
1	H1	S	-0.02214	-0.07197	0.03058	0.02816	0.00000
2	H1	S	0.05250	-0.00408	0.23581	-0.00180	0.00000
3	H1	PX	-0.00445	-0.00779	-0.00221	-0.01168	0.00000
4	H1	PY	-0.00326	0.01164	-0.00888	-0.00437	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.00499
6	C1	S	0.03655	-0.03055	0.00658	-0.02875	0.00000
7	C1	S	-0.08000	-0.10018	-0.15554	-0.35936	0.00000
8	C1	PX	0.09606	0.03557	0.17119	0.09098	0.00000
9	C1	PY	-0.04194	-0.24639	-0.19094	0.14172	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.39285
11	C1	S	-1.57939	0.97626	0.16734	0.99055	0.00000
12	C1	PX	0.79963	-0.82898	-0.83062	-0.13301	0.00000
13	C1	PY	-1.52800	1.48799	0.87577	-1.11391	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.22592
15	C1	DXX	-0.01367	-0.02354	0.00257	-0.02060	0.00000
16	C1	DYY	0.00703	-0.01193	-0.02371	-0.08736	0.00000
17	C1	DZZ	-0.00730	0.00724	-0.00246	0.01033	0.00000
18	C1	DXY	-0.00222	0.00382	-0.01766	0.01736	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.02037
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00087
21	C2	S	0.05155	0.00570	-0.04356	0.00031	0.00000
22	C2	S	-0.05986	-0.13560	-0.07273	-0.39537	0.00000
23	C2	PX	-0.09690	-0.00643	0.02584	-0.22485	0.00000
24	C2	PY	-0.06147	-0.23413	-0.09724	0.06433	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.27615
26	C2	S	-1.09914	-0.77693	0.78526	0.68042	0.00000
27	C2	PX	-1.42402	0.35524	0.44102	0.33207	0.00000
28	C2	PY	0.49070	-1.24798	-1.11538	0.94469	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.22033
30	C2	DXX	0.03067	-0.02730	0.03461	-0.05723	0.00000
31	C2	DYY	-0.00775	-0.03370	-0.06489	-0.02206	0.00000
32	C2	DZZ	-0.01130	0.01242	0.00784	-0.00320	0.00000
33	C2	DXY	0.02065	0.00031	0.01001	-0.00264	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.01075
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01175
36	C3	S	0.02226	0.06136	0.03554	-0.01333	0.00000
37	C3	S	-0.00940	-0.08697	-0.11687	-0.39652	0.00000
38	C3	PX	-0.02852	0.13058	0.29684	-0.04529	0.00000
39	C3	PY	0.06318	0.07251	-0.05399	-0.18580	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.22618
41	C3	S	-1.97308	-1.76512	-0.04394	0.34096	0.00000
42	C3	PX	-0.21480	0.09130	2.22315	-1.34958	0.00000
43	C3	PY	0.26489	1.89734	0.14592	-0.48129	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.11839
45	C3	DXX	-0.02034	-0.02330	0.00175	-0.04372	0.00000
46	C3	DYY	-0.01716	0.02846	0.01091	-0.07882	0.00000
47	C3	DZZ	0.00792	-0.01495	-0.01773	0.00983	0.00000
48	C3	DXY	0.00339	0.02002	-0.01651	-0.05335	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00616
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00257
51	C4	S	0.01064	0.01230	-0.04342	0.01066	0.00000
52	C4	S	-0.13799	-0.26770	-0.13339	-0.57257	0.00000
53	C4	PX	0.25538	-0.13119	-0.02023	0.04503	0.00000

54	C4	PY	0.00477	0.06809	0.06079	0.00210	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.41199
56	C4	S	0.52568	-0.03650	0.47506	0.62108	0.00000
57	C4	PX	2.41324	-1.52799	-1.07419	0.62250	0.00000
58	C4	PY	-0.15601	1.15105	-0.06069	0.88991	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.43417
60	C4	DXX	-0.00784	-0.03772	-0.05903	-0.10070	0.00000
61	C4	DYY	-0.00096	0.00369	-0.01822	0.01006	0.00000
62	C4	DZZ	-0.00708	0.00115	0.02011	-0.00551	0.00000
63	C4	DXY	0.03845	0.03989	0.02946	-0.00950	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00242
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00718
66	C5	S	-0.05598	-0.02694	0.03542	-0.01582	0.00000
67	C5	S	-0.00002	-0.11995	-0.26084	-0.35636	0.00000
68	C5	PX	0.13229	0.00892	-0.12102	-0.17820	0.00000
69	C5	PY	0.05106	0.06618	0.18002	0.00906	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.30558
71	C5	S	1.81306	0.70773	-0.01676	0.09647	0.00000
72	C5	PX	1.40973	-0.95829	-1.02646	0.79472	0.00000
73	C5	PY	0.21460	-1.88406	-0.58568	0.47903	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.14726
75	C5	DXX	-0.00087	-0.01195	-0.01327	-0.05744	0.00000
76	C5	DYY	-0.01680	-0.04494	-0.00834	-0.06544	0.00000
77	C5	DZZ	0.01168	0.01265	-0.01610	0.01240	0.00000
78	C5	DXY	-0.03489	-0.01494	-0.04329	-0.00335	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00456
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.01064
81	C6	S	-0.03653	-0.03283	0.01811	-0.00832	0.00000
82	C6	S	0.10496	-0.08631	-0.16880	-0.38049	0.00000
83	C6	PX	-0.13689	0.12932	0.23478	-0.16669	0.00000
84	C6	PY	-0.07563	-0.11427	0.05924	-0.08941	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	-0.29158
86	C6	S	0.92531	1.54867	-0.28528	0.50854	0.00000
87	C6	PX	-0.38031	1.08897	2.47459	-1.23598	0.00000
88	C6	PY	1.50929	-1.45598	1.01888	-1.08391	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.19210
90	C6	DXX	0.00660	-0.02098	-0.05345	-0.07946	0.00000
91	C6	DYY	0.00880	0.00861	0.03081	-0.03861	0.00000
92	C6	DZZ	0.00285	0.00973	-0.01247	0.00887	0.00000
93	C6	DXY	0.01770	-0.04577	-0.01593	0.03688	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00318
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00259
96	C7	S	-0.08098	-0.02843	0.01688	-0.00638	0.00000
97	C7	S	0.03392	0.18669	-0.07987	-0.18399	0.00000
98	C7	PX	-0.17825	-0.04943	0.06137	-0.03114	0.00000
99	C7	PY	-0.28287	-0.01273	0.22012	0.12138	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.17807
101	C7	S	2.42396	1.07181	-0.15627	0.19260	0.00000
102	C7	PX	-1.65369	-1.17378	0.00619	0.39456	0.00000
103	C7	PY	-0.18954	1.16211	-2.02885	0.53314	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.14268
105	C7	DXX	-0.00594	0.03333	-0.00720	-0.06447	0.00000
106	C7	DYY	0.00557	0.01380	-0.01127	-0.00654	0.00000
107	C7	DZZ	0.01011	0.00703	-0.00043	0.01090	0.00000

108	C7	DXY	-0.00809	0.00469	0.00240	-0.01603	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.01387
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00847
111	O1	S	0.00035	0.00743	0.00282	0.01571	0.00000
112	O1	S	0.05550	0.09873	0.01678	0.01763	0.00000
113	O1	PX	0.01815	-0.03638	-0.02659	0.09615	0.00000
114	O1	PY	0.01303	0.01645	0.04922	-0.07680	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	-0.13988
116	O1	S	-0.36978	-0.67935	-0.12198	-0.64793	0.00000
117	O1	PX	-0.36442	0.17322	0.09971	0.04986	0.00000
118	O1	PY	0.01300	0.35598	0.10212	0.31482	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	-0.19079
120	O1	DXX	-0.02116	0.01907	-0.01436	0.02425	0.00000
121	O1	DYY	0.00209	0.01886	0.02380	-0.05204	0.00000
122	O1	DZZ	0.03612	0.05265	0.01877	0.04502	0.00000
123	O1	DXY	-0.04706	-0.02459	-0.01460	-0.01036	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00899
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.02841
126	H4	S	0.02488	-0.01376	0.15678	-0.08690	0.00000
127	H4	S	0.13576	0.20434	-0.39925	0.01694	0.00000
128	H4	PX	-0.00151	0.00100	-0.00317	0.01977	0.00000
129	H4	PY	-0.00169	-0.01227	0.00336	-0.00776	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.00546
131	N1	S	0.00037	-0.00751	0.01717	0.00856	0.00000
132	N1	S	-0.01053	0.02781	-0.01378	0.03161	0.00000
133	N1	PX	-0.07537	0.15298	-0.16694	0.11491	0.00000
134	N1	PY	0.07414	-0.13387	0.22944	-0.06660	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.03543
136	N1	S	0.65280	-0.39675	-0.67569	-0.53338	0.00000
137	N1	PX	0.22740	0.41545	-1.46898	0.48381	0.00000
138	N1	PY	0.41532	-1.13591	1.23094	-0.69583	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00351
140	N1	DXX	-0.01076	-0.01901	-0.02025	0.01571	0.00000
141	N1	DYY	0.04433	-0.01309	-0.01710	-0.00450	0.00000
142	N1	DZZ	-0.01398	0.01130	0.02366	0.03036	0.00000
143	N1	DXY	-0.01530	0.03447	0.03130	-0.02522	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00634
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.02011
146	H6	S	0.15257	-0.03793	0.08113	-0.04443	0.00000
147	H6	S	-0.60046	0.02456	-0.23432	0.20497	0.00000
148	H6	PX	-0.01503	0.00972	-0.00346	0.01852	0.00000
149	H6	PY	0.00050	0.00359	0.00859	0.00093	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	-0.00289
151	C8	S	0.04083	0.05874	-0.04585	0.00097	0.00000
152	C8	S	0.00181	0.00842	-0.21833	-0.10959	0.00000
153	C8	PX	-0.16341	0.31643	-0.11036	-0.05228	0.00000
154	C8	PY	-0.11161	-0.09029	0.00942	-0.03201	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.10566
156	C8	S	-1.10207	-0.69664	1.26873	0.17717	0.00000
157	C8	PX	-0.98769	1.12815	-2.50200	1.01674	0.00000
158	C8	PY	-1.50762	-0.48600	-0.26252	-0.14141	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.03593
160	C8	DXX	-0.00384	0.01772	-0.05363	0.00350	0.00000
161	C8	DYY	0.01558	0.04752	-0.02548	-0.04971	0.00000

162	C8	DZZ	-0.01133	-0.02715	0.02500	0.00347	0.00000
163	C8	DXY	0.05242	-0.01123	-0.03516	-0.00576	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00635
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00346
166	H8	S	-0.07205	0.06647	0.03516	-0.15878	0.00000
167	H8	S	0.69414	0.60993	-0.08608	-0.14436	0.00000
168	H8	PX	-0.00559	0.00214	0.00129	-0.00885	0.00000
169	H8	PY	-0.00811	0.01047	-0.00283	-0.00413	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	-0.00181
171	C10	S	-0.00273	-0.00509	0.00237	0.00374	0.00000
172	C10	S	0.04547	0.17485	-0.17768	-0.07142	0.00000
173	C10	PX	0.10144	0.04493	-0.09694	-0.05289	0.00000
174	C10	PY	0.03960	0.18831	-0.07058	-0.10797	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.11684
176	C10	S	-0.65557	-0.53620	0.14951	-0.17203	0.00000
177	C10	PX	0.68870	-0.59696	1.17864	-0.14487	0.00000
178	C10	PY	-0.17063	-0.53273	-0.13276	-0.11814	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.11198
180	C10	DXX	0.02773	0.01325	-0.04470	-0.01408	0.00000
181	C10	DYY	-0.02183	0.01269	-0.02594	0.00920	0.00000
182	C10	DZZ	-0.00170	0.00363	0.01386	-0.00427	0.00000
183	C10	DXY	-0.05939	0.01035	-0.01548	0.02653	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00302
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00918
186	H16	S	0.15829	0.01980	-0.08961	-0.10939	0.00000
187	H16	S	-0.59553	0.38825	-0.67956	0.11663	0.00000
188	H16	PX	0.00278	-0.00496	0.00202	-0.00126	0.00000
189	H16	PY	-0.01224	-0.00336	-0.00985	0.01239	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.00109
191	H18	S	-0.15292	-0.03680	-0.09506	0.10254	0.00000
192	H18	S	0.53293	-0.39746	0.38803	-0.21731	0.00000
193	H18	PX	-0.00288	-0.01181	0.01311	0.00578	0.00000
194	H18	PY	0.01580	-0.00276	0.01319	-0.00409	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	-0.00191
196	C9	S	0.01261	0.00283	-0.00050	0.00303	0.00000
197	C9	S	-0.13042	-0.08604	-0.04005	0.01314	0.00000
198	C9	PX	0.25695	0.05664	0.06748	0.09728	0.00000
199	C9	PY	0.04496	0.21855	0.09266	-0.08915	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	-0.38886
201	C9	S	0.32476	0.14383	0.07442	-0.10641	0.00000
202	C9	PX	-0.44834	0.18276	0.00504	-0.01005	0.00000
203	C9	PY	0.08864	-0.28389	-0.20948	0.28886	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	1.03858
205	C9	DXX	0.00789	-0.01342	0.00167	-0.00501	0.00000
206	C9	DYY	0.00117	0.03289	0.00637	0.00875	0.00000
207	C9	DZZ	-0.00274	-0.03287	-0.01374	0.00322	0.00000
208	C9	DXY	0.02187	-0.00638	-0.00907	0.03039	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	-0.03675
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.03229
211	H3	S	-0.01668	0.14942	0.05198	-0.04958	0.00000
212	H3	S	-0.18083	-0.07693	0.04829	-0.11050	0.00000
213	H3	PX	0.00844	0.00414	-0.00012	0.00635	0.00000
214	H3	PY	0.00756	-0.00473	-0.00342	0.00914	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.01690

216	H5	S	0.04061	-0.07852	-0.01623	-0.00513	0.26634
217	H5	S	0.01372	-0.11491	-0.06462	0.03506	0.28097
218	H5	PX	-0.00073	0.00428	0.00346	-0.00686	-0.00126
219	H5	PY	0.00601	-0.01022	-0.00381	0.00692	0.00358
220	H5	PZ	0.00290	0.00534	0.00467	0.00492	0.01944
221	H7	S	0.04061	-0.07852	-0.01623	-0.00513	-0.26634
222	H7	S	0.01372	-0.11491	-0.06462	0.03506	-0.28097
223	H7	PX	-0.00073	0.00428	0.00346	-0.00686	0.00126
224	H7	PY	0.00601	-0.01022	-0.00381	0.00692	-0.00358
225	H7	PZ	-0.00290	-0.00534	-0.00467	-0.00492	0.01944

MO:	71	72	73	74	75
Eigenvalues:	0.74659	0.74936	0.75623	0.77139	0.78976
(ev):	20.31564	20.39120	20.57810	20.99055	21.49039

		A	A	A	A	A	
1	H1	S	0.00000	0.01786	0.04667	0.00000	-0.33877
2	H1	S	0.00000	0.25864	0.15780	0.00000	-0.38812
3	H1	PX	0.00000	0.01043	0.00589	0.00000	-0.01791
4	H1	PY	0.00000	0.00294	0.00165	0.00000	0.00102
5	H1	PZ	-0.00619	0.00000	0.00000	-0.00128	0.00000
6	C1	S	0.00000	0.00295	-0.00666	0.00000	-0.04424
7	C1	S	0.00000	0.18971	0.22697	0.00000	-0.21474
8	C1	PX	0.00000	-0.08825	0.01120	0.00000	-0.08771
9	C1	PY	0.00000	-0.14588	-0.34666	0.00000	-0.13472
10	C1	PZ	-0.13790	0.00000	0.00000	-0.02067	0.00000
11	C1	S	0.00000	-0.18013	-0.66310	0.00000	0.58356
12	C1	PX	0.00000	0.25814	-0.01426	0.00000	0.53620
13	C1	PY	0.00000	-0.97803	-0.16037	0.00000	-0.33202
14	C1	PZ	0.15321	0.00000	0.00000	-0.00236	0.00000
15	C1	DXX	0.00000	0.01825	0.04551	0.00000	-0.07313
16	C1	DYY	0.00000	0.03195	-0.00609	0.00000	-0.07239
17	C1	DZZ	0.00000	0.00304	0.01334	0.00000	0.03701
18	C1	DXY	0.00000	0.00163	-0.01295	0.00000	-0.02663
19	C1	DXZ	-0.00189	0.00000	0.00000	0.00180	0.00000
20	C1	DYZ	-0.00764	0.00000	0.00000	-0.00743	0.00000
21	C2	S	0.00000	-0.03906	0.06265	0.00000	0.00416
22	C2	S	0.00000	-0.13306	0.00410	0.00000	0.14159
23	C2	PX	0.00000	0.10459	-0.25475	0.00000	0.11007
24	C2	PY	0.00000	-0.23276	0.30301	0.00000	-0.14977
25	C2	PZ	-0.26567	0.00000	0.00000	-0.36375	0.00000
26	C2	S	0.00000	1.01820	-0.42117	0.00000	-0.10384
27	C2	PX	0.00000	0.06812	-0.25035	0.00000	-0.08450
28	C2	PY	0.00000	2.22504	-0.70717	0.00000	0.29131
29	C2	PZ	0.18913	0.00000	0.00000	0.33126	0.00000
30	C2	DXX	0.00000	-0.05115	0.05102	0.00000	0.01539
31	C2	DYY	0.00000	-0.03044	0.05394	0.00000	0.05213
32	C2	DZZ	0.00000	0.02321	-0.05306	0.00000	-0.01351
33	C2	DXY	0.00000	-0.01454	-0.01605	0.00000	-0.00792
34	C2	DXZ	-0.01662	0.00000	0.00000	-0.01358	0.00000
35	C2	DYZ	-0.01218	0.00000	0.00000	-0.02867	0.00000
36	C3	S	0.00000	-0.01941	0.07731	0.00000	0.00138
37	C3	S	0.00000	0.17429	0.22161	0.00000	-0.15355
38	C3	PX	0.00000	-0.03611	0.17400	0.00000	-0.26829

39	C3	PY	0.00000	-0.06865	-0.12336	0.00000	-0.23862
40	C3	PZ	-0.26519	0.00000	0.00000	-0.02789	0.00000
41	C3	S	0.00000	1.50361	-1.29506	0.00000	0.25350
42	C3	PX	0.00000	-0.97332	-0.15550	0.00000	-0.03327
43	C3	PY	0.00000	-1.65632	0.65957	0.00000	-0.42889
44	C3	PZ	0.14269	0.00000	0.00000	0.06319	0.00000
45	C3	DXX	0.00000	0.00466	0.08622	0.00000	-0.02192
46	C3	DYY	0.00000	0.06131	0.07520	0.00000	0.00199
47	C3	DZZ	0.00000	-0.00113	-0.05252	0.00000	-0.00482
48	C3	DXY	0.00000	0.01593	0.00006	0.00000	0.05169
49	C3	DXZ	-0.00580	0.00000	0.00000	0.01678	0.00000
50	C3	DYZ	0.02275	0.00000	0.00000	-0.01582	0.00000
51	C4	S	0.00000	0.03318	-0.00644	0.00000	0.02109
52	C4	S	0.00000	-0.11281	-0.16887	0.00000	-0.45775
53	C4	PX	0.00000	0.16508	0.00585	0.00000	-0.16318
54	C4	PY	0.00000	-0.08252	-0.12508	0.00000	-0.28989
55	C4	PZ	-0.00708	0.00000	0.00000	-0.21618	0.00000
56	C4	S	0.00000	0.33029	0.27333	0.00000	0.98382
57	C4	PX	0.00000	0.80911	0.61746	0.00000	0.40337
58	C4	PY	0.00000	-0.19591	0.52436	0.00000	0.08768
59	C4	PZ	-0.11190	0.00000	0.00000	0.15656	0.00000
60	C4	DXX	0.00000	0.04429	-0.06945	0.00000	-0.02809
61	C4	DYY	0.00000	0.00771	0.01824	0.00000	0.01041
62	C4	DZZ	0.00000	-0.02975	0.00185	0.00000	-0.02739
63	C4	DXY	0.00000	0.04418	0.02322	0.00000	0.00091
64	C4	DXZ	-0.01448	0.00000	0.00000	0.00587	0.00000
65	C4	DYZ	0.00626	0.00000	0.00000	-0.00011	0.00000
66	C5	S	0.00000	-0.02105	-0.01475	0.00000	-0.00715
67	C5	S	0.00000	-0.00781	0.20775	0.00000	0.07749
68	C5	PX	0.00000	0.35951	-0.15337	0.00000	0.08008
69	C5	PY	0.00000	0.25831	-0.22839	0.00000	-0.07583
70	C5	PZ	-0.27032	0.00000	0.00000	-0.39111	0.00000
71	C5	S	0.00000	-1.24815	0.70698	0.00000	-0.12047
72	C5	PX	0.00000	0.38958	0.63800	0.00000	-0.18167
73	C5	PY	0.00000	1.00719	-0.09551	0.00000	0.27317
74	C5	PZ	0.25202	0.00000	0.00000	0.32177	0.00000
75	C5	DXX	0.00000	-0.04017	0.03173	0.00000	0.01751
76	C5	DYY	0.00000	-0.04493	0.01267	0.00000	-0.02845
77	C5	DZZ	0.00000	0.03737	0.00331	0.00000	0.01220
78	C5	DXY	0.00000	0.00702	0.01479	0.00000	-0.00973
79	C5	DXZ	0.00728	0.00000	0.00000	-0.00680	0.00000
80	C5	DYZ	0.01995	0.00000	0.00000	0.02882	0.00000
81	C6	S	0.00000	0.02909	-0.07405	0.00000	0.02788
82	C6	S	0.00000	-0.11572	0.37076	0.00000	0.29849
83	C6	PX	0.00000	-0.06517	0.04683	0.00000	-0.03619
84	C6	PY	0.00000	0.03806	0.30733	0.00000	0.09183
85	C6	PZ	-0.28922	0.00000	0.00000	-0.04337	0.00000
86	C6	S	0.00000	-0.03697	-0.07768	0.00000	-1.23083
87	C6	PX	0.00000	-1.69422	0.31665	0.00000	-0.22166
88	C6	PY	0.00000	-0.63205	0.10215	0.00000	0.55391
89	C6	PZ	0.21552	0.00000	0.00000	-0.03109	0.00000
90	C6	DXX	0.00000	0.02883	0.00062	0.00000	0.09978
91	C6	DYY	0.00000	-0.01194	-0.01906	0.00000	-0.00828
92	C6	DZZ	0.00000	-0.01264	0.04237	0.00000	-0.01246

93	C6	DXY	0.00000	-0.03877	0.03541	0.00000	-0.00772
94	C6	DXZ	0.00153	0.00000	0.00000	-0.00610	0.00000
95	C6	DYZ	0.00090	0.00000	0.00000	-0.01170	0.00000
96	C7	S	0.00000	0.05252	-0.00042	0.00000	-0.00480
97	C7	S	0.00000	0.03147	0.25086	0.00000	-0.27617
98	C7	PX	0.00000	0.10139	-0.03520	0.00000	0.01647
99	C7	PY	0.00000	0.15158	0.36029	0.00000	-0.12944
100	C7	PZ	-0.31421	0.00000	0.00000	0.46153	0.00000
101	C7	S	0.00000	-1.89340	0.57830	0.00000	0.23888
102	C7	PX	0.00000	1.61096	-0.39612	0.00000	0.30806
103	C7	PY	0.00000	-0.05182	-0.08851	0.00000	0.03717
104	C7	PZ	0.26234	0.00000	0.00000	-0.38629	0.00000
105	C7	DXX	0.00000	0.06418	0.04741	0.00000	-0.01315
106	C7	DYY	0.00000	-0.02643	0.04027	0.00000	-0.04424
107	C7	DZZ	0.00000	-0.02317	-0.01778	0.00000	-0.00934
108	C7	DXY	0.00000	-0.01101	0.01148	0.00000	-0.01733
109	C7	DXZ	0.02040	0.00000	0.00000	-0.01090	0.00000
110	C7	DYZ	-0.01302	0.00000	0.00000	0.00037	0.00000
111	O1	S	0.00000	-0.01422	0.00294	0.00000	-0.01105
112	O1	S	0.00000	0.11774	0.00883	0.00000	0.07925
113	O1	PX	0.00000	0.15663	0.11156	0.00000	-0.08539
114	O1	PY	0.00000	-0.02240	-0.01012	0.00000	-0.08217
115	O1	PZ	0.10989	0.00000	0.00000	0.01526	0.00000
116	O1	S	0.00000	-0.38667	-0.41096	0.00000	-0.12953
117	O1	PX	0.00000	-0.17666	-0.08784	0.00000	-0.03609
118	O1	PY	0.00000	-0.09418	0.19575	0.00000	0.09936
119	O1	PZ	0.17474	0.00000	0.00000	0.03723	0.00000
120	O1	DXX	0.00000	-0.03103	-0.01722	0.00000	0.06269
121	O1	DYY	0.00000	-0.00555	-0.04652	0.00000	-0.05735
122	O1	DZZ	0.00000	0.05339	0.02973	0.00000	0.03499
123	O1	DXY	0.00000	-0.07272	-0.03263	0.00000	0.00006
124	O1	DXZ	0.01078	0.00000	0.00000	-0.00032	0.00000
125	O1	DYZ	-0.01093	0.00000	0.00000	0.00823	0.00000
126	H4	S	0.00000	-0.17371	0.01827	0.00000	-0.07669
127	H4	S	0.00000	-0.04965	0.29580	0.00000	-0.15551
128	H4	PX	0.00000	0.01262	0.01047	0.00000	-0.00451
129	H4	PY	0.00000	-0.01004	0.00841	0.00000	-0.00030
130	H4	PZ	-0.00373	0.00000	0.00000	-0.00125	0.00000
131	N1	S	0.00000	0.00707	-0.00164	0.00000	-0.00874
132	N1	S	0.00000	0.01531	-0.09166	0.00000	0.02701
133	N1	PX	0.00000	-0.10136	-0.01403	0.00000	-0.15133
134	N1	PY	0.00000	-0.04224	-0.13857	0.00000	-0.01193
135	N1	PZ	-0.08089	0.00000	0.00000	0.08546	0.00000
136	N1	S	0.00000	-0.76198	0.52654	0.00000	0.57432
137	N1	PX	0.00000	0.06385	0.12382	0.00000	-0.01809
138	N1	PY	0.00000	-0.31884	0.30071	0.00000	0.57721
139	N1	PZ	0.00180	0.00000	0.00000	0.02094	0.00000
140	N1	DXX	0.00000	0.02142	0.00522	0.00000	0.03358
141	N1	DYY	0.00000	-0.02578	-0.00933	0.00000	0.02857
142	N1	DZZ	0.00000	0.01694	-0.02578	0.00000	-0.01779
143	N1	DXY	0.00000	0.01225	-0.02550	0.00000	-0.01648
144	N1	DXZ	-0.00808	0.00000	0.00000	-0.00045	0.00000
145	N1	DYZ	-0.01897	0.00000	0.00000	0.00181	0.00000
146	H6	S	0.00000	-0.17789	0.17405	0.00000	-0.01821

147	H6	S	0.00000	0.31468	-0.27155	0.00000	0.08003
148	H6	PX	0.00000	0.01253	-0.01309	0.00000	-0.00636
149	H6	PY	0.00000	0.01767	-0.00534	0.00000	0.00360
150	H6	PZ	-0.00108	0.00000	0.00000	-0.00212	0.00000
151	C8	S	0.00000	-0.02783	-0.01809	0.00000	-0.01677
152	C8	S	0.00000	0.04108	0.18952	0.00000	-0.04256
153	C8	PX	0.00000	0.02424	-0.05352	0.00000	-0.21254
154	C8	PY	0.00000	0.02849	0.10280	0.00000	-0.01250
155	C8	PZ	-0.20251	0.00000	0.00000	0.32522	0.00000
156	C8	S	0.00000	0.68604	-0.50138	0.00000	0.23690
157	C8	PX	0.00000	0.30456	0.12555	0.00000	-0.09083
158	C8	PY	0.00000	1.41085	-0.36785	0.00000	0.09925
159	C8	PZ	0.10206	0.00000	0.00000	-0.22853	0.00000
160	C8	DXX	0.00000	-0.02451	0.00652	0.00000	-0.01733
161	C8	DYY	0.00000	0.01935	-0.01194	0.00000	-0.00877
162	C8	DZZ	0.00000	0.01163	0.01788	0.00000	0.00752
163	C8	DXY	0.00000	-0.03008	-0.00836	0.00000	0.01759
164	C8	DXZ	-0.00820	0.00000	0.00000	0.01648	0.00000
165	C8	DYZ	0.01074	0.00000	0.00000	-0.02827	0.00000
166	H8	S	0.00000	0.22018	0.05915	0.00000	-0.08471
167	H8	S	0.00000	-0.88019	0.11050	0.00000	-0.30648
168	H8	PX	0.00000	0.01775	0.00969	0.00000	-0.00155
169	H8	PY	0.00000	-0.00400	0.00009	0.00000	-0.00174
170	H8	PZ	-0.00336	0.00000	0.00000	0.00920	0.00000
171	C10	S	0.00000	0.00318	0.00366	0.00000	0.00044
172	C10	S	0.00000	0.01084	-0.02804	0.00000	-0.06510
173	C10	PX	0.00000	-0.06136	-0.04517	0.00000	-0.04914
174	C10	PY	0.00000	0.06382	-0.09214	0.00000	-0.05434
175	C10	PZ	-0.28450	0.00000	0.00000	0.64844	0.00000
176	C10	S	0.00000	0.69607	-0.13941	0.00000	0.08103
177	C10	PX	0.00000	-0.20092	0.10698	0.00000	0.22343
178	C10	PY	0.00000	0.21825	0.13750	0.00000	0.20121
179	C10	PZ	0.26010	0.00000	0.00000	-0.58269	0.00000
180	C10	DXX	0.00000	-0.00751	-0.00641	0.00000	-0.00382
181	C10	DYY	0.00000	0.01633	0.00914	0.00000	-0.00854
182	C10	DZZ	0.00000	0.00244	-0.00517	0.00000	-0.00061
183	C10	DXY	0.00000	0.02767	0.02619	0.00000	-0.00579
184	C10	DXZ	0.00630	0.00000	0.00000	-0.01044	0.00000
185	C10	DYZ	-0.01699	0.00000	0.00000	0.02751	0.00000
186	H16	S	0.00000	-0.07778	-0.05736	0.00000	-0.01368
187	H16	S	0.00000	0.19577	0.03101	0.00000	-0.11026
188	H16	PX	0.00000	0.00461	0.00108	0.00000	0.00528
189	H16	PY	0.00000	0.00410	0.00813	0.00000	0.00409
190	H16	PZ	-0.00341	0.00000	0.00000	0.00925	0.00000
191	H18	S	0.00000	0.08509	0.11536	0.00000	0.03244
192	H18	S	0.00000	-0.12631	0.02167	0.00000	0.20076
193	H18	PX	0.00000	-0.00009	0.00518	0.00000	0.00710
194	H18	PY	0.00000	-0.01243	-0.00665	0.00000	-0.00141
195	H18	PZ	-0.00512	0.00000	0.00000	0.01215	0.00000
196	C9	S	0.00000	0.01713	0.01140	0.00000	0.00643
197	C9	S	0.00000	-0.21008	-0.09373	0.00000	0.04466
198	C9	PX	0.00000	0.44790	0.16778	0.00000	-0.19420
199	C9	PY	0.00000	0.13925	0.09299	0.00000	0.18039
200	C9	PZ	0.51230	0.00000	0.00000	0.16317	0.00000

201	C9	S	0.00000	0.35114	0.11523	0.00000	-0.13970
202	C9	PX	0.00000	-0.69038	-0.09987	0.00000	0.41417
203	C9	PY	0.00000	-0.07685	-0.00533	0.00000	-0.39658
204	C9	PZ	-1.21351	0.00000	0.00000	-0.38146	0.00000
205	C9	DXX	0.00000	0.02163	0.00539	0.00000	-0.03861
206	C9	DYY	0.00000	-0.01038	0.02469	0.00000	0.10200
207	C9	DZZ	0.00000	-0.01177	-0.02300	0.00000	-0.04292
208	C9	DXY	0.00000	0.04128	0.02606	0.00000	-0.00153
209	C9	DXZ	0.03546	0.00000	0.00000	0.01087	0.00000
210	C9	DYZ	-0.04599	0.00000	0.00000	-0.01677	0.00000
211	H3	S	0.00000	-0.01034	0.06264	0.00000	0.33631
212	H3	S	0.00000	-0.10329	-0.13773	0.00000	-0.07031
213	H3	PX	0.00000	0.01506	0.00940	0.00000	0.00911
214	H3	PY	0.00000	0.00465	0.00455	0.00000	0.00486
215	H3	PZ	-0.02192	0.00000	0.00000	-0.00833	0.00000
216	H5	S	-0.29670	0.05861	-0.03654	-0.09153	-0.16146
217	H5	S	-0.25033	0.04521	-0.00697	-0.06997	0.02982
218	H5	PX	0.00946	0.00260	0.00059	0.00418	-0.00024
219	H5	PY	0.00277	0.01319	-0.00128	0.00239	-0.02371
220	H5	PZ	-0.02735	0.00731	0.00747	-0.00903	0.00242
221	H7	S	0.29670	0.05861	-0.03654	0.09153	-0.16146
222	H7	S	0.25033	0.04521	-0.00697	0.06997	0.02982
223	H7	PX	-0.00946	0.00260	0.00059	-0.00418	-0.00024
224	H7	PY	-0.00277	0.01319	-0.00128	-0.00239	-0.02371
225	H7	PZ	-0.02735	-0.00731	-0.00747	-0.00903	-0.00242

MO:		76	77	78	79	80
Eigenvalues:		0.79398	0.81386	0.81512	0.81972	0.84843
(ev):		21.60542	22.14624	22.18057	22.30575	23.08688

		A	A	A	A	A	
1	H1	S	0.02840	0.00000	-0.02220	0.13827	0.00000
2	H1	S	0.03542	0.00000	-0.08125	-0.11507	0.00000
3	H1	PX	0.00215	0.00000	-0.00685	0.00359	0.00000
4	H1	PY	0.00859	0.00000	0.01078	0.00794	0.00000
5	H1	PZ	0.00000	-0.00455	0.00000	0.00000	-0.00116
6	C1	S	-0.02650	0.00000	0.00384	0.03057	0.00000
7	C1	S	0.00182	0.00000	-0.34518	-0.17788	0.00000
8	C1	PX	-0.08284	0.00000	0.05447	0.12238	0.00000
9	C1	PY	0.00609	0.00000	0.11568	0.11422	0.00000
10	C1	PZ	0.00000	-0.59400	0.00000	0.00000	-0.30439
11	C1	S	0.71472	0.00000	0.62580	0.25262	0.00000
12	C1	PX	-0.39540	0.00000	-0.21370	-0.08153	0.00000
13	C1	PY	0.31985	0.00000	0.20750	-0.10674	0.00000
14	C1	PZ	0.00000	0.60741	0.00000	0.00000	0.29751
15	C1	DXX	-0.00109	0.00000	-0.02891	0.03974	0.00000
16	C1	DYY	-0.01808	0.00000	-0.03533	-0.01918	0.00000
17	C1	DZZ	0.00980	0.00000	-0.01037	-0.02617	0.00000
18	C1	DXY	0.04578	0.00000	0.00179	-0.00900	0.00000
19	C1	DXZ	0.00000	0.02903	0.00000	0.00000	0.02749
20	C1	DYZ	0.00000	0.00749	0.00000	0.00000	-0.01865
21	C2	S	0.00246	0.00000	-0.02105	-0.01981	0.00000
22	C2	S	0.42459	0.00000	0.29734	0.06648	0.00000
23	C2	PX	0.13939	0.00000	-0.03542	0.03984	0.00000

24	C2	PY	-0.05631	0.00000	0.30941	-0.10373	0.00000
25	C2	PZ	0.00000	0.39949	0.00000	0.00000	0.34998
26	C2	S	-0.73535	0.00000	0.55690	0.35392	0.00000
27	C2	PX	0.13231	0.00000	0.51129	0.51342	0.00000
28	C2	PY	-0.38125	0.00000	0.53304	0.32520	0.00000
29	C2	PZ	0.00000	-0.36451	0.00000	0.00000	-0.34422
30	C2	DXX	0.04130	0.00000	0.04651	-0.02133	0.00000
31	C2	DYY	0.05534	0.00000	0.00926	0.03181	0.00000
32	C2	DZZ	0.00293	0.00000	0.00456	0.00804	0.00000
33	C2	DXY	-0.00193	0.00000	-0.02521	0.00105	0.00000
34	C2	DXZ	0.00000	0.02436	0.00000	0.00000	0.02197
35	C2	DYZ	0.00000	0.02176	0.00000	0.00000	-0.02819
36	C3	S	0.01658	0.00000	-0.05583	-0.06316	0.00000
37	C3	S	0.02811	0.00000	-0.30291	0.37524	0.00000
38	C3	PX	-0.27998	0.00000	0.13563	0.09471	0.00000
39	C3	PY	0.06304	0.00000	0.04101	-0.16229	0.00000
40	C3	PZ	0.00000	-0.28737	0.00000	0.00000	0.21913
41	C3	S	-1.35894	0.00000	1.60593	0.69218	0.00000
42	C3	PX	-0.19306	0.00000	0.11486	-0.13526	0.00000
43	C3	PY	0.68377	0.00000	-0.66720	-0.32876	0.00000
44	C3	PZ	0.00000	0.15150	0.00000	0.00000	-0.18422
45	C3	DXX	-0.02329	0.00000	-0.06502	0.03381	0.00000
46	C3	DYY	0.00913	0.00000	-0.07191	-0.01933	0.00000
47	C3	DZZ	0.01050	0.00000	0.03372	0.02682	0.00000
48	C3	DXY	-0.03146	0.00000	0.01258	0.02477	0.00000
49	C3	DXZ	0.00000	-0.00260	0.00000	0.00000	-0.00812
50	C3	DYZ	0.00000	-0.00154	0.00000	0.00000	-0.01821
51	C4	S	0.00632	0.00000	-0.01025	-0.01935	0.00000
52	C4	S	0.03072	0.00000	0.12745	-0.30071	0.00000
53	C4	PX	-0.23354	0.00000	-0.35787	-0.00115	0.00000
54	C4	PY	0.05978	0.00000	-0.24421	-0.37485	0.00000
55	C4	PZ	0.00000	-0.02103	0.00000	0.00000	-0.42796
56	C4	S	-0.16443	0.00000	-0.52527	0.66870	0.00000
57	C4	PX	-0.56683	0.00000	0.00133	-0.22838	0.00000
58	C4	PY	0.56211	0.00000	-0.19709	0.40413	0.00000
59	C4	PZ	0.00000	0.00723	0.00000	0.00000	0.44037
60	C4	DXX	0.01552	0.00000	-0.01237	-0.09334	0.00000
61	C4	DYY	0.01088	0.00000	0.01284	0.02129	0.00000
62	C4	DZZ	0.00014	0.00000	0.01580	0.00653	0.00000
63	C4	DXY	-0.00045	0.00000	0.01163	0.01076	0.00000
64	C4	DXZ	0.00000	-0.03801	0.00000	0.00000	-0.00303
65	C4	DYZ	0.00000	0.02438	0.00000	0.00000	0.02415
66	C5	S	0.02072	0.00000	0.08017	0.01417	0.00000
67	C5	S	0.27094	0.00000	0.23584	-0.22059	0.00000
68	C5	PX	-0.03198	0.00000	-0.17934	-0.21673	0.00000
69	C5	PY	-0.02721	0.00000	0.05375	-0.06915	0.00000
70	C5	PZ	0.00000	0.26688	0.00000	0.00000	-0.33736
71	C5	S	-0.36082	0.00000	-1.49611	-0.31082	0.00000
72	C5	PX	-0.32577	0.00000	0.13141	-0.07889	0.00000
73	C5	PY	-0.52719	0.00000	0.73648	0.34140	0.00000
74	C5	PZ	0.00000	-0.27442	0.00000	0.00000	0.32998
75	C5	DXX	0.04238	0.00000	0.09981	-0.01100	0.00000
76	C5	DYY	0.04448	0.00000	0.08961	-0.04735	0.00000
77	C5	DZZ	-0.01265	0.00000	-0.06081	-0.00580	0.00000

78	C5	DXY	0.00318	0.00000	0.00220	-0.02829	0.00000
79	C5	DXZ	0.00000	0.01324	0.00000	0.00000	-0.02112
80	C5	DYZ	0.00000	-0.03595	0.00000	0.00000	-0.01259
81	C6	S	0.02314	0.00000	-0.00331	0.02492	0.00000
82	C6	S	0.24805	0.00000	-0.27694	0.23650	0.00000
83	C6	PX	-0.13659	0.00000	-0.14130	-0.05060	0.00000
84	C6	PY	-0.17443	0.00000	0.06973	-0.27843	0.00000
85	C6	PZ	0.00000	0.07776	0.00000	0.00000	0.48543
86	C6	S	-0.09771	0.00000	0.18065	-0.68935	0.00000
87	C6	PX	0.41986	0.00000	-0.19137	-0.16602	0.00000
88	C6	PY	-0.21704	0.00000	-0.36112	-0.13320	0.00000
89	C6	PZ	0.00000	-0.07347	0.00000	0.00000	-0.47453
90	C6	DXX	0.05608	0.00000	-0.06802	0.05182	0.00000
91	C6	DYY	0.03906	0.00000	-0.02251	0.01894	0.00000
92	C6	DZZ	-0.01501	0.00000	0.00820	-0.01274	0.00000
93	C6	DXY	-0.00642	0.00000	-0.00707	0.00341	0.00000
94	C6	DXZ	0.00000	-0.01643	0.00000	0.00000	-0.00734
95	C6	DYZ	0.00000	-0.00284	0.00000	0.00000	0.01865
96	C7	S	-0.03668	0.00000	0.02300	0.08130	0.00000
97	C7	S	-0.29411	0.00000	-0.05353	0.19937	0.00000
98	C7	PX	0.04490	0.00000	0.02113	0.10928	0.00000
99	C7	PY	0.21340	0.00000	-0.27114	-0.10568	0.00000
100	C7	PZ	0.00000	-0.40536	0.00000	0.00000	0.21539
101	C7	S	1.40513	0.00000	-1.10053	-1.31108	0.00000
102	C7	PX	-0.69500	0.00000	0.64875	0.46094	0.00000
103	C7	PY	0.71217	0.00000	-0.23841	0.00825	0.00000
104	C7	PZ	0.00000	0.48071	0.00000	0.00000	-0.14824
105	C7	DXX	-0.08594	0.00000	0.00757	0.07973	0.00000
106	C7	DYY	-0.03001	0.00000	-0.01342	0.10492	0.00000
107	C7	DZZ	0.01954	0.00000	0.00338	-0.05519	0.00000
108	C7	DXY	0.01884	0.00000	-0.01828	0.00312	0.00000
109	C7	DXZ	0.00000	0.02906	0.00000	0.00000	-0.00720
110	C7	DYZ	0.00000	-0.00059	0.00000	0.00000	0.00013
111	O1	S	0.00032	0.00000	-0.02172	-0.00459	0.00000
112	O1	S	0.08432	0.00000	0.13436	0.02993	0.00000
113	O1	PX	0.16872	0.00000	0.18121	0.04093	0.00000
114	O1	PY	0.04880	0.00000	0.02651	-0.11391	0.00000
115	O1	PZ	0.00000	-0.01266	0.00000	0.00000	-0.08163
116	O1	S	-0.53726	0.00000	-0.14228	-0.27372	0.00000
117	O1	PX	0.02396	0.00000	-0.10484	0.06555	0.00000
118	O1	PY	0.08550	0.00000	-0.22172	0.05775	0.00000
119	O1	PZ	0.00000	0.03108	0.00000	0.00000	0.03991
120	O1	DXX	-0.03552	0.00000	-0.02867	0.02386	0.00000
121	O1	DYY	0.01809	0.00000	0.00275	-0.08048	0.00000
122	O1	DZZ	0.04770	0.00000	0.05414	0.04070	0.00000
123	O1	DXY	-0.03289	0.00000	-0.03882	-0.00906	0.00000
124	O1	DXZ	0.00000	0.01784	0.00000	0.00000	0.00520
125	O1	DYZ	0.00000	-0.00539	0.00000	0.00000	0.01154
126	H4	S	0.08880	0.00000	0.28539	0.01787	0.00000
127	H4	S	0.12619	0.00000	-0.15453	-0.28611	0.00000
128	H4	PX	-0.00310	0.00000	-0.00473	0.00609	0.00000
129	H4	PY	0.00465	0.00000	0.01932	0.00220	0.00000
130	H4	PZ	0.00000	-0.00595	0.00000	0.00000	-0.00393
131	N1	S	0.00403	0.00000	-0.00089	0.01267	0.00000

132	N1	S	0.00089	0.00000	0.03261	-0.04696	0.00000
133	N1	PX	0.04230	0.00000	0.02997	-0.04100	0.00000
134	N1	PY	0.06357	0.00000	-0.03564	0.12805	0.00000
135	N1	PZ	0.00000	0.13439	0.00000	0.00000	0.13369
136	N1	S	-0.04827	0.00000	-0.42442	0.05288	0.00000
137	N1	PX	0.08685	0.00000	-0.11865	0.13840	0.00000
138	N1	PY	-0.29893	0.00000	-0.12868	-0.30033	0.00000
139	N1	PZ	0.00000	-0.05387	0.00000	0.00000	0.00262
140	N1	DXX	-0.04190	0.00000	0.00918	-0.03036	0.00000
141	N1	DYY	0.02296	0.00000	-0.02264	0.03528	0.00000
142	N1	DZZ	0.00879	0.00000	0.01982	-0.03166	0.00000
143	N1	DXY	0.01165	0.00000	0.00641	0.00030	0.00000
144	N1	DXZ	0.00000	0.01634	0.00000	0.00000	0.01984
145	N1	DYZ	0.00000	0.01159	0.00000	0.00000	0.01629
146	H6	S	0.06823	0.00000	0.05642	-0.00999	0.00000
147	H6	S	0.21149	0.00000	0.35246	0.39355	0.00000
148	H6	PX	-0.00771	0.00000	-0.00156	0.00657	0.00000
149	H6	PY	-0.00392	0.00000	0.00327	0.00160	0.00000
150	H6	PZ	0.00000	0.00017	0.00000	0.00000	0.00312
151	C8	S	-0.02972	0.00000	0.03303	-0.04821	0.00000
152	C8	S	-0.53701	0.00000	0.17198	0.26498	0.00000
153	C8	PX	0.16477	0.00000	-0.02077	0.32616	0.00000
154	C8	PY	0.00445	0.00000	-0.06717	0.17482	0.00000
155	C8	PZ	0.00000	0.16225	0.00000	0.00000	0.19660
156	C8	S	0.94269	0.00000	-0.25310	0.15199	0.00000
157	C8	PX	0.34532	0.00000	-0.08399	0.17230	0.00000
158	C8	PY	-0.74691	0.00000	0.69385	0.04875	0.00000
159	C8	PZ	0.00000	-0.22681	0.00000	0.00000	-0.24304
160	C8	DXX	-0.04784	0.00000	0.02403	0.03091	0.00000
161	C8	DYY	-0.10876	0.00000	0.06038	-0.02279	0.00000
162	C8	DZZ	0.01333	0.00000	-0.01894	0.02440	0.00000
163	C8	DXY	-0.00756	0.00000	-0.00644	0.02540	0.00000
164	C8	DXZ	0.00000	-0.01152	0.00000	0.00000	-0.00740
165	C8	DYZ	0.00000	-0.04423	0.00000	0.00000	0.03261
166	H8	S	-0.21038	0.00000	0.09179	0.26167	0.00000
167	H8	S	0.33755	0.00000	-0.26704	-0.14738	0.00000
168	H8	PX	-0.01975	0.00000	0.00440	0.02166	0.00000
169	H8	PY	0.02075	0.00000	-0.00997	-0.00232	0.00000
170	H8	PZ	0.00000	0.00015	0.00000	0.00000	0.00374
171	C10	S	-0.00619	0.00000	0.00100	0.02000	0.00000
172	C10	S	-0.42047	0.00000	0.31220	-0.09482	0.00000
173	C10	PX	0.07998	0.00000	-0.04695	0.24388	0.00000
174	C10	PY	-0.22428	0.00000	0.20974	-0.21459	0.00000
175	C10	PZ	0.00000	0.47762	0.00000	0.00000	-0.48884
176	C10	S	-0.07050	0.00000	0.05089	-0.04912	0.00000
177	C10	PX	-0.16073	0.00000	-0.02351	-0.75725	0.00000
178	C10	PY	-0.33241	0.00000	0.09056	0.10536	0.00000
179	C10	PZ	0.00000	-0.44474	0.00000	0.00000	0.55813
180	C10	DXX	-0.08093	0.00000	0.05101	0.01308	0.00000
181	C10	DYY	-0.03804	0.00000	0.02949	0.00741	0.00000
182	C10	DZZ	0.00863	0.00000	-0.00089	-0.02073	0.00000
183	C10	DXY	0.00554	0.00000	0.00192	-0.02203	0.00000
184	C10	DXZ	0.00000	0.00189	0.00000	0.00000	-0.00215
185	C10	DYZ	0.00000	0.02291	0.00000	0.00000	0.00048

186	H16	S	-0.14138	0.00000	0.07748	0.21110	0.00000
187	H16	S	0.04524	0.00000	0.05448	0.30130	0.00000
188	H16	PX	-0.02136	0.00000	0.01201	-0.01609	0.00000
189	H16	PY	0.00307	0.00000	-0.00183	-0.01452	0.00000
190	H16	PZ	0.00000	0.00802	0.00000	0.00000	-0.00808
191	H18	S	-0.13001	0.00000	0.06995	-0.07815	0.00000
192	H18	S	-0.29837	0.00000	0.07772	-0.27716	0.00000
193	H18	PX	0.00794	0.00000	-0.00868	-0.01278	0.00000
194	H18	PY	0.01142	0.00000	-0.00638	0.00370	0.00000
195	H18	PZ	0.00000	0.00459	0.00000	0.00000	-0.00745
196	C9	S	0.01318	0.00000	0.02188	-0.00078	0.00000
197	C9	S	-0.16643	0.00000	-0.17775	0.00659	0.00000
198	C9	PX	0.37650	0.00000	0.37873	0.02036	0.00000
199	C9	PY	0.08221	0.00000	0.18471	-0.03736	0.00000
200	C9	PZ	0.00000	0.16172	0.00000	0.00000	0.19759
201	C9	S	0.20466	0.00000	0.21412	-0.04040	0.00000
202	C9	PX	-0.44843	0.00000	-0.53530	-0.00958	0.00000
203	C9	PY	0.02303	0.00000	-0.18449	0.13576	0.00000
204	C9	PZ	0.00000	-0.23287	0.00000	0.00000	-0.35931
205	C9	DXX	0.03182	0.00000	0.03011	-0.01955	0.00000
206	C9	DYY	-0.02583	0.00000	0.00970	0.02208	0.00000
207	C9	DZZ	-0.01142	0.00000	-0.02658	-0.00268	0.00000
208	C9	DXY	0.03203	0.00000	0.04092	0.02738	0.00000
209	C9	DXZ	0.00000	-0.00913	0.00000	0.00000	0.00036
210	C9	DYZ	0.00000	-0.01194	0.00000	0.00000	-0.02089
211	H3	S	-0.07516	0.00000	0.06196	0.03393	0.00000
212	H3	S	-0.03451	0.00000	-0.05247	-0.12164	0.00000
213	H3	PX	0.01072	0.00000	0.01877	0.00924	0.00000
214	H3	PY	0.00188	0.00000	0.00526	0.00823	0.00000
215	H3	PZ	0.00000	-0.00242	0.00000	0.00000	-0.00863
216	H5	S	0.04797	-0.01364	0.01401	-0.03885	-0.04682
217	H5	S	0.00210	-0.01284	0.07023	0.06829	-0.03726
218	H5	PX	0.00286	0.01153	0.00400	-0.00730	0.01377
219	H5	PY	0.01145	0.00574	0.00542	0.00322	0.00876
220	H5	PZ	0.00877	-0.01142	0.00855	0.00201	-0.01339
221	H7	S	0.04797	0.01364	0.01401	-0.03885	0.04682
222	H7	S	0.00210	0.01284	0.07023	0.06829	0.03726
223	H7	PX	0.00286	-0.01153	0.00400	-0.00730	-0.01377
224	H7	PY	0.01145	-0.00574	0.00542	0.00322	-0.00876
225	H7	PZ	-0.00877	-0.01142	-0.00855	-0.00201	-0.01339

MO:	81	82	83	84	85
Eigenvalues:	0.85238	0.87614	0.87640	0.89436	0.91131
(ev):	23.19457	23.84103	23.84796	24.33683	24.79810

		A	A	A	A	A	
1	H1	S	0.09784	0.00000	-0.23481	0.00000	0.18368
2	H1	S	0.08025	0.00000	0.11908	0.00000	0.10641
3	H1	PX	0.00870	0.00000	-0.01304	0.00000	0.00979
4	H1	PY	0.01464	0.00000	-0.00181	0.00000	0.00124
5	H1	PZ	0.00000	0.00007	0.00000	-0.00276	0.00000
6	C1	S	0.01561	0.00000	-0.06156	0.00000	0.02476
7	C1	S	0.22409	0.00000	-0.06639	0.00000	0.16070
8	C1	PX	-0.13001	0.00000	-0.14963	0.00000	0.07363

9	C1	PY	0.23045	0.00000	-0.00669	0.00000	-0.09446
10	C1	PZ	0.00000	-0.10311	0.00000	0.47764	0.00000
11	C1	S	0.43231	0.00000	0.66852	0.00000	-0.21869
12	C1	PX	-0.61504	0.00000	-0.16032	0.00000	-0.40983
13	C1	PY	0.98470	0.00000	0.12024	0.00000	0.51449
14	C1	PZ	0.00000	-0.02551	0.00000	-0.69219	0.00000
15	C1	DXX	0.06674	0.00000	-0.08132	0.00000	0.06294
16	C1	DYY	0.03590	0.00000	-0.05118	0.00000	0.03670
17	C1	DZZ	-0.02139	0.00000	0.04968	0.00000	-0.01946
18	C1	DXY	0.00259	0.00000	0.01293	0.00000	-0.00017
19	C1	DXZ	0.00000	0.01191	0.00000	-0.01370	0.00000
20	C1	DYZ	0.00000	0.00720	0.00000	-0.00937	0.00000
21	C2	S	-0.03424	0.00000	-0.04866	0.00000	0.02237
22	C2	S	-0.11525	0.00000	-0.18517	0.00000	0.21413
23	C2	PX	0.06323	0.00000	0.01389	0.00000	0.08727
24	C2	PY	0.05394	0.00000	0.20276	0.00000	-0.25221
25	C2	PZ	0.00000	0.23750	0.00000	0.60821	0.00000
26	C2	S	-0.36495	0.00000	0.74084	0.00000	-0.88094
27	C2	PX	0.10714	0.00000	0.30583	0.00000	-0.17778
28	C2	PY	-1.74042	0.00000	-0.25637	0.00000	0.03092
29	C2	PZ	0.00000	-0.33700	0.00000	-0.89955	0.00000
30	C2	DXX	-0.06255	0.00000	-0.05028	0.00000	0.03773
31	C2	DYY	-0.04614	0.00000	-0.08882	0.00000	0.05088
32	C2	DZZ	0.02972	0.00000	0.03540	0.00000	-0.00785
33	C2	DXY	-0.02834	0.00000	0.01260	0.00000	0.01848
34	C2	DXZ	0.00000	0.03018	0.00000	0.00901	0.00000
35	C2	DYZ	0.00000	0.03606	0.00000	-0.01199	0.00000
36	C3	S	0.01964	0.00000	0.03054	0.00000	0.00526
37	C3	S	0.10749	0.00000	0.00850	0.00000	-0.13551
38	C3	PX	0.05601	0.00000	-0.05994	0.00000	0.00775
39	C3	PY	0.24774	0.00000	-0.27177	0.00000	0.20699
40	C3	PZ	0.00000	-0.10660	0.00000	-0.11645	0.00000
41	C3	S	-1.34345	0.00000	-0.09195	0.00000	-0.41714
42	C3	PX	0.80748	0.00000	0.31858	0.00000	0.26676
43	C3	PY	1.42970	0.00000	-0.11758	0.00000	0.55602
44	C3	PZ	0.00000	0.09814	0.00000	0.21658	0.00000
45	C3	DXX	0.07716	0.00000	0.03420	0.00000	-0.03557
46	C3	DYY	-0.02359	0.00000	0.01215	0.00000	-0.01130
47	C3	DZZ	-0.01561	0.00000	-0.02342	0.00000	0.01180
48	C3	DXY	0.00103	0.00000	0.00237	0.00000	0.00498
49	C3	DXZ	0.00000	0.01682	0.00000	-0.01210	0.00000
50	C3	DYZ	0.00000	-0.04407	0.00000	0.02090	0.00000
51	C4	S	0.02413	0.00000	0.02051	0.00000	-0.01158
52	C4	S	-0.15859	0.00000	0.07739	0.00000	-0.01085
53	C4	PX	-0.05495	0.00000	-0.20238	0.00000	0.12753
54	C4	PY	-0.44171	0.00000	0.36953	0.00000	-0.09656
55	C4	PZ	0.00000	-0.39994	0.00000	-0.26554	0.00000
56	C4	S	0.01235	0.00000	-0.34414	0.00000	-0.08849
57	C4	PX	-1.69996	0.00000	-0.25646	0.00000	-0.55625
58	C4	PY	1.57922	0.00000	-0.55078	0.00000	0.57315
59	C4	PZ	0.00000	0.67617	0.00000	0.34279	0.00000
60	C4	DXX	-0.00865	0.00000	0.06538	0.00000	-0.04269
61	C4	DYY	0.04377	0.00000	-0.02465	0.00000	0.02143
62	C4	DZZ	-0.02732	0.00000	-0.00763	0.00000	0.01071

63	C4	DXY	-0.01661	0.00000	-0.03058	0.00000	0.02222
64	C4	DXZ	0.00000	-0.01784	0.00000	0.03734	0.00000
65	C4	DYZ	0.00000	-0.01236	0.00000	-0.01208	0.00000
66	C5	S	0.00043	0.00000	0.03335	0.00000	-0.01857
67	C5	S	-0.22116	0.00000	-0.00719	0.00000	0.01489
68	C5	PX	-0.03823	0.00000	0.17434	0.00000	-0.09375
69	C5	PY	0.07424	0.00000	0.18762	0.00000	-0.11255
70	C5	PZ	0.00000	0.46553	0.00000	-0.50393	0.00000
71	C5	S	0.80954	0.00000	-0.50311	0.00000	0.17208
72	C5	PX	-0.95662	0.00000	-0.52267	0.00000	-0.01635
73	C5	PY	-1.53713	0.00000	0.10884	0.00000	-0.42465
74	C5	PZ	0.00000	-0.65053	0.00000	0.70076	0.00000
75	C5	DXX	-0.03980	0.00000	-0.01059	0.00000	-0.00305
76	C5	DYY	-0.01855	0.00000	0.06933	0.00000	-0.03776
77	C5	DZZ	0.00464	0.00000	-0.01489	0.00000	0.01454
78	C5	DXY	0.05185	0.00000	0.02387	0.00000	-0.03634
79	C5	DXZ	0.00000	0.01951	0.00000	-0.02823	0.00000
80	C5	DYZ	0.00000	-0.04022	0.00000	-0.02646	0.00000
81	C6	S	0.01053	0.00000	-0.00790	0.00000	-0.00063
82	C6	S	0.13540	0.00000	0.06339	0.00000	-0.00196
83	C6	PX	0.43682	0.00000	0.30853	0.00000	-0.05325
84	C6	PY	0.15271	0.00000	-0.20912	0.00000	-0.04044
85	C6	PZ	0.00000	-0.48219	0.00000	-0.09535	0.00000
86	C6	S	-0.70020	0.00000	-0.25069	0.00000	0.56499
87	C6	PX	1.23486	0.00000	-0.09528	0.00000	0.25634
88	C6	PY	0.34160	0.00000	0.16275	0.00000	0.07300
89	C6	PZ	0.00000	0.71731	0.00000	0.25094	0.00000
90	C6	DXX	-0.00502	0.00000	0.00448	0.00000	0.00576
91	C6	DYY	0.03737	0.00000	-0.01294	0.00000	-0.01980
92	C6	DZZ	-0.00286	0.00000	0.00556	0.00000	0.00661
93	C6	DXY	0.00041	0.00000	0.03309	0.00000	-0.02660
94	C6	DXZ	0.00000	-0.01070	0.00000	-0.00117	0.00000
95	C6	DYZ	0.00000	0.02370	0.00000	0.00975	0.00000
96	C7	S	-0.06178	0.00000	0.00764	0.00000	-0.03640
97	C7	S	-0.02343	0.00000	0.18641	0.00000	-0.36076
98	C7	PX	-0.04706	0.00000	-0.04896	0.00000	0.19145
99	C7	PY	-0.13242	0.00000	0.02304	0.00000	0.13235
100	C7	PZ	0.00000	0.60355	0.00000	-0.15546	0.00000
101	C7	S	1.82572	0.00000	-0.48436	0.00000	1.04408
102	C7	PX	-1.49090	0.00000	0.08057	0.00000	-0.95128
103	C7	PY	-0.03240	0.00000	-0.08161	0.00000	-0.04938
104	C7	PZ	0.00000	-0.85059	0.00000	-0.00833	0.00000
105	C7	DXX	-0.08790	0.00000	-0.00842	0.00000	-0.09595
106	C7	DYY	0.01833	0.00000	0.05876	0.00000	-0.05765
107	C7	DZZ	0.03232	0.00000	-0.00773	0.00000	0.03787
108	C7	DXY	0.01353	0.00000	0.00184	0.00000	0.00132
109	C7	DXZ	0.00000	-0.03506	0.00000	0.00570	0.00000
110	C7	DYZ	0.00000	-0.00181	0.00000	-0.00027	0.00000
111	O1	S	-0.00717	0.00000	-0.00169	0.00000	0.00676
112	O1	S	0.09103	0.00000	0.08217	0.00000	-0.05542
113	O1	PX	0.16988	0.00000	0.06838	0.00000	-0.02046
114	O1	PY	-0.12904	0.00000	0.10628	0.00000	-0.04851
115	O1	PZ	0.00000	0.01604	0.00000	-0.05199	0.00000
116	O1	S	-0.78626	0.00000	0.05441	0.00000	-0.14466

117	O1	PX	0.15651	0.00000	-0.04200	0.00000	0.11565
118	O1	PY	0.11852	0.00000	-0.09659	0.00000	0.14831
119	O1	PZ	0.00000	-0.06869	0.00000	-0.00518	0.00000
120	O1	DXX	0.01259	0.00000	-0.01748	0.00000	-0.00636
121	O1	DYY	-0.09578	0.00000	0.10010	0.00000	-0.04003
122	O1	DZZ	0.06589	0.00000	0.00535	0.00000	-0.00060
123	O1	DXY	-0.02507	0.00000	0.00564	0.00000	-0.00553
124	O1	DXZ	0.00000	0.01944	0.00000	-0.03078	0.00000
125	O1	DYZ	0.00000	0.02337	0.00000	0.00992	0.00000
126	H4	S	-0.21659	0.00000	0.07321	0.00000	-0.00380
127	H4	S	0.17630	0.00000	-0.13389	0.00000	0.04255
128	H4	PX	0.02334	0.00000	-0.00536	0.00000	-0.00168
129	H4	PY	-0.00680	0.00000	0.00999	0.00000	-0.00630
130	H4	PZ	0.00000	-0.00780	0.00000	-0.00252	0.00000
131	N1	S	-0.01260	0.00000	0.01581	0.00000	0.00699
132	N1	S	0.02038	0.00000	-0.06815	0.00000	0.00989
133	N1	PX	0.11042	0.00000	-0.05303	0.00000	-0.17831
134	N1	PY	0.10199	0.00000	0.04603	0.00000	-0.06151
135	N1	PZ	0.00000	-0.15115	0.00000	0.06565	0.00000
136	N1	S	0.55006	0.00000	0.40273	0.00000	-0.32647
137	N1	PX	-0.37202	0.00000	0.18751	0.00000	-0.04333
138	N1	PY	0.58911	0.00000	-0.04819	0.00000	-0.01638
139	N1	PZ	0.00000	-0.06299	0.00000	-0.22620	0.00000
140	N1	DXX	0.02146	0.00000	0.00995	0.00000	-0.01106
141	N1	DYY	-0.02181	0.00000	0.03966	0.00000	0.01327
142	N1	DZZ	-0.01889	0.00000	-0.04135	0.00000	0.02923
143	N1	DXY	0.00811	0.00000	-0.04159	0.00000	0.00867
144	N1	DXZ	0.00000	-0.02133	0.00000	-0.00054	0.00000
145	N1	DYZ	0.00000	-0.03640	0.00000	0.00054	0.00000
146	H6	S	-0.24512	0.00000	-0.16397	0.00000	0.14713
147	H6	S	-0.11608	0.00000	0.02561	0.00000	0.01340
148	H6	PX	0.01858	0.00000	0.00783	0.00000	-0.00672
149	H6	PY	0.00091	0.00000	0.00411	0.00000	-0.00853
150	H6	PZ	0.00000	-0.00967	0.00000	0.00170	0.00000
151	C8	S	0.02882	0.00000	-0.04853	0.00000	-0.04591
152	C8	S	0.00749	0.00000	0.43293	0.00000	0.09510
153	C8	PX	-0.20835	0.00000	-0.08793	0.00000	0.02292
154	C8	PY	-0.03254	0.00000	-0.11832	0.00000	-0.46663
155	C8	PZ	0.00000	-0.27001	0.00000	-0.44768	0.00000
156	C8	S	-0.55725	0.00000	-0.20012	0.00000	-0.06071
157	C8	PX	-0.54332	0.00000	0.39702	0.00000	-0.34087
158	C8	PY	-1.02123	0.00000	-0.33149	0.00000	0.05370
159	C8	PZ	0.00000	0.48300	0.00000	0.66663	0.00000
160	C8	DXX	0.02431	0.00000	0.05669	0.00000	-0.01864
161	C8	DYY	0.01403	0.00000	-0.04488	0.00000	-0.09506
162	C8	DZZ	-0.01649	0.00000	0.02926	0.00000	0.04281
163	C8	DXY	0.00963	0.00000	0.06314	0.00000	0.01108
164	C8	DXZ	0.00000	0.01257	0.00000	-0.00449	0.00000
165	C8	DYZ	0.00000	0.03293	0.00000	-0.01304	0.00000
166	H8	S	-0.29557	0.00000	-0.10073	0.00000	-0.11294
167	H8	S	0.85416	0.00000	0.12151	0.00000	0.48349
168	H8	PX	-0.02851	0.00000	-0.00394	0.00000	-0.02843
169	H8	PY	-0.00299	0.00000	0.00201	0.00000	0.01026
170	H8	PZ	0.00000	-0.00648	0.00000	-0.00451	0.00000

171	C10	S	-0.00860	0.00000	0.05513	0.00000	0.07885
172	C10	S	0.07080	0.00000	0.11322	0.00000	0.45964
173	C10	PX	-0.07025	0.00000	0.11399	0.00000	-0.02502
174	C10	PY	0.01753	0.00000	-0.39407	0.00000	-0.29143
175	C10	PZ	0.00000	-0.01667	0.00000	0.33851	0.00000
176	C10	S	-0.53161	0.00000	-0.92507	0.00000	-1.40023
177	C10	PX	0.52250	0.00000	-0.20005	0.00000	0.31852
178	C10	PY	-0.09412	0.00000	0.25380	0.00000	0.33500
179	C10	PZ	0.00000	-0.06091	0.00000	-0.51099	0.00000
180	C10	DXX	0.01349	0.00000	0.07318	0.00000	0.11999
181	C10	DYY	-0.02294	0.00000	0.07700	0.00000	0.16867
182	C10	DZZ	0.00682	0.00000	-0.05733	0.00000	-0.07052
183	C10	DXY	-0.03341	0.00000	-0.03045	0.00000	-0.00694
184	C10	DXZ	0.00000	-0.00664	0.00000	0.00720	0.00000
185	C10	DYZ	0.00000	-0.02679	0.00000	-0.01586	0.00000
186	H16	S	0.03736	0.00000	0.29469	0.00000	0.36124
187	H16	S	-0.31175	0.00000	0.05732	0.00000	-0.01681
188	H16	PX	0.00651	0.00000	0.00361	0.00000	0.02126
189	H16	PY	-0.00413	0.00000	-0.00812	0.00000	-0.01239
190	H16	PZ	0.00000	-0.00059	0.00000	0.00549	0.00000
191	H18	S	-0.06046	0.00000	0.19439	0.00000	0.43865
192	H18	S	0.33605	0.00000	0.09860	0.00000	0.31388
193	H18	PX	0.00753	0.00000	0.00132	0.00000	-0.00204
194	H18	PY	0.01369	0.00000	-0.00916	0.00000	-0.01708
195	H18	PZ	0.00000	0.00601	0.00000	0.00421	0.00000
196	C9	S	0.00492	0.00000	0.01228	0.00000	-0.00963
197	C9	S	-0.09949	0.00000	-0.02118	0.00000	-0.01051
198	C9	PX	0.22409	0.00000	0.15919	0.00000	-0.03529
199	C9	PY	-0.01130	0.00000	0.13336	0.00000	-0.06838
200	C9	PZ	0.00000	0.14791	0.00000	-0.08375	0.00000
201	C9	S	0.10245	0.00000	-0.03912	0.00000	0.05151
202	C9	PX	-0.27470	0.00000	-0.22414	0.00000	0.09281
203	C9	PY	0.21273	0.00000	-0.30930	0.00000	0.18107
204	C9	PZ	0.00000	-0.29104	0.00000	0.05261	0.00000
205	C9	DXX	-0.00263	0.00000	0.04381	0.00000	-0.01621
206	C9	DYY	0.00222	0.00000	-0.01622	0.00000	-0.01238
207	C9	DZZ	-0.00663	0.00000	-0.00647	0.00000	0.00646
208	C9	DXY	0.05010	0.00000	-0.00966	0.00000	0.00022
209	C9	DXZ	0.00000	-0.00775	0.00000	0.02976	0.00000
210	C9	DYZ	0.00000	-0.02486	0.00000	-0.00303	0.00000
211	H3	S	-0.02165	0.00000	0.00156	0.00000	-0.06189
212	H3	S	-0.17468	0.00000	0.20443	0.00000	-0.07219
213	H3	PX	0.01547	0.00000	-0.00217	0.00000	-0.00244
214	H3	PY	0.01011	0.00000	-0.00809	0.00000	-0.00044
215	H3	PZ	0.00000	-0.01020	0.00000	-0.00603	0.00000
216	H5	S	-0.01015	-0.03438	0.05344	-0.06594	-0.01105
217	H5	S	0.06683	-0.05369	-0.02044	0.04675	-0.02836
218	H5	PX	-0.00534	0.01039	0.01084	-0.01001	-0.00413
219	H5	PY	0.00989	0.00781	-0.00110	-0.00142	0.00333
220	H5	PZ	0.00605	-0.01059	0.00420	0.00844	-0.00014
221	H7	S	-0.01015	0.03438	0.05344	0.06594	-0.01105
222	H7	S	0.06683	0.05369	-0.02044	-0.04675	-0.02836
223	H7	PX	-0.00534	-0.01039	0.01084	0.01001	-0.00413
224	H7	PY	0.00989	-0.00781	-0.00110	0.00142	0.00333

225	H7	PZ	-0.00605	-0.01059	-0.00420	0.00844	0.00014
MO:			86	87	88	89	90
Eigenvalues:			0.92840	0.96524	0.97925	0.98288	0.99443
(ev):			25.26314	26.26542	26.64664	26.74547	27.05974
			A	A	A	A	A
1	H1	S	-0.22739	0.00000	-0.08795	0.00000	0.01319
2	H1	S	0.66028	0.00000	0.28861	0.00000	0.27057
3	H1	PX	-0.01928	0.00000	0.00135	0.00000	0.00319
4	H1	PY	0.00009	0.00000	-0.01430	0.00000	0.01922
5	H1	PZ	0.00000	-0.00060	0.00000	-0.02139	0.00000
6	C1	S	-0.06019	0.00000	-0.00180	0.00000	-0.00057
7	C1	S	-0.07939	0.00000	-0.10237	0.00000	-0.05336
8	C1	PX	-0.25856	0.00000	0.00946	0.00000	-0.05233
9	C1	PY	0.32233	0.00000	-0.11620	0.00000	-0.01527
10	C1	PZ	0.00000	-0.15672	0.00000	0.46187	0.00000
11	C1	S	0.70415	0.00000	-1.10229	0.00000	0.14230
12	C1	PX	-0.84845	0.00000	0.33114	0.00000	-0.33809
13	C1	PY	0.86298	0.00000	-0.65986	0.00000	0.27074
14	C1	PZ	0.00000	0.22774	0.00000	-0.95542	0.00000
15	C1	DXX	-0.12183	0.00000	-0.03698	0.00000	-0.02373
16	C1	DYY	-0.05436	0.00000	-0.03478	0.00000	0.01358
17	C1	DZZ	0.08502	0.00000	0.00783	0.00000	0.00287
18	C1	DXY	0.00584	0.00000	0.01709	0.00000	0.03253
19	C1	DXZ	0.00000	-0.01644	0.00000	-0.02301	0.00000
20	C1	DYZ	0.00000	0.02710	0.00000	-0.02791	0.00000
21	C2	S	0.05445	0.00000	-0.01156	0.00000	-0.02222
22	C2	S	0.08319	0.00000	0.07179	0.00000	-0.12196
23	C2	PX	-0.03129	0.00000	0.06610	0.00000	0.03511
24	C2	PY	-0.23285	0.00000	0.08509	0.00000	-0.02970
25	C2	PZ	0.00000	0.29503	0.00000	0.06911	0.00000
26	C2	S	-0.58379	0.00000	-0.33960	0.00000	0.18629
27	C2	PX	0.34225	0.00000	-0.68502	0.00000	0.29006
28	C2	PY	-1.50115	0.00000	0.46260	0.00000	-0.12505
29	C2	PZ	0.00000	-0.59174	0.00000	-0.05907	0.00000
30	C2	DXX	0.09618	0.00000	0.01214	0.00000	-0.05094
31	C2	DYY	0.06226	0.00000	-0.05582	0.00000	-0.01831
32	C2	DZZ	-0.06793	0.00000	0.01615	0.00000	0.02551
33	C2	DXY	0.00868	0.00000	-0.01874	0.00000	0.02665
34	C2	DXZ	0.00000	0.01525	0.00000	0.02282	0.00000
35	C2	DYZ	0.00000	-0.00253	0.00000	0.00610	0.00000
36	C3	S	-0.01582	0.00000	0.00863	0.00000	0.00126
37	C3	S	-0.19146	0.00000	0.17739	0.00000	-0.10964
38	C3	PX	0.24530	0.00000	-0.04789	0.00000	0.15762
39	C3	PY	-0.22289	0.00000	-0.05450	0.00000	0.21939
40	C3	PZ	0.00000	-0.65606	0.00000	-0.32864	0.00000
41	C3	S	0.09985	0.00000	-0.33674	0.00000	-0.25453
42	C3	PX	0.99313	0.00000	-0.52446	0.00000	0.08703
43	C3	PY	1.03287	0.00000	0.32220	0.00000	-0.20462
44	C3	PZ	0.00000	0.98464	0.00000	0.55541	0.00000
45	C3	DXX	-0.03010	0.00000	0.01574	0.00000	-0.01374
46	C3	DYY	-0.06806	0.00000	0.02953	0.00000	0.00150
47	C3	DZZ	0.01526	0.00000	-0.00399	0.00000	-0.00064

48	C3	DXY	0.00308	0.00000	-0.02449	0.00000	0.04554
49	C3	DXZ	0.00000	0.02360	0.00000	0.00930	0.00000
50	C3	DYZ	0.00000	-0.02928	0.00000	0.06100	0.00000
51	C4	S	0.03968	0.00000	-0.00085	0.00000	-0.00046
52	C4	S	-0.42280	0.00000	-0.10270	0.00000	-0.12075
53	C4	PX	-0.09967	0.00000	-0.24993	0.00000	-0.22286
54	C4	PY	0.30436	0.00000	-0.18184	0.00000	-0.02685
55	C4	PZ	0.00000	0.57123	0.00000	-0.35352	0.00000
56	C4	S	0.24497	0.00000	0.16905	0.00000	0.04372
57	C4	PX	-1.61764	0.00000	2.18827	0.00000	0.17054
58	C4	PY	0.66486	0.00000	0.40570	0.00000	0.25751
59	C4	PZ	0.00000	-1.05073	0.00000	0.83654	0.00000
60	C4	DXX	0.02670	0.00000	0.02731	0.00000	-0.00776
61	C4	DYY	-0.00806	0.00000	-0.01026	0.00000	0.01808
62	C4	DZZ	-0.04244	0.00000	-0.01901	0.00000	-0.00926
63	C4	DXY	-0.05513	0.00000	-0.00604	0.00000	-0.00057
64	C4	DXZ	0.00000	-0.00308	0.00000	-0.00181	0.00000
65	C4	DYZ	0.00000	0.00274	0.00000	-0.03244	0.00000
66	C5	S	-0.04468	0.00000	0.00929	0.00000	0.02025
67	C5	S	0.20510	0.00000	0.22005	0.00000	0.01768
68	C5	PX	0.09496	0.00000	0.13582	0.00000	0.07697
69	C5	PY	-0.18193	0.00000	0.28917	0.00000	-0.03707
70	C5	PZ	0.00000	-0.34308	0.00000	0.18726	0.00000
71	C5	S	0.30636	0.00000	0.63749	0.00000	-0.00097
72	C5	PX	-1.20725	0.00000	1.06499	0.00000	-0.33890
73	C5	PY	-1.33336	0.00000	-0.23281	0.00000	0.08220
74	C5	PZ	0.00000	0.80194	0.00000	-0.42748	0.00000
75	C5	DXX	-0.02576	0.00000	0.08261	0.00000	0.03927
76	C5	DYY	-0.03889	0.00000	0.05840	0.00000	0.01858
77	C5	DZZ	0.05420	0.00000	-0.03352	0.00000	-0.01455
78	C5	DXY	0.01276	0.00000	0.01603	0.00000	-0.03728
79	C5	DXZ	0.00000	0.00210	0.00000	0.01801	0.00000
80	C5	DYZ	0.00000	-0.01292	0.00000	-0.01392	0.00000
81	C6	S	0.00153	0.00000	0.02067	0.00000	-0.05143
82	C6	S	0.25154	0.00000	-0.18898	0.00000	0.08236
83	C6	PX	-0.09277	0.00000	0.02622	0.00000	0.13379
84	C6	PY	0.29305	0.00000	0.15482	0.00000	-0.39844
85	C6	PZ	0.00000	-0.05743	0.00000	-0.24174	0.00000
86	C6	S	-0.49502	0.00000	0.74267	0.00000	-0.17584
87	C6	PX	1.81713	0.00000	-0.61606	0.00000	0.03615
88	C6	PY	-0.46637	0.00000	-0.20521	0.00000	0.44290
89	C6	PZ	0.00000	0.03948	0.00000	0.25618	0.00000
90	C6	DXX	0.01698	0.00000	-0.03489	0.00000	0.02796
91	C6	DYY	0.05590	0.00000	0.06795	0.00000	-0.14939
92	C6	DZZ	0.00450	0.00000	-0.02703	0.00000	0.05653
93	C6	DXY	-0.01589	0.00000	-0.00790	0.00000	-0.00547
94	C6	DXZ	0.00000	-0.02291	0.00000	-0.02952	0.00000
95	C6	DYZ	0.00000	0.01448	0.00000	-0.00149	0.00000
96	C7	S	0.03062	0.00000	-0.00724	0.00000	-0.00276
97	C7	S	-0.02730	0.00000	0.13868	0.00000	-0.03185
98	C7	PX	0.11182	0.00000	-0.05371	0.00000	0.16538
99	C7	PY	-0.07571	0.00000	0.11411	0.00000	-0.00520
100	C7	PZ	0.00000	0.45724	0.00000	-0.17679	0.00000
101	C7	S	0.48636	0.00000	0.23891	0.00000	0.14995

102	C7	PX	-0.49509	0.00000	0.06416	0.00000	-0.79854
103	C7	PY	-0.81085	0.00000	0.02140	0.00000	0.25584
104	C7	PZ	0.00000	-0.78415	0.00000	0.38328	0.00000
105	C7	DXX	0.03612	0.00000	-0.00905	0.00000	0.03184
106	C7	DYY	0.04948	0.00000	0.02094	0.00000	-0.01289
107	C7	DZZ	-0.03690	0.00000	0.00678	0.00000	-0.00672
108	C7	DXY	-0.01621	0.00000	-0.01986	0.00000	0.03674
109	C7	DXZ	0.00000	-0.00995	0.00000	0.01139	0.00000
110	C7	DYZ	0.00000	-0.01842	0.00000	-0.02856	0.00000
111	O1	S	0.00894	0.00000	0.00058	0.00000	0.00404
112	O1	S	0.01789	0.00000	-0.17890	0.00000	-0.09474
113	O1	PX	0.06824	0.00000	-0.27921	0.00000	-0.08834
114	O1	PY	-0.08245	0.00000	-0.02057	0.00000	-0.04542
115	O1	PZ	0.00000	0.08761	0.00000	0.01137	0.00000
116	O1	S	-0.36982	0.00000	0.21415	0.00000	0.03654
117	O1	PX	0.22220	0.00000	-0.08799	0.00000	0.06574
118	O1	PY	0.15115	0.00000	-0.15725	0.00000	-0.02579
119	O1	PZ	0.00000	0.03685	0.00000	-0.13447	0.00000
120	O1	DXX	0.00140	0.00000	0.01741	0.00000	-0.00606
121	O1	DYY	0.00212	0.00000	-0.11471	0.00000	-0.05759
122	O1	DZZ	0.01727	0.00000	-0.04325	0.00000	-0.01168
123	O1	DXY	0.01307	0.00000	-0.02009	0.00000	0.00139
124	O1	DXZ	0.00000	-0.02201	0.00000	-0.02728	0.00000
125	O1	DYZ	0.00000	-0.02331	0.00000	0.01362	0.00000
126	H4	S	-0.22350	0.00000	0.13963	0.00000	0.17361
127	H4	S	0.23587	0.00000	0.41663	0.00000	-0.31007
128	H4	PX	-0.00223	0.00000	-0.00424	0.00000	-0.02445
129	H4	PY	-0.01488	0.00000	-0.00969	0.00000	0.01085
130	H4	PZ	0.00000	0.00416	0.00000	-0.01005	0.00000
131	N1	S	-0.00401	0.00000	-0.01076	0.00000	0.02509
132	N1	S	0.04179	0.00000	-0.00154	0.00000	-0.04174
133	N1	PX	0.00605	0.00000	0.23705	0.00000	-0.52713
134	N1	PY	0.07243	0.00000	0.16293	0.00000	-0.35099
135	N1	PZ	0.00000	0.03789	0.00000	0.14075	0.00000
136	N1	S	-0.37754	0.00000	-0.53573	0.00000	0.91469
137	N1	PX	-0.56519	0.00000	-0.21224	0.00000	0.82705
138	N1	PY	0.35273	0.00000	-0.20536	0.00000	0.11667
139	N1	PZ	0.00000	-0.03380	0.00000	0.03233	0.00000
140	N1	DXX	0.00986	0.00000	-0.04723	0.00000	0.08964
141	N1	DYY	-0.03924	0.00000	-0.08362	0.00000	0.15134
142	N1	DZZ	0.01075	0.00000	0.03039	0.00000	-0.04902
143	N1	DXY	0.02064	0.00000	0.01038	0.00000	-0.02072
144	N1	DXZ	0.00000	0.02497	0.00000	0.03435	0.00000
145	N1	DYZ	0.00000	-0.01414	0.00000	-0.01616	0.00000
146	H6	S	0.24167	0.00000	-0.07412	0.00000	-0.02869
147	H6	S	-0.22961	0.00000	-0.22849	0.00000	0.19131
148	H6	PX	-0.01792	0.00000	-0.00119	0.00000	0.00098
149	H6	PY	-0.00930	0.00000	0.00590	0.00000	-0.00339
150	H6	PZ	0.00000	-0.00855	0.00000	-0.00622	0.00000
151	C8	S	0.01030	0.00000	-0.00277	0.00000	-0.00701
152	C8	S	0.16149	0.00000	-0.13576	0.00000	0.24649
153	C8	PX	0.08873	0.00000	0.14909	0.00000	-0.31373
154	C8	PY	0.10064	0.00000	-0.16715	0.00000	0.27296
155	C8	PZ	0.00000	0.12806	0.00000	0.72622	0.00000

156	C8	S	-0.35120	0.00000	0.37545	0.00000	-1.07949
157	C8	PX	-1.02773	0.00000	-0.33543	0.00000	0.90358
158	C8	PY	-0.55340	0.00000	0.42030	0.00000	-0.89606
159	C8	PZ	0.00000	-0.09818	0.00000	-1.27280	0.00000
160	C8	DXX	0.01000	0.00000	0.02415	0.00000	-0.06812
161	C8	DYY	0.03283	0.00000	-0.03588	0.00000	0.04277
162	C8	DZZ	0.00230	0.00000	-0.00695	0.00000	0.02738
163	C8	DXY	-0.03100	0.00000	-0.02628	0.00000	0.05697
164	C8	DXZ	0.00000	-0.01367	0.00000	-0.01873	0.00000
165	C8	DYZ	0.00000	0.04628	0.00000	0.03309	0.00000
166	H8	S	0.13098	0.00000	-0.00663	0.00000	0.03386
167	H8	S	0.06326	0.00000	-0.02369	0.00000	0.36900
168	H8	PX	0.00491	0.00000	-0.00011	0.00000	-0.01372
169	H8	PY	-0.01404	0.00000	-0.00314	0.00000	0.00639
170	H8	PZ	0.00000	-0.00923	0.00000	0.01094	0.00000
171	C10	S	-0.00015	0.00000	0.01482	0.00000	-0.02336
172	C10	S	0.15640	0.00000	0.03953	0.00000	-0.15118
173	C10	PX	-0.08370	0.00000	0.00808	0.00000	-0.04121
174	C10	PY	0.05822	0.00000	-0.08002	0.00000	0.09289
175	C10	PZ	0.00000	-0.18885	0.00000	-0.26368	0.00000
176	C10	S	-0.38094	0.00000	0.02799	0.00000	0.00759
177	C10	PX	0.47880	0.00000	0.03097	0.00000	0.02850
178	C10	PY	-0.05516	0.00000	0.09845	0.00000	-0.11322
179	C10	PZ	0.00000	0.27487	0.00000	0.64716	0.00000
180	C10	DXX	0.02142	0.00000	0.00682	0.00000	-0.01809
181	C10	DYY	-0.00313	0.00000	0.03757	0.00000	-0.06296
182	C10	DZZ	0.00489	0.00000	-0.01541	0.00000	0.02370
183	C10	DXY	-0.00588	0.00000	-0.00204	0.00000	0.00431
184	C10	DXZ	0.00000	-0.01134	0.00000	0.00449	0.00000
185	C10	DYZ	0.00000	-0.01745	0.00000	0.00594	0.00000
186	H16	S	0.06160	0.00000	0.04543	0.00000	-0.11075
187	H16	S	-0.21335	0.00000	0.01788	0.00000	-0.07932
188	H16	PX	0.00837	0.00000	-0.00060	0.00000	0.00480
189	H16	PY	-0.01045	0.00000	-0.01035	0.00000	0.02196
190	H16	PZ	0.00000	-0.00077	0.00000	0.00816	0.00000
191	H18	S	-0.01020	0.00000	0.04418	0.00000	-0.03795
192	H18	S	0.22168	0.00000	-0.00319	0.00000	0.03310
193	H18	PX	-0.00048	0.00000	0.00039	0.00000	0.00272
194	H18	PY	0.01279	0.00000	0.00140	0.00000	-0.00552
195	H18	PZ	0.00000	0.00649	0.00000	0.00355	0.00000
196	C9	S	-0.01667	0.00000	-0.04403	0.00000	-0.03362
197	C9	S	0.07124	0.00000	-0.11890	0.00000	-0.07189
198	C9	PX	0.18050	0.00000	-0.02766	0.00000	0.07048
199	C9	PY	-0.20128	0.00000	-0.60655	0.00000	-0.30858
200	C9	PZ	0.00000	-0.14874	0.00000	-0.17265	0.00000
201	C9	S	0.01042	0.00000	0.85278	0.00000	0.51585
202	C9	PX	-0.23178	0.00000	-0.03914	0.00000	-0.10921
203	C9	PY	0.58116	0.00000	1.66054	0.00000	0.91428
204	C9	PZ	0.00000	0.32304	0.00000	0.19766	0.00000
205	C9	DXX	0.01338	0.00000	-0.11671	0.00000	-0.04676
206	C9	DYY	-0.04070	0.00000	0.07667	0.00000	-0.00633
207	C9	DZZ	0.01510	0.00000	-0.04431	0.00000	-0.01481
208	C9	DXY	0.01926	0.00000	0.03792	0.00000	0.03050
209	C9	DXZ	0.00000	0.00711	0.00000	0.05762	0.00000

210	C9	DYZ	0.00000	0.03534	0.00000	-0.02829	0.00000
211	H3	S	-0.25672	0.00000	-0.10202	0.00000	-0.21540
212	H3	S	-0.15471	0.00000	-1.27083	0.00000	-0.57564
213	H3	PX	-0.00150	0.00000	0.02033	0.00000	0.00999
214	H3	PY	0.00351	0.00000	0.06183	0.00000	0.01947
215	H3	PZ	0.00000	0.01590	0.00000	-0.01793	0.00000
216	H5	S	0.00874	0.02411	-0.26379	-0.15642	-0.13565
217	H5	S	0.02044	0.07300	0.17017	0.22212	0.05723
218	H5	PX	-0.00858	-0.01544	-0.04466	-0.02015	-0.02384
219	H5	PY	0.01640	-0.01355	0.00540	0.00499	0.01525
220	H5	PZ	0.01613	0.01128	0.02346	0.01714	0.01656
221	H7	S	0.00874	-0.02411	-0.26379	0.15642	-0.13565
222	H7	S	0.02044	-0.07300	0.17017	-0.22212	0.05723
223	H7	PX	-0.00858	0.01544	-0.04466	0.02015	-0.02384
224	H7	PY	0.01640	0.01355	0.00540	-0.00499	0.01525
225	H7	PZ	-0.01613	0.01128	-0.02346	0.01714	-0.01656

MO:	91	92	93	94	95
Eigenvalues:	1.03696	1.05039	1.05945	1.08470	1.09571
(ev):	28.21712	28.58250	28.82904	29.51622	29.81568

		A	A	A	A	A	
1	H1	S	0.00000	-0.03631	-0.15787	-0.24662	0.05396
2	H1	S	0.00000	-0.18511	0.99060	1.69870	-0.46265
3	H1	PX	0.00000	0.00583	-0.05003	-0.09496	0.02362
4	H1	PY	0.00000	0.00476	-0.03914	-0.04044	-0.00215
5	H1	PZ	-0.02666	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	-0.00128	-0.02001	-0.02458	0.01016
7	C1	S	0.00000	0.12555	0.20064	0.28612	-0.04367
8	C1	PX	0.00000	-0.12678	0.31169	0.55259	-0.14050
9	C1	PY	0.00000	0.01865	0.04827	0.28326	-0.05161
10	C1	PZ	0.12260	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.13628	-0.37854	-0.24934	-0.95596
12	C1	PX	0.00000	0.36586	-1.12336	-2.05295	0.87377
13	C1	PY	0.00000	0.08707	-0.29613	-1.01430	0.48399
14	C1	PZ	-0.70709	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.01169	-0.04465	-0.08361	0.00533
16	C1	DYY	0.00000	-0.00295	0.01047	0.06174	-0.00869
17	C1	DZZ	0.00000	0.00592	0.05267	0.04646	-0.00736
18	C1	DXY	0.00000	-0.00881	-0.06935	-0.04084	0.01642
19	C1	DXZ	-0.01467	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.01162	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.00532	0.00078	-0.01145	0.02793
22	C2	S	0.00000	-0.25025	-0.10659	0.14916	-0.41492
23	C2	PX	0.00000	0.10230	0.05869	-0.26949	0.57143
24	C2	PY	0.00000	0.05687	0.11160	-0.12437	0.19551
25	C2	PZ	-0.34990	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.35057	0.04718	0.32318	0.91828
27	C2	PX	0.00000	-0.55561	-0.28901	1.28879	-2.08669
28	C2	PY	0.00000	-0.42664	-0.23626	0.58434	-0.54618
29	C2	PZ	1.03970	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.01552	0.01682	-0.04066	0.07138
31	C2	DYY	0.00000	-0.02843	-0.02017	0.05691	-0.04275
32	C2	DZZ	0.00000	0.00337	-0.01192	0.01716	-0.05721

33	C2	DXY	0.00000	0.01592	0.00812	0.00467	0.07006
34	C2	DXZ	-0.01632	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02082	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.00077	-0.01559	0.00988	-0.00206
37	C3	S	0.00000	0.06431	-0.19429	0.21427	0.09247
38	C3	PX	0.00000	0.06778	-0.03138	-0.21534	0.00341
39	C3	PY	0.00000	-0.13295	-0.09612	0.12525	0.07870
40	C3	PZ	-0.55244	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	-0.23682	-1.02897	-1.11290	-0.09854
42	C3	PX	0.00000	-0.45898	0.44022	1.04085	0.35349
43	C3	PY	0.00000	0.59842	0.56292	-0.68465	0.33064
44	C3	PZ	1.42463	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.00435	-0.00628	0.04126	-0.01991
46	C3	DYY	0.00000	0.00039	-0.10795	-0.03508	0.03570
47	C3	DZZ	0.00000	0.01075	0.03117	0.00802	0.00634
48	C3	DXY	0.00000	0.03313	0.03595	-0.02265	0.00239
49	C3	DXZ	-0.01113	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00228	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00982	0.00137	-0.00570	-0.03230
52	C4	S	0.00000	0.14070	0.05695	-0.04576	-0.00212
53	C4	PX	0.00000	-0.06726	0.08550	-0.06239	-0.03773
54	C4	PY	0.00000	-0.03284	-0.03421	-0.01374	0.09524
55	C4	PZ	-0.24153	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.10206	-0.22687	-0.10039	-0.55333
57	C4	PX	0.00000	-0.02167	-0.17409	0.19109	0.66243
58	C4	PY	0.00000	0.41599	0.46689	0.34399	-1.50605
59	C4	PZ	0.75603	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.01456	0.01540	0.02035	-0.03016
61	C4	DYY	0.00000	0.03085	-0.01206	-0.04563	-0.11498
62	C4	DZZ	0.00000	-0.00533	0.00606	0.00856	0.03968
63	C4	DXY	0.00000	-0.02447	0.02419	0.04012	-0.06221
64	C4	DXZ	-0.00939	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.02157	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.00395	0.01022	0.01747	-0.00484
67	C5	S	0.00000	0.08271	0.03889	-0.09143	-0.60564
68	C5	PX	0.00000	-0.11692	0.15902	0.24441	0.03173
69	C5	PY	0.00000	-0.00030	-0.02739	-0.24496	-0.34615
70	C5	PZ	0.28413	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.33898	0.13620	-0.21827	1.91362
72	C5	PX	0.00000	0.25490	-0.32178	-0.83575	0.31499
73	C5	PY	0.00000	-0.53402	0.01922	1.05320	1.09794
74	C5	PZ	-0.82824	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.00910	0.01528	0.04339	-0.06258
76	C5	DYY	0.00000	0.01089	0.02702	-0.02812	0.01455
77	C5	DZZ	0.00000	0.00798	-0.01086	-0.02255	-0.03272
78	C5	DXY	0.00000	0.02302	-0.02535	-0.05637	-0.03494
79	C5	DXZ	0.00850	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00531	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00145	0.00849	-0.00332	-0.01131
82	C6	S	0.00000	-0.51445	-0.12791	-0.13738	0.01389
83	C6	PX	0.00000	0.12802	0.03015	-0.01099	-0.06690
84	C6	PY	0.00000	0.32950	0.18391	-0.00062	-0.07714
85	C6	PZ	0.61103	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.40963	0.03941	0.66179	0.52865

87	C6	PX	0.00000	-0.49228	-0.03284	0.29020	0.40371
88	C6	PY	0.00000	0.47921	0.34456	-0.33203	1.19635
89	C6	PZ	-1.45643	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.07163	-0.00733	0.01753	0.00777
91	C6	DYY	0.00000	-0.08556	-0.00911	-0.02179	0.00964
92	C6	DZZ	0.00000	0.01326	-0.00382	-0.00748	-0.00035
93	C6	DXY	0.00000	0.04219	0.02026	0.04583	-0.03169
94	C6	DXZ	0.02212	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.03439	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.01274	-0.03250	-0.00345	-0.00045
97	C7	S	0.00000	-0.01508	0.17870	0.26854	-0.06528
98	C7	PX	0.00000	-0.08260	0.73399	0.04456	0.00203
99	C7	PY	0.00000	-0.18322	0.02451	0.11007	0.01669
100	C7	PZ	0.16376	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	1.10378	0.11877	-0.16220	0.24397
102	C7	PX	0.00000	-0.30898	-3.10671	-0.34940	-0.07334
103	C7	PY	0.00000	0.31428	0.06300	-0.63836	-0.18943
104	C7	PZ	-0.71505	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.03544	-0.06211	0.00245	-0.00053
106	C7	DYY	0.00000	0.03177	0.04087	0.04434	-0.00892
107	C7	DZZ	0.00000	-0.01744	0.05805	0.00770	-0.00380
108	C7	DXY	0.00000	-0.02436	-0.01239	0.04876	0.00348
109	C7	DXZ	0.01713	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.00476	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	0.00353	0.00103	0.00106	-0.01010
112	O1	S	0.00000	-0.00739	0.03450	0.09153	0.14602
113	O1	PX	0.00000	0.05402	0.00064	-0.00665	0.02284
114	O1	PY	0.00000	-0.00856	-0.00443	0.02611	0.33820
115	O1	PZ	0.05845	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	-0.17232	-0.18604	-0.25715	0.45353
117	O1	PX	0.00000	-0.02427	0.05826	0.07036	-0.05283
118	O1	PY	0.00000	0.12283	0.08360	0.01320	-0.79896
119	O1	PZ	-0.18666	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.00775	0.01303	0.03607	0.06983
121	O1	DYY	0.00000	-0.01199	0.00309	0.01809	0.08832
122	O1	DZZ	0.00000	0.00131	0.01074	0.03348	0.02293
123	O1	DXY	0.00000	0.00550	-0.00517	0.01055	0.00777
124	O1	DXZ	-0.01964	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00163	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	-0.06353	0.05412	0.18933	0.01884
127	H4	S	0.00000	0.33268	-0.25393	-0.94894	-0.76371
128	H4	PX	0.00000	0.00485	-0.01243	-0.04372	-0.04017
129	H4	PY	0.00000	-0.01919	0.01665	0.04080	0.03091
130	H4	PZ	-0.01797	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	-0.06139	-0.01427	-0.00338	0.00197
132	N1	S	0.00000	0.20014	0.00156	0.06143	-0.07354
133	N1	PX	0.00000	-0.31201	-0.01927	0.03029	0.09529
134	N1	PY	0.00000	-0.17821	0.02157	-0.04711	-0.08478
135	N1	PZ	0.15801	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	0.26729	1.13423	-0.84569	0.37370
137	N1	PX	0.00000	0.89785	0.38862	-0.14733	-0.32382
138	N1	PY	0.00000	1.23290	0.31677	0.08477	0.33164
139	N1	PZ	-0.05732	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.05617	0.03979	-0.02669	-0.02835

141	N1	DYY	0.00000	0.01344	-0.02460	-0.01630	0.00675
142	N1	DZZ	0.00000	0.14508	0.00343	0.04399	-0.01890
143	N1	DXY	0.00000	-0.01980	-0.01701	0.02206	0.00533
144	N1	DXZ	0.01472	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.03651	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00000	0.00307	-0.01421	-0.11910	0.25773
147	H6	S	0.00000	-0.36641	-0.27609	0.94293	-1.74895
148	H6	PX	0.00000	-0.01099	-0.01355	0.04506	-0.10102
149	H6	PY	0.00000	-0.03275	-0.00063	0.01719	-0.02803
150	H6	PZ	0.02315	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.01741	-0.00655	0.00975	0.00239
152	C8	S	0.00000	-0.61982	-0.05829	0.01649	-0.04311
153	C8	PX	0.00000	0.41679	-0.06480	0.22705	0.07429
154	C8	PY	0.00000	-0.08129	0.09239	0.10183	-0.04054
155	C8	PZ	-0.39775	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	0.82808	-0.89763	-0.02811	0.04669
157	C8	PX	0.00000	-0.82734	1.00103	-1.31261	-0.58011
158	C8	PY	0.00000	-0.93337	-1.52459	-0.78680	0.33858
159	C8	PZ	0.84236	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.05058	-0.01243	0.00327	0.01097
161	C8	DYY	0.00000	-0.11508	-0.07989	0.01489	0.00053
162	C8	DZZ	0.00000	0.01426	0.03002	-0.00670	-0.00780
163	C8	DXY	0.00000	0.06506	-0.07396	0.02839	-0.01177
164	C8	DXZ	-0.01327	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	-0.00430	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	0.14150	-0.11305	-0.07125	0.02550
167	H8	S	0.00000	-0.03840	2.01648	0.28866	-0.03398
168	H8	PX	0.00000	0.02297	-0.10216	-0.01605	0.00340
169	H8	PY	0.00000	0.00128	-0.00089	0.02127	0.00316
170	H8	PZ	-0.01513	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	0.01214	-0.00780	0.00094	-0.00108
172	C10	S	0.00000	-0.31063	0.06965	0.07535	0.02058
173	C10	PX	0.00000	-0.03724	0.57430	-0.58020	-0.09354
174	C10	PY	0.00000	-0.08205	0.07567	-0.08537	0.00643
175	C10	PZ	0.04703	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	-0.41712	-1.11317	-0.45587	0.27666
177	C10	PX	0.00000	0.40253	-1.63362	1.94013	0.33411
178	C10	PY	0.00000	0.02398	-0.56424	0.16725	0.17763
179	C10	PZ	-0.27803	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	0.01870	-0.03795	0.03882	-0.00232
181	C10	DYY	0.00000	-0.03435	0.01310	-0.03512	0.00807
182	C10	DZZ	0.00000	-0.00664	0.03087	0.00388	-0.00128
183	C10	DXY	0.00000	-0.01927	0.07426	-0.06973	-0.00275
184	C10	DXZ	-0.01220	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	-0.00561	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.25316	-0.13287	0.15370	0.00266
187	H16	S	0.00000	-0.32481	1.12618	-1.15014	-0.16444
188	H16	PX	0.00000	0.02252	-0.06796	0.06196	0.00869
189	H16	PY	0.00000	-0.01067	0.03120	-0.02695	-0.00740
190	H16	PZ	-0.00925	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	0.01201	0.07663	-0.12122	-0.00549
192	H18	S	0.00000	0.25150	-0.89571	1.09647	0.17847
193	H18	PX	0.00000	-0.02242	-0.04171	0.04027	0.00722

194	H18	PY	0.00000	0.02029	-0.03224	0.05666	0.00444
195	H18	PZ	-0.00128	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00333	0.00963	0.01478	0.03405
197	C9	S	0.00000	-0.02887	0.14752	0.27062	0.14285
198	C9	PX	0.00000	0.00873	0.05535	0.11913	0.28249
199	C9	PY	0.00000	0.04174	-0.03653	-0.07906	-0.30126
200	C9	PZ	-0.21984	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	0.00383	-0.41942	-0.71182	-0.40406
202	C9	PX	0.00000	0.04803	-0.07737	-0.21799	-0.75477
203	C9	PY	0.00000	-0.08407	-0.00970	0.05053	0.62353
204	C9	PZ	0.34077	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	0.00842	0.00900	0.01505	0.00726
206	C9	DYY	0.00000	0.00102	0.03709	0.05100	0.13463
207	C9	DZZ	0.00000	-0.00880	-0.01012	-0.01185	-0.05328
208	C9	DXY	0.00000	0.00105	-0.01823	-0.01545	0.02061
209	C9	DXZ	0.07300	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	-0.03997	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.01570	0.14102	0.19946	0.40569
212	H3	S	0.00000	0.03447	-0.02227	-0.04524	-0.71288
213	H3	PX	0.00000	-0.00060	-0.00655	-0.00402	0.02257
214	H3	PY	0.00000	-0.00291	0.01040	0.01852	0.08000
215	H3	PZ	-0.02139	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.19797	-0.00566	0.00141	-0.00477	-0.03266
217	H5	S	0.36973	-0.02492	0.11218	0.23761	0.56014
218	H5	PX	-0.02508	0.00381	0.00374	0.00196	-0.01597
219	H5	PY	0.00906	-0.00353	-0.01003	-0.00827	-0.00741
220	H5	PZ	0.02066	0.00100	0.01157	0.01812	0.01825
221	H7	S	0.19797	-0.00566	0.00141	-0.00477	-0.03266
222	H7	S	-0.36973	-0.02492	0.11218	0.23761	0.56014
223	H7	PX	0.02508	0.00381	0.00374	0.00196	-0.01597
224	H7	PY	-0.00906	-0.00353	-0.01003	-0.00827	-0.00741
225	H7	PZ	0.02066	-0.00100	-0.01157	-0.01812	-0.01825

MO:	96	97	98	99	100
Eigenvalues:	1.10661	1.10759	1.11104	1.12374	1.12979
(ev):	30.11254	30.13895	30.23296	30.57848	30.74320

		A	A	A	A	A	
1	H1	S	0.00000	-0.12310	0.02617	-0.08109	0.00000
2	H1	S	0.00000	0.48044	-0.04944	1.10620	0.00000
3	H1	PX	0.00000	-0.03682	-0.00091	-0.06812	0.00000
4	H1	PY	0.00000	0.01376	0.01604	-0.02380	0.00000
5	H1	PZ	-0.00294	0.00000	0.00000	0.00000	0.00691
6	C1	S	0.00000	-0.00688	-0.00136	0.00052	0.00000
7	C1	S	0.00000	0.18057	-0.08169	0.83559	0.00000
8	C1	PX	0.00000	0.11062	0.01919	0.24713	0.00000
9	C1	PY	0.00000	0.09633	-0.10158	0.32793	0.00000
10	C1	PZ	0.26121	0.00000	0.00000	0.00000	-0.16921
11	C1	S	0.00000	0.14131	-0.03635	-0.76144	0.00000
12	C1	PX	0.00000	-0.39458	-0.04108	-1.15092	0.00000
13	C1	PY	0.00000	-0.36692	0.07331	-0.88008	0.00000
14	C1	PZ	-0.60198	0.00000	0.00000	0.00000	0.50524
15	C1	DXX	0.00000	-0.05470	-0.00448	0.01079	0.00000
16	C1	DYY	0.00000	0.07652	-0.00759	0.07349	0.00000

17	C1	DZZ	0.00000	0.00829	0.00496	0.04204	0.00000
18	C1	DXY	0.00000	-0.00110	-0.00019	-0.02287	0.00000
19	C1	DXZ	-0.02607	0.00000	0.00000	0.00000	-0.00789
20	C1	DYZ	0.01079	0.00000	0.00000	0.00000	0.00745
21	C2	S	0.00000	-0.00367	0.00936	-0.00087	0.00000
22	C2	S	0.00000	0.00427	-0.23269	-0.37780	0.00000
23	C2	PX	0.00000	-0.23634	0.43430	0.27037	0.00000
24	C2	PY	0.00000	0.03148	0.22316	0.19806	0.00000
25	C2	PZ	-0.08248	0.00000	0.00000	0.00000	-0.03746
26	C2	S	0.00000	0.42342	0.21412	0.10231	0.00000
27	C2	PX	0.00000	1.45364	-1.57363	-0.41177	0.00000
28	C2	PY	0.00000	-0.20443	-0.31815	-2.15579	0.00000
29	C2	PZ	0.19596	0.00000	0.00000	0.00000	-0.23564
30	C2	DXX	0.00000	0.03515	0.07615	0.07596	0.00000
31	C2	DYY	0.00000	0.00039	-0.05886	-0.10486	0.00000
32	C2	DZZ	0.00000	-0.00907	-0.04459	-0.03773	0.00000
33	C2	DXY	0.00000	0.01954	0.05636	0.01331	0.00000
34	C2	DXZ	-0.00378	0.00000	0.00000	0.00000	0.01890
35	C2	DYZ	0.01694	0.00000	0.00000	0.00000	0.02131
36	C3	S	0.00000	0.01331	-0.00525	-0.00724	0.00000
37	C3	S	0.00000	0.26712	0.09902	0.01158	0.00000
38	C3	PX	0.00000	0.12081	-0.04166	0.08093	0.00000
39	C3	PY	0.00000	0.14603	-0.13078	-0.07326	0.00000
40	C3	PZ	-0.22691	0.00000	0.00000	0.00000	0.28134
41	C3	S	0.00000	0.20817	-1.13588	-1.73929	0.00000
42	C3	PX	0.00000	-0.45432	0.09280	-0.05805	0.00000
43	C3	PY	0.00000	-1.10329	0.65167	0.54324	0.00000
44	C3	PZ	0.55827	0.00000	0.00000	0.00000	-0.77311
45	C3	DXX	0.00000	0.01882	-0.02461	-0.06886	0.00000
46	C3	DYY	0.00000	0.05903	-0.01857	-0.01261	0.00000
47	C3	DZZ	0.00000	-0.00896	0.01873	0.02304	0.00000
48	C3	DXY	0.00000	0.00980	0.03922	0.00555	0.00000
49	C3	DXZ	-0.01640	0.00000	0.00000	0.00000	-0.02958
50	C3	DYZ	0.00395	0.00000	0.00000	0.00000	0.00369
51	C4	S	0.00000	-0.00434	0.00518	0.00888	0.00000
52	C4	S	0.00000	-0.28591	-0.26529	-0.13134	0.00000
53	C4	PX	0.00000	-0.09314	0.05617	-0.02509	0.00000
54	C4	PY	0.00000	-0.03449	-0.13379	-0.06985	0.00000
55	C4	PZ	-0.03548	0.00000	0.00000	0.00000	0.09916
56	C4	S	0.00000	1.20742	0.77795	1.62247	0.00000
57	C4	PX	0.00000	-0.33350	-0.25338	-0.87793	0.00000
58	C4	PY	0.00000	-0.23271	0.19370	1.93784	0.00000
59	C4	PZ	0.24800	0.00000	0.00000	0.00000	-0.29024
60	C4	DXX	0.00000	-0.00468	-0.03120	0.05925	0.00000
61	C4	DYY	0.00000	-0.01145	0.06622	0.04234	0.00000
62	C4	DZZ	0.00000	-0.01424	-0.01968	-0.05136	0.00000
63	C4	DXY	0.00000	0.02392	0.04915	-0.02492	0.00000
64	C4	DXZ	0.01505	0.00000	0.00000	0.00000	0.00082
65	C4	DYZ	-0.04071	0.00000	0.00000	0.00000	0.00493
66	C5	S	0.00000	0.01821	0.02677	0.01295	0.00000
67	C5	S	0.00000	-0.44611	-0.09187	0.36228	0.00000
68	C5	PX	0.00000	0.41630	0.30704	-0.03581	0.00000
69	C5	PY	0.00000	-0.33856	-0.09491	0.35723	0.00000
70	C5	PZ	0.05867	0.00000	0.00000	0.00000	0.01515

71	C5	S	0.00000	0.41183	0.33283	0.06862	0.00000
72	C5	PX	0.00000	-1.85431	-0.51560	-0.61322	0.00000
73	C5	PY	0.00000	0.94078	0.12176	-2.55360	0.00000
74	C5	PZ	-0.20466	0.00000	0.00000	0.00000	0.09982
75	C5	DXX	0.00000	0.01083	0.01935	0.01205	0.00000
76	C5	DYY	0.00000	-0.01670	0.07655	0.06477	0.00000
77	C5	DZZ	0.00000	-0.04878	-0.06202	0.00834	0.00000
78	C5	DXY	0.00000	-0.09138	-0.12005	0.01054	0.00000
79	C5	DXZ	0.01055	0.00000	0.00000	0.00000	0.01517
80	C5	DYZ	-0.00657	0.00000	0.00000	0.00000	-0.01928
81	C6	S	0.00000	-0.00580	-0.00824	-0.00384	0.00000
82	C6	S	0.00000	0.06274	-0.07998	-0.03556	0.00000
83	C6	PX	0.00000	0.01521	-0.02924	-0.26281	0.00000
84	C6	PY	0.00000	0.13068	-0.05521	-0.19904	0.00000
85	C6	PZ	0.00165	0.00000	0.00000	0.00000	-0.34314
86	C6	S	0.00000	-1.33537	0.62073	0.02159	0.00000
87	C6	PX	0.00000	0.08634	0.10393	1.92689	0.00000
88	C6	PY	0.00000	-0.28912	1.05211	-0.30993	0.00000
89	C6	PZ	-0.05813	0.00000	0.00000	0.00000	1.08485
90	C6	DXX	0.00000	-0.03009	0.01508	-0.04735	0.00000
91	C6	DYY	0.00000	-0.00611	-0.01441	0.02500	0.00000
92	C6	DZZ	0.00000	0.01325	-0.00704	0.00962	0.00000
93	C6	DXY	0.00000	0.02705	-0.03213	0.00798	0.00000
94	C6	DXZ	0.02269	0.00000	0.00000	0.00000	0.02420
95	C6	DYZ	-0.03587	0.00000	0.00000	0.00000	-0.06000
96	C7	S	0.00000	0.00596	-0.00362	0.01124	0.00000
97	C7	S	0.00000	-0.17344	0.07891	-0.29183	0.00000
98	C7	PX	0.00000	-0.50565	0.20985	-0.23492	0.00000
99	C7	PY	0.00000	-0.11700	-0.08792	-0.00217	0.00000
100	C7	PZ	0.02435	0.00000	0.00000	0.00000	0.04102
101	C7	S	0.00000	-1.00091	0.62783	1.19777	0.00000
102	C7	PX	0.00000	2.39636	-1.03053	0.48004	0.00000
103	C7	PY	0.00000	0.48318	0.34285	0.44170	0.00000
104	C7	PZ	-0.23068	0.00000	0.00000	0.00000	-0.02069
105	C7	DXX	0.00000	0.02130	-0.01657	0.05903	0.00000
106	C7	DYY	0.00000	-0.08268	0.05736	-0.03969	0.00000
107	C7	DZZ	0.00000	-0.00001	-0.00380	-0.03997	0.00000
108	C7	DXY	0.00000	-0.04523	-0.01474	-0.03086	0.00000
109	C7	DXZ	-0.00879	0.00000	0.00000	0.00000	-0.01799
110	C7	DYZ	-0.01491	0.00000	0.00000	0.00000	-0.04032
111	O1	S	0.00000	0.00064	0.00010	0.01148	0.00000
112	O1	S	0.00000	0.02287	-0.15680	-0.05236	0.00000
113	O1	PX	0.00000	-0.03241	0.00498	0.02490	0.00000
114	O1	PY	0.00000	-0.03556	-0.24423	-0.12963	0.00000
115	O1	PZ	-0.09121	0.00000	0.00000	0.00000	0.13667
116	O1	S	0.00000	-0.10509	0.06502	-0.91737	0.00000
117	O1	PX	0.00000	0.10794	-0.02441	0.14578	0.00000
118	O1	PY	0.00000	0.03113	0.38263	0.73669	0.00000
119	O1	PZ	0.13415	0.00000	0.00000	0.00000	-0.14026
120	O1	DXX	0.00000	0.00473	-0.07386	-0.03915	0.00000
121	O1	DYY	0.00000	-0.01534	-0.08508	-0.08923	0.00000
122	O1	DZZ	0.00000	0.03261	-0.01705	0.03496	0.00000
123	O1	DXY	0.00000	0.02911	0.01296	0.00575	0.00000
124	O1	DXZ	0.08596	0.00000	0.00000	0.00000	-0.02087

125	O1	DYZ	0.04799	0.00000	0.00000	0.00000	-0.01454
126	H4	S	0.00000	0.29226	0.31306	-0.01356	0.00000
127	H4	S	0.00000	-1.56954	-0.79139	0.88323	0.00000
128	H4	PX	0.00000	-0.07144	-0.03879	0.01422	0.00000
129	H4	PY	0.00000	0.06728	0.04574	-0.04316	0.00000
130	H4	PZ	-0.00797	0.00000	0.00000	0.00000	-0.00452
131	N1	S	0.00000	-0.00885	-0.00187	0.01754	0.00000
132	N1	S	0.00000	-0.04551	-0.06977	0.05095	0.00000
133	N1	PX	0.00000	0.00077	0.20621	-0.01683	0.00000
134	N1	PY	0.00000	0.03069	-0.08081	0.04653	0.00000
135	N1	PZ	0.39910	0.00000	0.00000	0.00000	0.85409
136	N1	S	0.00000	0.22344	0.32528	-0.06610	0.00000
137	N1	PX	0.00000	-0.05061	-0.37009	-0.20380	0.00000
138	N1	PY	0.00000	0.09484	0.39755	-0.37490	0.00000
139	N1	PZ	-0.53171	0.00000	0.00000	0.00000	-1.41006
140	N1	DXX	0.00000	-0.03827	-0.03035	0.03460	0.00000
141	N1	DYY	0.00000	-0.00471	-0.01251	0.05812	0.00000
142	N1	DZZ	0.00000	0.00841	-0.01260	-0.02607	0.00000
143	N1	DXY	0.00000	-0.03253	0.00618	-0.03514	0.00000
144	N1	DXZ	0.03315	0.00000	0.00000	0.00000	0.03053
145	N1	DYZ	0.01458	0.00000	0.00000	0.00000	0.02780
146	H6	S	0.00000	0.04588	0.17155	0.29442	0.00000
147	H6	S	0.00000	0.59361	-1.31207	-1.01172	0.00000
148	H6	PX	0.00000	0.01904	-0.07703	-0.06533	0.00000
149	H6	PY	0.00000	0.01743	0.00001	-0.02046	0.00000
150	H6	PZ	0.00492	0.00000	0.00000	0.00000	-0.01641
151	C8	S	0.00000	-0.00703	0.00239	0.00318	0.00000
152	C8	S	0.00000	-0.31267	-0.06004	0.17059	0.00000
153	C8	PX	0.00000	-0.14901	0.10459	-0.12418	0.00000
154	C8	PY	0.00000	-0.23060	0.01525	0.02715	0.00000
155	C8	PZ	-0.04838	0.00000	0.00000	0.00000	-0.16153
156	C8	S	0.00000	1.43045	0.05383	-0.08289	0.00000
157	C8	PX	0.00000	0.91244	-0.65861	0.46430	0.00000
158	C8	PY	0.00000	1.40360	-0.17447	-0.24691	0.00000
159	C8	PZ	0.23707	0.00000	0.00000	0.00000	0.59227
160	C8	DXX	0.00000	-0.00516	0.04171	0.00441	0.00000
161	C8	DYY	0.00000	-0.02207	-0.02293	0.02499	0.00000
162	C8	DZZ	0.00000	-0.01093	-0.01018	0.00246	0.00000
163	C8	DXY	0.00000	0.00975	-0.00426	0.00654	0.00000
164	C8	DXZ	-0.01329	0.00000	0.00000	0.00000	0.01639
165	C8	DYZ	0.02923	0.00000	0.00000	0.00000	0.04491
166	H8	S	0.00000	0.09932	-0.05044	0.17192	0.00000
167	H8	S	0.00000	-1.41085	0.61681	-0.75540	0.00000
168	H8	PX	0.00000	0.06508	-0.02869	0.04991	0.00000
169	H8	PY	0.00000	-0.01281	0.01306	0.00240	0.00000
170	H8	PZ	-0.01101	0.00000	0.00000	0.00000	-0.00538
171	C10	S	0.00000	0.01145	-0.00736	0.00385	0.00000
172	C10	S	0.00000	-0.16354	0.00065	-0.06058	0.00000
173	C10	PX	0.00000	0.49806	-0.30519	-0.00499	0.00000
174	C10	PY	0.00000	0.10267	-0.10071	-0.04762	0.00000
175	C10	PZ	-0.04429	0.00000	0.00000	0.00000	-0.04432
176	C10	S	0.00000	0.67639	-0.05208	-0.11576	0.00000
177	C10	PX	0.00000	-1.61045	0.96337	-0.03210	0.00000
178	C10	PY	0.00000	-0.16464	0.33807	-0.08762	0.00000

179	C10	PZ	0.00923	0.00000	0.00000	0.00000	-0.08386
180	C10	DXX	0.00000	-0.01163	-0.00840	-0.00096	0.00000
181	C10	DYY	0.00000	0.03615	-0.01842	0.00186	0.00000
182	C10	DZZ	0.00000	-0.02662	0.01607	-0.01443	0.00000
183	C10	DXY	0.00000	0.07423	-0.03469	0.01821	0.00000
184	C10	DXZ	0.01172	0.00000	0.00000	0.00000	0.04713
185	C10	DYZ	-0.00757	0.00000	0.00000	0.00000	0.00100
186	H16	S	0.00000	-0.05860	0.02185	-0.04270	0.00000
187	H16	S	0.00000	0.86784	-0.46282	0.03970	0.00000
188	H16	PX	0.00000	-0.04096	0.02717	0.00137	0.00000
189	H16	PY	0.00000	0.02645	-0.01580	0.00538	0.00000
190	H16	PZ	0.00337	0.00000	0.00000	0.00000	0.00890
191	H18	S	0.00000	0.22636	-0.08757	0.06514	0.00000
192	H18	S	0.00000	-1.05406	0.65494	-0.11473	0.00000
193	H18	PX	0.00000	-0.04747	0.02954	0.00289	0.00000
194	H18	PY	0.00000	-0.05997	0.03145	-0.00793	0.00000
195	H18	PZ	-0.00145	0.00000	0.00000	0.00000	-0.01404
196	C9	S	0.00000	-0.01379	-0.03222	0.00169	0.00000
197	C9	S	0.00000	0.14500	-0.11783	0.00645	0.00000
198	C9	PX	0.00000	0.03967	-0.24027	-0.01292	0.00000
199	C9	PY	0.00000	0.07162	0.36112	0.01730	0.00000
200	C9	PZ	0.65349	0.00000	0.00000	0.00000	-0.23725
201	C9	S	0.00000	-0.25677	0.41047	-0.25680	0.00000
202	C9	PX	0.00000	-0.03070	0.57413	0.30956	0.00000
203	C9	PY	0.00000	-0.08792	-0.60743	-0.29425	0.00000
204	C9	PZ	-1.24135	0.00000	0.00000	0.00000	0.51949
205	C9	DXX	0.00000	0.00856	0.00673	-0.00343	0.00000
206	C9	DYY	0.00000	-0.05052	-0.16258	0.03810	0.00000
207	C9	DZZ	0.00000	0.02434	0.07880	-0.04540	0.00000
208	C9	DXY	0.00000	0.01610	0.01285	-0.03949	0.00000
209	C9	DXZ	-0.22602	0.00000	0.00000	0.00000	0.07476
210	C9	DYZ	0.08996	0.00000	0.00000	0.00000	-0.02756
211	H3	S	0.00000	-0.19684	-0.54593	0.24388	0.00000
212	H3	S	0.00000	0.29124	0.83694	0.02800	0.00000
213	H3	PX	0.00000	0.00589	-0.00605	-0.01923	0.00000
214	H3	PY	0.00000	-0.02620	-0.08865	0.00281	0.00000
215	H3	PZ	0.04292	0.00000	0.00000	0.00000	-0.01032
216	H5	S	0.56050	-0.02906	0.05695	-0.06884	-0.18971
217	H5	S	-1.31884	0.01506	-0.53167	-0.02543	0.50794
218	H5	PX	0.07106	-0.00516	0.00812	0.01675	-0.02734
219	H5	PY	-0.03182	0.01417	0.01972	-0.02320	0.00940
220	H5	PZ	-0.05455	0.00487	-0.02594	0.01866	0.01875
221	H7	S	-0.56050	-0.02906	0.05695	-0.06884	0.18971
222	H7	S	1.31884	0.01506	-0.53167	-0.02543	-0.50794
223	H7	PX	-0.07106	-0.00516	0.00812	0.01675	0.02734
224	H7	PY	0.03182	0.01417	0.01972	-0.02320	-0.00940
225	H7	PZ	-0.05455	-0.00487	0.02594	-0.01866	0.01875

MO:	101	102	103	104	105
Eigenvalues:	1.14664	1.16819	1.17462	1.17763	1.18515
(ev):	31.20181	31.78807	31.96313	32.04497	32.24946

	A	A	A	A	A	
1 H1	S	-0.20003	-0.10678	-0.07597	-0.03766	0.20388

2	H1	S	0.71477	0.08673	-0.04791	-0.20105	-0.76487
3	H1	PX	-0.06381	-0.00576	-0.01092	0.00718	0.03012
4	H1	PY	0.00834	-0.01348	-0.00066	-0.00058	0.01067
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00517	-0.00421	0.00882	0.00360	0.00527
7	C1	S	0.23802	-0.16266	-0.11574	-0.02955	0.17839
8	C1	PX	0.31079	0.13350	0.09571	-0.09085	-0.10577
9	C1	PY	-0.02818	-0.13247	0.06422	0.09048	-0.26580
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-1.97572	0.36233	0.24354	0.23597	0.66077
12	C1	PX	-0.50863	-0.40600	0.15311	0.38846	0.13263
13	C1	PY	-0.07102	0.49643	-0.17097	-0.42434	1.72866
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.03522	-0.00371	-0.04389	-0.01244	0.10264
16	C1	DYY	0.02461	-0.03018	0.02760	0.01572	-0.01403
17	C1	DZZ	0.02002	-0.00103	0.00462	-0.00710	-0.03640
18	C1	DXY	-0.00780	-0.05125	-0.00122	0.01815	-0.03325
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.01003	-0.01340	-0.00048	0.00017	0.00660
22	C2	S	-0.40351	-0.43948	0.13696	-0.03262	0.24628
23	C2	PX	0.24318	0.06706	0.13840	0.05281	-0.25618
24	C2	PY	-0.41579	0.10610	0.05520	-0.04797	0.05644
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	2.13108	1.41619	-0.26466	-0.03010	-1.12690
27	C2	PX	-1.17262	-0.32245	-0.53244	0.07503	0.77765
28	C2	PY	2.69939	-0.38033	0.43029	0.11130	-0.72908
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.04808	-0.05834	0.02595	0.00361	0.02626
31	C2	DYY	0.04337	-0.00939	-0.01056	-0.00443	-0.00198
32	C2	DZZ	-0.03181	-0.00858	0.00633	0.00256	0.00992
33	C2	DXY	0.03384	-0.01454	-0.00637	0.02619	-0.02312
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00746	-0.00663	0.00896	0.00932	-0.01646
37	C3	S	0.33260	-0.49182	0.38194	0.11574	-0.14504
38	C3	PX	-0.05598	-0.23292	0.00089	-0.07874	0.14432
39	C3	PY	-0.11090	0.09772	0.12692	0.14647	-0.30911
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00417	1.91913	-0.95726	-0.16243	0.37743
42	C3	PX	0.08389	1.22261	-0.37803	0.00190	-0.42078
43	C3	PY	0.38254	-0.72858	0.05381	-0.44663	1.15124
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.03359	0.00696	0.04153	0.00810	-0.06133
46	C3	DYY	0.03777	-0.01560	0.02091	0.02493	-0.00837
47	C3	DZZ	-0.01213	-0.02157	0.00487	-0.00730	0.01960
48	C3	DXY	0.04566	-0.03620	0.00872	-0.03989	0.08011
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01340	0.00639	-0.02221	-0.00987	0.01364
52	C4	S	0.55998	0.43003	-0.37387	-0.16071	0.33612
53	C4	PX	-0.36640	0.06716	0.08937	-0.04315	0.28486
54	C4	PY	0.10435	-0.08804	-0.04799	-0.08676	0.13624
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

56	C4	S	-3.31086	-1.67128	0.63601	0.85785	-0.60503
57	C4	PX	2.86900	0.06246	-0.27039	-0.02735	-2.05858
58	C4	PY	-0.99787	-0.39285	-0.03118	0.09385	0.11786
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.03837	0.00701	-0.03389	0.00735	-0.00176
61	C4	DYY	0.04362	0.03497	-0.10707	-0.03353	0.07447
62	C4	DZZ	0.02924	0.00960	0.03048	-0.00013	-0.01699
63	C4	DXY	0.01620	0.04213	-0.05009	-0.03124	0.02666
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02245	-0.00303	0.00132	0.00040	0.00022
67	C5	S	-0.08779	-0.01442	0.26844	0.12159	-0.16350
68	C5	PX	-0.53361	-0.00820	-0.24957	-0.04508	0.16941
69	C5	PY	-0.25572	-0.09504	0.31706	-0.01248	0.04165
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.12638	0.34511	-1.28885	-0.47871	0.03664
72	C5	PX	3.12324	0.24173	0.87239	-0.04849	-1.29526
73	C5	PY	2.38858	0.63313	-0.74333	-0.17157	-0.72941
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.07795	0.02342	-0.04619	-0.00166	-0.02823
76	C5	DYY	-0.11619	-0.01614	0.01927	-0.00204	0.01967
77	C5	DZZ	0.01540	0.00121	0.04160	0.01353	-0.01723
78	C5	DXY	0.00191	0.01464	0.03390	-0.00040	-0.01996
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01434	0.00688	0.00259	-0.00850	0.00502
82	C6	S	-0.19986	0.18584	0.03687	-0.37448	0.13800
83	C6	PX	0.13007	-0.00079	0.02739	-0.00194	-0.09570
84	C6	PY	0.05052	0.04822	-0.02766	0.07218	-0.03917
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	2.44592	-0.83770	0.79772	0.75735	-1.19029
87	C6	PX	-1.16233	0.39477	-0.46039	-0.04088	0.32666
88	C6	PY	-0.76368	0.65884	-0.56410	-0.29969	0.26450
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.04021	0.01217	0.01778	-0.04381	0.00422
91	C6	DYY	0.04488	0.02006	0.02550	-0.01239	-0.04127
92	C6	DZZ	-0.04330	-0.00252	-0.00851	0.00041	0.01380
93	C6	DXY	-0.01902	0.03373	-0.00708	0.03095	-0.02493
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00940	-0.01745	-0.00404	0.00425	0.01578
97	C7	S	0.22431	-0.62707	0.20511	0.20731	-0.03401
98	C7	PX	-0.04728	-0.15428	0.05009	-0.12853	0.09941
99	C7	PY	-0.22602	0.44943	-0.07338	0.08027	-0.44542
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.21570	1.28348	-0.28850	-0.45449	-0.13912
102	C7	PX	0.63799	0.22417	-0.26508	0.59969	-0.14113
103	C7	PY	0.87035	-2.26304	0.65825	-0.13855	1.46064
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00498	-0.00213	-0.00180	0.03879	-0.01930
106	C7	DYY	0.01714	-0.09689	0.01458	-0.00935	0.03687
107	C7	DZZ	0.00124	-0.00603	0.00961	-0.00068	-0.00515
108	C7	DXY	-0.04715	0.09715	-0.01574	0.02069	-0.06391
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00805	-0.01061	-0.00213	0.00012	0.00301
112	O1	S	-0.16892	-0.17014	0.27850	0.08461	-0.19641
113	O1	PX	0.20919	0.04696	-0.22833	-0.07138	0.02161
114	O1	PY	-0.11630	-0.11409	0.11984	0.05714	-0.04909
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.98819	0.80080	-0.25642	-0.20035	0.41087
117	O1	PX	-0.58907	-0.10741	0.39592	0.14497	0.20031
118	O1	PY	-0.24601	-0.09421	-0.20476	-0.01953	0.18589
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.05067	-0.04089	0.10763	0.03338	-0.06025
121	O1	DYY	0.00201	-0.03771	0.08308	0.00317	-0.02923
122	O1	DZZ	-0.12072	-0.10013	0.08868	0.04461	-0.08757
123	O1	DXY	0.00029	-0.01674	0.04787	0.02606	-0.02959
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.08356	-0.06733	-0.09411	0.00378	0.03941
127	H4	S	0.28429	-0.17680	1.09115	0.16408	-0.36203
128	H4	PX	0.00739	0.00269	0.04635	-0.00265	-0.00521
129	H4	PY	-0.03811	0.00439	-0.03816	-0.01229	0.02089
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00694	-0.00940	0.01110	-0.00949	-0.00052
132	N1	S	-0.06107	0.10825	-0.07349	-0.00858	0.08266
133	N1	PX	-0.00161	-0.01208	-0.00775	-0.18097	0.15605
134	N1	PY	0.13209	0.03397	-0.04997	0.03489	-0.05709
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.77712	0.29957	-0.38373	-0.12056	0.15982
137	N1	PX	0.09621	0.02421	0.10865	0.42586	-0.42377
138	N1	PY	-0.88707	0.49606	-0.42717	-0.13631	0.34839
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00403	0.02726	-0.00965	-0.01500	0.00250
141	N1	DYY	-0.07636	0.03173	-0.02322	-0.02890	0.05091
142	N1	DZZ	0.00528	-0.01196	0.00131	0.04060	-0.00545
143	N1	DXY	-0.01663	0.03105	-0.00978	-0.01820	-0.01485
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.05383	-0.13782	0.07007	0.09683	-0.02689
147	H6	S	-0.45080	-0.39645	-0.22824	-0.00484	0.49298
148	H6	PX	-0.03034	-0.01162	-0.01878	-0.00721	0.03164
149	H6	PY	-0.02271	-0.01437	0.00146	-0.01346	0.02268
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.00600	0.01925	-0.00445	0.00047	-0.00974
152	C8	S	-0.04913	0.36273	-0.19416	0.18178	-0.16815
153	C8	PX	-0.26067	0.34130	-0.13295	0.01867	-0.05912
154	C8	PY	-0.12096	0.23742	-0.03568	-0.11802	-0.13126
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.40313	-1.38695	0.49358	-0.46983	0.87188
157	C8	PX	1.02411	-1.46553	0.55939	0.17345	0.27864
158	C8	PY	1.37325	-1.15792	0.11697	0.15788	0.84439
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00762	-0.02302	-0.01013	-0.02792	0.06430
161	C8	DYY	0.00616	0.06587	-0.01005	-0.00308	-0.05683
162	C8	DZZ	-0.01090	0.00481	-0.00527	0.01636	-0.00512
163	C8	DXY	0.02515	-0.06768	0.01432	0.02978	0.03386

164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.09255	0.03154	-0.02469	0.01918	0.03142
167	H8	S	-0.09934	-0.59593	0.31407	-0.39009	0.20660
168	H8	PX	-0.00910	0.04253	-0.01394	0.00620	-0.00813
169	H8	PY	0.00406	-0.00823	0.00511	-0.00798	0.02037
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00556	0.00740	0.00715	-0.01893	-0.01301
172	C10	S	-0.05148	0.19632	-0.33812	0.99306	-0.03232
173	C10	PX	0.04867	0.07408	-0.05942	0.16977	-0.11219
174	C10	PY	-0.00343	0.18581	0.14558	-0.50497	-0.25379
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.80049	-0.42904	0.60750	-2.06809	0.18155
177	C10	PX	-0.42862	0.01508	0.11369	-0.31916	0.14401
178	C10	PY	0.27929	-0.54960	-0.27087	0.87379	0.74511
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.02112	0.05039	0.04248	-0.14717	-0.06652
181	C10	DYY	0.00741	0.00742	-0.03067	0.10789	-0.00411
182	C10	DZZ	0.00526	-0.02615	-0.03945	0.12961	0.04740
183	C10	DXY	-0.00121	0.00623	0.03136	-0.05484	-0.03679
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.12297	0.16498	0.09960	-0.54482	-0.10191
187	H16	S	0.25178	-0.17985	-0.37392	1.31945	0.19548
188	H16	PX	-0.00667	-0.00559	0.03711	-0.11270	-0.00428
189	H16	PY	0.01229	-0.02209	0.01251	0.00644	-0.00422
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.02860	-0.08736	0.24363	-0.47483	-0.14578
192	H18	S	-0.15377	-0.21689	-0.39165	1.15214	0.57292
193	H18	PX	0.00672	-0.02756	-0.02522	0.09174	0.03810
194	H18	PY	-0.01658	0.01203	-0.02070	0.03124	0.01759
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.01236	-0.02849	0.00799	0.00547	-0.03432
197	C9	S	-0.06911	0.57228	1.25476	0.40205	0.51909
198	C9	PX	0.07609	0.16679	0.17055	0.03054	0.29920
199	C9	PY	-0.02740	0.10872	0.23477	0.13860	-0.05993
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.47601	-1.17172	-3.04260	-1.04100	-1.25220
202	C9	PX	-0.21715	-0.24607	-0.36210	-0.03775	-0.32452
203	C9	PY	0.24417	-0.17398	-0.32523	-0.24162	-0.06693
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.03379	0.04808	0.05331	0.01569	0.04232
206	C9	DYY	-0.00624	0.00176	-0.02027	-0.01486	0.07522
207	C9	DZZ	-0.04445	-0.04389	0.08540	0.03831	-0.14096
208	C9	DXY	0.02616	0.03219	0.05260	0.02504	-0.00925
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.18089	-0.27685	-0.30122	-0.10247	0.01494
212	H3	S	-0.20351	0.47793	1.15773	0.49988	0.08984
213	H3	PX	-0.00377	0.00831	0.04010	0.01852	-0.00587
214	H3	PY	-0.01167	-0.05317	-0.06557	-0.02706	-0.01898
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.11222	-0.27764	-0.07562	-0.00761	-0.43512
217	H5	S	0.02722	0.48511	0.75554	0.20346	0.76038

218	H5	PX	0.00496	-0.00882	-0.03493	-0.01149	-0.00289
219	H5	PY	0.00447	0.01474	0.03049	0.01029	-0.00099
220	H5	PZ	0.01744	0.04893	0.02318	0.00138	0.08127
221	H7	S	-0.11222	-0.27764	-0.07562	-0.00761	-0.43512
222	H7	S	0.02722	0.48511	0.75554	0.20346	0.76038
223	H7	PX	0.00496	-0.00882	-0.03493	-0.01149	-0.00289
224	H7	PY	0.00447	0.01474	0.03049	0.01029	-0.00099
225	H7	PZ	-0.01744	-0.04893	-0.02318	-0.00138	-0.08127

M0:	106	107	108	109	110
Eigenvalues:	1.21214	1.24414	1.26238	1.28992	1.31200
(ev):	32.98403	33.85491	34.35121	35.10064	35.70137

			A	A	A	A	A
1	H1	S	-0.21684	0.10511	0.14845	-0.02904	0.00000
2	H1	S	0.92582	0.69236	0.51114	0.70170	0.00000
3	H1	PX	-0.04564	-0.03309	-0.00218	-0.01319	0.00000
4	H1	PY	0.00637	0.00951	0.02277	-0.01011	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.03548
6	C1	S	0.00014	-0.00323	-0.00353	-0.00175	0.00000
7	C1	S	0.14693	-0.13303	0.57927	0.17415	0.00000
8	C1	PX	0.24925	0.37690	-0.01844	0.21698	0.00000
9	C1	PY	-0.07951	-0.06265	-0.33775	-0.30189	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.01390
11	C1	S	-0.87398	0.36068	-0.44056	-0.30671	0.00000
12	C1	PX	-0.77387	-1.07033	-1.28753	-0.71555	0.00000
13	C1	PY	-0.03738	0.29432	1.66558	0.20174	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.21785
15	C1	DXX	-0.05619	-0.04457	0.07925	-0.00427	0.00000
16	C1	DYY	0.05271	-0.01272	0.01317	0.02305	0.00000
17	C1	DZZ	0.02848	0.03999	0.01289	0.02255	0.00000
18	C1	DXY	-0.02345	-0.02680	0.01112	-0.06611	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.08396
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00360
21	C2	S	-0.02085	0.00693	0.00160	0.01114	0.00000
22	C2	S	-0.35139	0.31731	0.05248	0.02432	0.00000
23	C2	PX	-0.15789	0.26498	-0.10126	0.02719	0.00000
24	C2	PY	0.35363	-0.06370	0.06379	-0.12691	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.04122
26	C2	S	1.55560	-0.52828	-0.36334	0.09000	0.00000
27	C2	PX	0.35162	-1.36803	0.82629	-0.06519	0.00000
28	C2	PY	-1.81122	2.08660	-0.25918	0.45881	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.01100
30	C2	DXX	-0.03936	0.03295	0.04439	0.00069	0.00000
31	C2	DYY	-0.03216	0.04995	-0.05189	0.02117	0.00000
32	C2	DZZ	0.02102	-0.03604	0.02401	-0.01806	0.00000
33	C2	DXY	-0.13341	0.03193	-0.00570	0.02561	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.03471
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00073
36	C3	S	-0.00013	-0.00937	-0.01052	-0.02177	0.00000
37	C3	S	0.15695	-0.16640	0.22837	-0.67691	0.00000
38	C3	PX	0.07443	0.23517	-0.28117	0.22769	0.00000
39	C3	PY	0.01834	-0.01184	-0.32622	-0.09252	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.06487

41	C3	S	-1.14572	2.07966	0.68063	1.10364	0.00000
42	C3	PX	0.34925	-1.28077	1.57095	-1.37294	0.00000
43	C3	PY	0.07034	-0.84208	0.54933	0.00485	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.04037
45	C3	DXX	-0.00420	0.04583	-0.00273	-0.10594	0.00000
46	C3	DYY	0.00950	-0.02016	0.05300	-0.06192	0.00000
47	C3	DZZ	0.01496	-0.00625	0.00203	0.03893	0.00000
48	C3	DXY	0.06571	0.08598	0.03538	0.04433	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	-0.02804
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00753
51	C4	S	0.00976	-0.01933	-0.00720	-0.00344	0.00000
52	C4	S	0.12006	-0.44846	-0.18026	0.29140	0.00000
53	C4	PX	-0.19026	0.27922	-0.00718	-0.01154	0.00000
54	C4	PY	-0.02341	0.19748	0.06910	-0.24838	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.16381
56	C4	S	-1.57462	0.23481	-0.74958	-1.50099	0.00000
57	C4	PX	1.35779	-0.83939	-1.27590	0.43759	0.00000
58	C4	PY	-0.10404	-0.41852	0.58809	0.32299	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.69294
60	C4	DXX	-0.01790	-0.06747	-0.07124	0.03832	0.00000
61	C4	DYY	-0.03703	-0.04126	-0.03021	-0.09389	0.00000
62	C4	DZZ	0.02894	0.02705	0.03266	0.02599	0.00000
63	C4	DXY	-0.00380	0.05902	-0.02974	0.03162	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00700
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	-0.06147
66	C5	S	-0.01406	0.02573	-0.01000	-0.00792	0.00000
67	C5	S	-0.53880	0.62714	-0.30958	0.18540	0.00000
68	C5	PX	-0.15006	-0.00840	-0.06003	0.08041	0.00000
69	C5	PY	0.22151	0.11783	0.15149	-0.23924	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.06600
71	C5	S	2.54324	-3.06001	0.05453	0.22546	0.00000
72	C5	PX	0.80489	0.56768	-0.09964	0.03376	0.00000
73	C5	PY	-0.18922	0.50219	-1.04922	0.87647	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.07711
75	C5	DXX	-0.03524	0.00330	-0.06985	0.05628	0.00000
76	C5	DYY	-0.04361	0.07013	-0.01293	-0.01525	0.00000
77	C5	DZZ	0.01826	-0.00066	0.02794	-0.00231	0.00000
78	C5	DXY	0.10458	-0.06102	-0.01080	0.03842	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.05756
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	-0.05389
81	C6	S	0.02446	0.00443	-0.00344	0.00929	0.00000
82	C6	S	0.87775	0.27574	-0.39825	-0.24555	0.00000
83	C6	PX	-0.31966	0.49141	-0.17371	0.10802	0.00000
84	C6	PY	0.06245	0.07181	0.24238	0.08697	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.06706
86	C6	S	-3.18225	-0.44922	1.99264	0.27736	0.00000
87	C6	PX	1.91084	-3.11440	0.79990	-1.00934	0.00000
88	C6	PY	0.24671	0.28706	-1.69868	-0.57133	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	-0.16109
90	C6	DXX	0.06563	0.06516	0.01234	-0.10385	0.00000
91	C6	DYY	0.00035	-0.00958	0.01212	0.06077	0.00000
92	C6	DZZ	0.02516	-0.01305	-0.01937	0.00219	0.00000
93	C6	DXY	0.00626	-0.07061	0.05334	-0.02431	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00344

95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.02578
96	C7	S	-0.00066	-0.01154	0.01902	-0.00120	0.00000
97	C7	S	-0.35655	-0.59170	-0.42509	-0.15167	0.00000
98	C7	PX	0.11873	-0.23889	0.11479	-0.06216	0.00000
99	C7	PY	-0.15885	-0.13028	-0.15763	-0.10909	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.05110
101	C7	S	0.66998	0.80359	0.20595	0.29866	0.00000
102	C7	PX	-0.40449	1.17914	0.50624	-0.04455	0.00000
103	C7	PY	0.27831	0.34328	-0.29365	1.08222	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.12496
105	C7	DXX	0.00041	-0.04629	-0.06840	0.01228	0.00000
106	C7	DYY	-0.05436	-0.01509	0.02018	-0.00258	0.00000
107	C7	DZZ	0.00264	-0.01394	-0.02453	-0.00177	0.00000
108	C7	DXY	-0.03772	0.00323	0.01843	-0.01125	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.01754
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00090
111	O1	S	-0.00272	-0.00063	0.00932	-0.00154	0.00000
112	O1	S	0.18752	0.06420	0.17595	0.07162	0.00000
113	O1	PX	-0.08752	0.02307	-0.17924	-0.11557	0.00000
114	O1	PY	0.02853	-0.06486	0.09293	0.32979	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.89368
116	O1	S	-0.10384	0.03755	-0.55689	-0.06412	0.00000
117	O1	PX	-0.13813	0.08208	0.38265	0.04772	0.00000
118	O1	PY	-0.34777	0.03851	-0.09649	-0.71209	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	-1.30584
120	O1	DXX	0.05940	0.01518	0.02244	0.06313	0.00000
121	O1	DYY	0.08882	0.03872	0.07831	0.00208	0.00000
122	O1	DZZ	0.03487	0.00626	0.10047	0.04051	0.00000
123	O1	DXY	0.01417	-0.02438	0.02176	-0.00398	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.02743
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.01129
126	H4	S	-0.20388	0.08075	0.12908	-0.21431	0.00000
127	H4	S	0.37254	0.36507	0.31973	-0.23741	0.00000
128	H4	PX	0.02849	0.03560	0.00194	-0.00954	0.00000
129	H4	PY	-0.00097	-0.00161	0.00118	0.00052	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.03337
131	N1	S	0.00462	0.00087	-0.00902	-0.00385	0.00000
132	N1	S	0.18821	-0.01975	-0.05145	0.27352	0.00000
133	N1	PX	0.10133	0.05949	-0.13284	0.02056	0.00000
134	N1	PY	-0.20812	-0.22705	0.14274	0.28361	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.08362
136	N1	S	0.03652	-0.09087	-0.39746	0.01071	0.00000
137	N1	PX	-0.79117	0.28853	0.60960	0.50981	0.00000
138	N1	PY	0.95984	0.43751	-0.78939	-0.94533	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.18710
140	N1	DXX	0.01205	0.01095	0.02856	0.10460	0.00000
141	N1	DYY	0.11397	0.00096	-0.10642	0.02044	0.00000
142	N1	DZZ	-0.00600	-0.00726	0.02334	-0.00252	0.00000
143	N1	DXY	0.01198	0.02598	-0.05041	-0.02137	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00884
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01394
146	H6	S	-0.22127	-0.13569	0.23004	-0.04675	0.00000
147	H6	S	-0.10305	-0.36045	0.35207	0.02711	0.00000
148	H6	PX	0.00374	-0.01370	-0.00852	0.01046	0.00000

149	H6	PY	0.01106	0.01448	0.01363	-0.02725	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	-0.01043
151	C8	S	-0.00876	0.00163	0.01724	0.00824	0.00000
152	C8	S	-0.39288	0.03776	0.37415	0.52273	0.00000
153	C8	PX	0.11474	0.09484	0.00837	-0.08659	0.00000
154	C8	PY	-0.10454	0.01533	0.34543	-0.09524	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.02018
156	C8	S	1.31443	0.05389	-0.77535	-1.73110	0.00000
157	C8	PX	-0.78614	-0.24986	0.90102	1.32473	0.00000
158	C8	PY	-0.11046	0.74193	-1.01047	0.27627	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.10435
160	C8	DXX	-0.00308	0.04237	0.00866	0.05745	0.00000
161	C8	DYY	-0.04885	0.00022	0.06034	-0.00940	0.00000
162	C8	DZZ	0.00690	-0.01054	-0.02498	0.01696	0.00000
163	C8	DXY	-0.02782	0.00635	-0.00176	0.04306	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00463
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01434
166	H8	S	0.16773	-0.02269	-0.43883	0.18006	0.00000
167	H8	S	-0.04077	-0.85450	-0.18300	-0.11173	0.00000
168	H8	PX	0.00572	0.04548	-0.02534	0.02336	0.00000
169	H8	PY	0.00538	0.00500	0.00723	0.03225	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.01428
171	C10	S	-0.00069	-0.01109	-0.00352	-0.00650	0.00000
172	C10	S	0.34930	0.13360	0.21959	-0.60561	0.00000
173	C10	PX	-0.06801	0.09289	0.00996	-0.05760	0.00000
174	C10	PY	-0.17295	-0.05461	0.19299	-0.24572	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.01152
176	C10	S	-1.19547	0.22603	-0.75172	1.48110	0.00000
177	C10	PX	0.36691	-0.42311	-0.52336	-0.35827	0.00000
178	C10	PY	0.29228	0.42100	-0.73235	0.52709	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00637
180	C10	DXX	-0.04040	-0.03413	0.08028	-0.04491	0.00000
181	C10	DYY	0.02166	0.00058	-0.04783	-0.00945	0.00000
182	C10	DZZ	0.05376	0.03714	-0.01048	-0.02583	0.00000
183	C10	DXY	-0.00660	-0.02546	-0.03952	-0.05106	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00562
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00161
186	H16	S	-0.04818	-0.04376	0.18791	0.02707	0.00000
187	H16	S	0.25763	0.41301	0.00957	-0.08654	0.00000
188	H16	PX	-0.01735	-0.02579	0.00351	0.01965	0.00000
189	H16	PY	-0.00792	-0.01187	-0.01270	-0.01068	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.00139
191	H18	S	-0.09729	-0.19962	-0.19232	-0.13063	0.00000
192	H18	S	0.63962	0.18212	-0.28093	-0.10504	0.00000
193	H18	PX	0.03015	0.00378	-0.01844	0.01172	0.00000
194	H18	PY	0.02232	0.01301	0.02793	0.00491	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00115
196	C9	S	-0.00030	0.01094	-0.01323	0.00810	0.00000
197	C9	S	-0.25940	-0.00676	-0.24006	-0.00135	0.00000
198	C9	PX	-0.06453	-0.01280	0.05003	-0.03826	0.00000
199	C9	PY	-0.04055	-0.20053	-0.04761	0.07557	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.03576
201	C9	S	0.88392	0.07191	0.59488	0.15526	0.00000
202	C9	PX	-0.09423	-0.06363	-0.08421	-0.19331	0.00000

203	C9	PY	0.39010	0.29738	0.30830	0.21125	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.47754
205	C9	DXX	-0.03115	0.00638	-0.03902	-0.05157	0.00000
206	C9	DYY	-0.05500	0.01864	-0.04208	-0.04265	0.00000
207	C9	DZZ	0.06973	0.00588	0.02837	0.12195	0.00000
208	C9	DXY	0.01495	-0.03736	-0.01191	0.09204	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	-0.01271
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.13669
211	H3	S	-0.18435	0.16437	-0.10238	-0.19870	0.00000
212	H3	S	-0.23111	-0.32332	-0.22466	0.09266	0.00000
213	H3	PX	0.00897	-0.02624	0.00597	0.06077	0.00000
214	H3	PY	0.00694	0.03091	0.00976	0.00224	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.07959
216	H5	S	0.14212	0.11151	0.01905	0.13284	0.12674
217	H5	S	-0.31950	-0.02019	-0.15374	-0.13259	0.08823
218	H5	PX	-0.01206	0.00982	-0.01450	-0.03980	-0.02936
219	H5	PY	0.00926	-0.00147	0.00250	0.02351	-0.06824
220	H5	PZ	-0.03157	0.00016	-0.00870	-0.04583	0.00031
221	H7	S	0.14212	0.11151	0.01905	0.13284	-0.12674
222	H7	S	-0.31950	-0.02019	-0.15374	-0.13259	-0.08823
223	H7	PX	-0.01206	0.00982	-0.01450	-0.03980	0.02936
224	H7	PY	0.00926	-0.00147	0.00250	0.02351	0.06824
225	H7	PZ	0.03157	-0.00016	0.00870	0.04583	0.00031

M0:	111	112	113	114	115
Eigenvalues:	1.32518	1.38955	1.40283	1.43085	1.44189
(ev):	36.05988	37.81152	38.17308	38.93552	39.23593

			A	A	A	A	A
1	H1	S	0.24323	-0.18973	-0.15681	0.39863	0.41746
2	H1	S	-0.31426	0.20582	-0.30281	0.28971	0.52346
3	H1	PX	0.03043	-0.02886	-0.00866	-0.00712	0.00789
4	H1	PY	0.00012	-0.02112	-0.00137	-0.02258	0.00920
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00226	0.02531	0.01688	0.01250	0.01621
7	C1	S	0.37608	0.45633	0.30298	0.01441	0.49269
8	C1	PX	-0.31523	0.10331	-0.16626	0.22062	-0.08212
9	C1	PY	0.20206	0.09509	0.13929	0.19378	0.25830
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.97764	-2.56479	-1.60913	-2.67605	-1.76407
12	C1	PX	1.51170	0.44336	1.50669	0.44054	-0.88679
13	C1	PY	-3.94887	0.73740	-0.99287	-3.47423	-0.64809
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.04321	0.03832	-0.03234	0.05481	0.10750
16	C1	DYY	0.03874	0.01596	0.03994	-0.05737	-0.03212
17	C1	DZZ	-0.01780	-0.02297	0.01094	-0.00787	-0.01061
18	C1	DXY	0.11616	-0.03919	0.04169	0.12768	0.05879
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00416	0.02343	0.01165	0.00787	-0.01066
22	C2	S	-0.38503	0.59148	0.21648	0.63036	-0.28439
23	C2	PX	-0.15856	0.04926	-0.06282	0.29974	0.02257
24	C2	PY	-0.25834	-0.12448	0.02914	0.21034	-0.10859
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

26	C2	S	0.64566	-2.24522	-1.23886	-0.16494	0.89136
27	C2	PX	-0.89269	-0.34595	-0.14029	-0.41590	-0.96315
28	C2	PY	2.09254	0.37308	1.12802	-0.90981	0.72873
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.09734	0.06048	0.04620	0.05965	-0.06467
31	C2	DYY	0.03500	0.04792	-0.02036	0.02190	0.02150
32	C2	DZZ	-0.00864	-0.03573	0.00570	0.00317	0.01106
33	C2	DXY	0.01216	0.05762	-0.00293	-0.06686	-0.03878
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00843	0.00276	-0.00511	-0.00622	-0.02441
37	C3	S	0.34117	-0.25382	-0.08341	-0.10878	-0.73411
38	C3	PX	0.39302	-0.09602	-0.11995	0.29704	-0.18955
39	C3	PY	-0.05948	-0.25964	0.32786	0.02348	-0.03781
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-2.11717	1.91337	1.69674	-0.86518	2.60288
42	C3	PX	-2.69227	1.11612	-0.28756	-1.78607	1.39338
43	C3	PY	-2.19785	1.23906	-1.29306	-1.21229	-0.51876
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.02060	0.00579	0.00047	-0.02281	0.00166
46	C3	DYY	-0.01637	0.03353	0.03122	-0.03278	-0.05025
47	C3	DZZ	0.01668	-0.05734	-0.00703	0.01494	-0.01015
48	C3	DXY	-0.00902	-0.00304	-0.00244	-0.06955	-0.00822
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00828	-0.00474	-0.00471	0.00804	0.00679
52	C4	S	-0.17955	0.16306	-0.24883	-0.02840	-0.14671
53	C4	PX	-0.43119	0.00737	-0.15378	-0.37145	-0.13771
54	C4	PY	0.15094	-0.08479	0.08048	0.14315	0.19012
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	1.62738	-0.28058	1.76256	1.01312	-0.71170
57	C4	PX	4.15538	-0.08707	1.48868	4.94507	1.11645
58	C4	PY	0.06531	-0.99243	-0.76069	-1.22448	0.39803
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.03552	0.08391	-0.03413	0.02010	-0.03066
61	C4	DYY	0.01799	-0.06916	0.04795	0.03397	0.00170
62	C4	DZZ	-0.04420	-0.04393	-0.00839	-0.01827	-0.00295
63	C4	DXY	-0.06181	-0.04635	-0.06761	0.00009	-0.06036
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00170	0.00214	-0.01077	-0.03814	-0.00689
67	C5	S	0.25751	-0.19340	-0.37421	-0.62970	-0.04697
68	C5	PX	-0.06005	-0.09713	-0.17901	0.22268	-0.11751
69	C5	PY	-0.22758	0.04228	0.09477	0.03601	-0.07210
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.18830	0.48761	0.44628	4.74132	0.16194
72	C5	PX	2.16539	-0.43037	0.90094	0.61882	1.81747
73	C5	PY	1.59804	0.18840	0.27157	1.54207	0.19289
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.10789	-0.03357	-0.05696	-0.05394	-0.00621
76	C5	DYY	-0.02922	0.02669	-0.03635	-0.00980	-0.01157
77	C5	DZZ	-0.01558	-0.03596	0.03237	-0.00112	0.01858
78	C5	DXY	-0.03334	0.03949	-0.00109	0.13816	-0.03926
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00035	-0.02231	0.00423	-0.00236	0.01779
82	C6	S	0.05511	-0.19606	-0.07892	0.00874	0.54520
83	C6	PX	0.05306	0.16798	0.06233	-0.08332	0.11214
84	C6	PY	-0.09501	-0.46294	0.09580	0.14460	0.22395
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.95290	0.15908	-0.19989	-0.89825	-0.93891
87	C6	PX	-2.08402	-0.24963	-1.84162	0.21772	-0.56176
88	C6	PY	1.42065	2.20170	0.41451	-1.03758	0.42661
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01524	0.06493	0.00229	-0.04735	0.06447
91	C6	DYY	-0.04205	-0.13524	-0.03636	0.03031	0.02718
92	C6	DZZ	0.00517	0.00523	0.01387	0.01421	-0.01735
93	C6	DXY	-0.05356	-0.05620	-0.03953	-0.05661	0.00923
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00840	-0.00034	-0.01532	0.01666	-0.00271
97	C7	S	-0.54378	0.12312	-0.05757	0.24504	0.16078
98	C7	PX	0.22628	-0.09855	0.10957	-0.06683	-0.03049
99	C7	PY	0.03857	0.16623	0.16741	0.02780	-0.15762
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.73761	0.04372	-0.93031	-0.52063	-0.24779
102	C7	PX	0.25722	0.41346	0.20207	1.19984	-0.42775
103	C7	PY	0.82272	-1.43309	-0.94841	0.56331	-1.70423
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.10499	-0.00547	-0.02805	-0.03168	0.05217
106	C7	DYY	0.02021	0.02112	-0.02540	0.08943	-0.00955
107	C7	DZZ	-0.00679	-0.00613	0.02636	-0.02722	0.00208
108	C7	DXY	-0.06936	-0.00056	0.04233	-0.00026	0.08102
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00936	-0.01011	0.00257	-0.00689	0.00796
112	O1	S	-0.13271	-0.14846	0.11623	-0.09084	-0.03382
113	O1	PX	-0.01542	-0.03818	-0.03358	-0.08543	-0.20422
114	O1	PY	0.17242	0.28150	-0.18753	-0.14049	0.16030
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.06742	0.46115	-0.16238	0.56299	-0.25144
117	O1	PX	-0.28673	-0.18563	-0.02686	-0.47662	0.23509
118	O1	PY	0.21259	-0.86861	0.39587	0.26626	-0.04301
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00532	-0.04312	0.00467	0.00704	-0.06193
121	O1	DYY	-0.07358	-0.05462	0.05149	0.01127	0.00927
122	O1	DZZ	-0.01254	-0.01140	0.02639	-0.09812	0.07172
123	O1	DXY	0.02760	0.00124	0.03308	-0.05112	0.02564
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.24532	-0.29586	0.03924	-0.47545	0.32724
127	H4	S	0.07100	-0.16563	0.19434	-0.65234	0.43555
128	H4	PX	-0.02593	0.00688	0.00500	0.00323	0.00089
129	H4	PY	0.00622	-0.02287	-0.00497	0.01825	0.03306
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00108	0.01638	-0.00129	-0.00857	-0.01034
132	N1	S	0.13323	-0.13317	0.12693	-0.15497	-0.22945
133	N1	PX	0.16654	0.19043	0.14532	-0.19196	-0.04724

134	N1	PY	-0.05851	-0.47065	-0.19863	-0.01248	0.06398
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.66026	-0.15586	-0.03572	0.45536	0.09086
137	N1	PX	-0.16932	-1.13382	0.01918	0.54388	-0.05230
138	N1	PY	0.36282	1.81563	0.12648	-0.27014	0.65464
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.07098	-0.06692	0.06500	-0.01372	-0.09706
141	N1	DYY	0.03875	0.07078	0.02835	-0.05620	-0.04289
142	N1	DZZ	-0.02865	-0.01287	-0.01312	0.00056	0.00120
143	N1	DXY	0.05557	0.02458	-0.01846	0.00337	0.00416
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.20019	0.22357	0.18740	-0.05120	-0.28056
147	H6	S	-0.03485	0.12300	0.21197	-0.20600	-0.31056
148	H6	PX	0.01991	0.00059	-0.00573	-0.01344	0.00432
149	H6	PY	0.01688	0.00984	0.02623	-0.02785	0.01954
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.01295	-0.00776	0.03698	0.00210	0.01444
152	C8	S	-0.22683	-0.19863	0.97491	0.08825	0.25837
153	C8	PX	-0.00373	0.14467	0.18258	-0.06063	0.27689
154	C8	PY	0.07710	0.04746	-0.47018	0.06600	-0.03778
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	1.15944	1.06689	-4.86905	0.30701	-1.55296
157	C8	PX	0.60537	-2.42147	-0.60283	1.16673	-2.57434
158	C8	PY	0.33020	0.96963	3.14729	-0.44958	-0.46389
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00042	0.05795	0.10979	-0.00720	0.00483
161	C8	DYY	-0.02017	-0.01737	-0.05661	0.03292	0.01504
162	C8	DZZ	0.00422	-0.01514	0.02788	-0.01747	0.00093
163	C8	DXY	-0.06930	-0.04073	-0.00054	0.04317	0.02431
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.10264	-0.09844	0.04286	-0.25029	0.12811
167	H8	S	-0.13271	-0.22347	-0.00192	-0.37853	0.14519
168	H8	PX	-0.01951	0.00241	-0.01309	-0.01801	0.00531
169	H8	PY	-0.02732	-0.02821	-0.00645	-0.00310	-0.01173
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00112	-0.00484	-0.03301	0.00252	-0.00223
172	C10	S	0.22121	0.19612	-1.07890	-0.00060	-0.18095
173	C10	PX	-0.01205	0.10953	0.08257	0.05305	-0.01913
174	C10	PY	0.06332	0.13894	-0.17635	-0.02165	-0.02950
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.54625	0.41071	5.52727	-0.53744	0.79424
177	C10	PX	-0.72910	0.20724	-1.04782	-0.47740	1.59106
178	C10	PY	-0.23231	0.30781	2.01238	-0.36103	0.53351
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.03701	-0.02004	-0.14916	0.03196	-0.06231
181	C10	DYY	-0.04080	0.00116	0.06675	-0.02337	0.06799
182	C10	DZZ	0.02664	0.03501	-0.02755	-0.01638	-0.02324
183	C10	DXY	-0.06463	0.02885	-0.11032	-0.03103	0.10139
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.27649	-0.02991	0.05870	0.07743	-0.38380
187	H16	S	0.27556	0.07188	-0.03491	0.13563	-0.56041

188	H16	PX	0.00256	-0.02207	0.01008	-0.00446	-0.00504
189	H16	PY	-0.03580	-0.01039	-0.05071	0.00059	0.03778
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.25564	0.03231	-0.33475	-0.06506	0.35519
192	H18	S	-0.03152	0.13355	-0.30006	-0.19306	0.34519
193	H18	PX	-0.00710	-0.02096	-0.01411	-0.00383	0.00902
194	H18	PY	0.03849	-0.00596	-0.00588	0.00395	-0.04558
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.02871	-0.03967	-0.00292	0.00300	-0.02296
197	C9	S	0.42319	-0.52183	-0.03550	0.18153	-0.25532
198	C9	PX	-0.07277	0.00895	0.02327	-0.06194	0.04796
199	C9	PY	0.21236	0.15718	-0.00358	0.15183	0.16303
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-1.30888	1.56714	-0.00297	-0.54577	0.40380
202	C9	PX	0.24386	-0.23462	0.10161	0.20459	0.07209
203	C9	PY	-0.46923	-0.23025	-0.02020	-0.35806	-0.28556
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.00497	-0.05236	0.02080	-0.02768	-0.04877
206	C9	DYY	0.03582	-0.03904	-0.00053	0.04787	-0.02202
207	C9	DZZ	0.03291	0.01133	-0.04497	-0.02236	-0.00267
208	C9	DXY	0.05709	0.09287	-0.06027	-0.00158	-0.00247
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.06684	-0.24692	0.01435	-0.02269	-0.07856
212	H3	S	0.58276	-0.01640	-0.03052	0.32685	0.14905
213	H3	PX	0.03864	0.06118	-0.03495	-0.00234	0.02210
214	H3	PY	-0.02135	-0.01105	-0.00827	-0.03345	-0.01628
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.01183	-0.16666	-0.03465	-0.08042	-0.13525
217	H5	S	0.19060	-0.23123	-0.00305	0.11290	-0.07953
218	H5	PX	-0.01352	-0.02666	0.01724	0.00064	-0.01634
219	H5	PY	0.00174	0.00539	-0.01336	-0.00733	-0.01217
220	H5	PZ	-0.01554	-0.01834	0.01791	0.00143	-0.00109
221	H7	S	0.01183	-0.16666	-0.03465	-0.08042	-0.13525
222	H7	S	0.19060	-0.23123	-0.00305	0.11290	-0.07953
223	H7	PX	-0.01352	-0.02666	0.01724	0.00064	-0.01634
224	H7	PY	0.00174	0.00539	-0.01336	-0.00733	-0.01217
225	H7	PZ	0.01554	0.01834	-0.01791	-0.00143	0.00109

M0:	116	117	118	119	120
Eigenvalues:	1.47318	1.48252	1.51650	1.55009	1.58637
(ev):	40.08715	40.34143	41.26607	42.18025	43.16741

		A	A	A	A	A	
1	H1	S	0.00000	-0.08782	-0.18463	0.00000	0.00000
2	H1	S	0.00000	-0.14642	-0.45293	0.00000	0.00000
3	H1	PX	0.00000	0.01095	-0.02810	0.00000	0.00000
4	H1	PY	0.00000	-0.00672	-0.01599	0.00000	0.00000
5	H1	PZ	0.01441	0.00000	0.00000	-0.11751	0.08260
6	C1	S	0.00000	-0.01273	0.00339	0.00000	0.00000
7	C1	S	0.00000	0.00838	0.05028	0.00000	0.00000
8	C1	PX	0.00000	-0.14005	0.00576	0.00000	0.00000
9	C1	PY	0.00000	0.02018	0.16580	0.00000	0.00000
10	C1	PZ	-0.02292	0.00000	0.00000	-0.08732	0.07378

11	C1	S	0.00000	0.89229	-0.06489	0.00000	0.00000
12	C1	PX	0.00000	0.97679	1.03613	0.00000	0.00000
13	C1	PY	0.00000	-2.31024	-0.25144	0.00000	0.00000
14	C1	PZ	0.01278	0.00000	0.00000	0.06685	-0.06528
15	C1	DXX	0.00000	-0.04013	-0.00255	0.00000	0.00000
16	C1	DYY	0.00000	0.01504	0.02318	0.00000	0.00000
17	C1	DZZ	0.00000	0.02785	-0.01948	0.00000	0.00000
18	C1	DXY	0.00000	-0.00663	-0.03503	0.00000	0.00000
19	C1	DXZ	-0.04134	0.00000	0.00000	-0.27508	0.15174
20	C1	DYZ	0.29314	0.00000	0.00000	-0.00356	0.19797
21	C2	S	0.00000	0.01542	0.01909	0.00000	0.00000
22	C2	S	0.00000	0.37280	0.28068	0.00000	0.00000
23	C2	PX	0.00000	-0.02837	0.14259	0.00000	0.00000
24	C2	PY	0.00000	-0.13622	0.04154	0.00000	0.00000
25	C2	PZ	-0.01632	0.00000	0.00000	-0.03230	-0.06947
26	C2	S	0.00000	-1.96039	-0.82169	0.00000	0.00000
27	C2	PX	0.00000	0.51819	-1.64223	0.00000	0.00000
28	C2	PY	0.00000	2.27039	0.68768	0.00000	0.00000
29	C2	PZ	0.02475	0.00000	0.00000	-0.06969	0.01066
30	C2	DXX	0.00000	0.11598	-0.05272	0.00000	0.00000
31	C2	DYY	0.00000	-0.06735	0.06807	0.00000	0.00000
32	C2	DZZ	0.00000	0.01648	-0.01147	0.00000	0.00000
33	C2	DXY	0.00000	0.05408	0.01380	0.00000	0.00000
34	C2	DXZ	-0.15032	0.00000	0.00000	0.16973	0.17053
35	C2	DYZ	0.23215	0.00000	0.00000	0.08673	0.01933
36	C3	S	0.00000	-0.02874	0.00934	0.00000	0.00000
37	C3	S	0.00000	-0.26349	0.12225	0.00000	0.00000
38	C3	PX	0.00000	0.10225	0.12526	0.00000	0.00000
39	C3	PY	0.00000	0.26170	0.06411	0.00000	0.00000
40	C3	PZ	-0.01522	0.00000	0.00000	0.03593	-0.02248
41	C3	S	0.00000	0.06632	-1.18154	0.00000	0.00000
42	C3	PX	0.00000	-3.57130	-1.05017	0.00000	0.00000
43	C3	PY	0.00000	-1.98264	0.60807	0.00000	0.00000
44	C3	PZ	-0.03168	0.00000	0.00000	-0.05514	-0.04242
45	C3	DXX	0.00000	-0.00570	0.01650	0.00000	0.00000
46	C3	DYY	0.00000	-0.08255	-0.02201	0.00000	0.00000
47	C3	DZZ	0.00000	0.06860	-0.00750	0.00000	0.00000
48	C3	DXY	0.00000	0.05538	-0.02313	0.00000	0.00000
49	C3	DXZ	-0.17487	0.00000	0.00000	-0.07999	0.05513
50	C3	DYZ	-0.28175	0.00000	0.00000	0.11874	-0.18349
51	C4	S	0.00000	0.02017	-0.00030	0.00000	0.00000
52	C4	S	0.00000	0.33722	-0.14553	0.00000	0.00000
53	C4	PX	0.00000	-0.26129	0.21157	0.00000	0.00000
54	C4	PY	0.00000	-0.07400	0.05234	0.00000	0.00000
55	C4	PZ	-0.04041	0.00000	0.00000	0.08178	-0.03869
56	C4	S	0.00000	-0.09336	0.67669	0.00000	0.00000
57	C4	PX	0.00000	2.38520	-0.74554	0.00000	0.00000
58	C4	PY	0.00000	0.84262	-0.77986	0.00000	0.00000
59	C4	PZ	0.06677	0.00000	0.00000	-0.17715	0.04379
60	C4	DXX	0.00000	-0.01755	-0.05110	0.00000	0.00000
61	C4	DYY	0.00000	0.07168	0.01771	0.00000	0.00000
62	C4	DZZ	0.00000	0.01036	-0.00162	0.00000	0.00000
63	C4	DXY	0.00000	-0.03925	-0.06524	0.00000	0.00000
64	C4	DXZ	0.31383	0.00000	0.00000	0.14993	0.11573

65	C4	DYZ	0.00070	0.00000	0.00000	-0.27489	0.15813
66	C5	S	0.00000	-0.02844	0.00109	0.00000	0.00000
67	C5	S	0.00000	-0.61476	0.07941	0.00000	0.00000
68	C5	PX	0.00000	-0.08086	-0.13578	0.00000	0.00000
69	C5	PY	0.00000	0.13967	-0.22160	0.00000	0.00000
70	C5	PZ	-0.02849	0.00000	0.00000	-0.06514	0.02648
71	C5	S	0.00000	1.52300	-0.87181	0.00000	0.00000
72	C5	PX	0.00000	1.39936	0.63067	0.00000	0.00000
73	C5	PY	0.00000	0.40757	0.54516	0.00000	0.00000
74	C5	PZ	0.01838	0.00000	0.00000	0.14723	-0.02610
75	C5	DXX	0.00000	-0.02453	-0.08162	0.00000	0.00000
76	C5	DYY	0.00000	-0.07437	0.04546	0.00000	0.00000
77	C5	DZZ	0.00000	0.03758	0.00890	0.00000	0.00000
78	C5	DXY	0.00000	-0.00459	-0.01108	0.00000	0.00000
79	C5	DXZ	-0.23893	0.00000	0.00000	0.01188	-0.07217
80	C5	DYZ	-0.14357	0.00000	0.00000	-0.16385	-0.04011
81	C6	S	0.00000	0.00261	-0.00881	0.00000	0.00000
82	C6	S	0.00000	0.01590	-0.28440	0.00000	0.00000
83	C6	PX	0.00000	0.44602	0.07520	0.00000	0.00000
84	C6	PY	0.00000	0.07638	-0.00344	0.00000	0.00000
85	C6	PZ	-0.00017	0.00000	0.00000	0.01945	-0.02190
86	C6	S	0.00000	-0.83586	2.61537	0.00000	0.00000
87	C6	PX	0.00000	-4.12073	-1.14317	0.00000	0.00000
88	C6	PY	0.00000	-1.31299	-0.02725	0.00000	0.00000
89	C6	PZ	-0.03445	0.00000	0.00000	0.00997	0.17687
90	C6	DXX	0.00000	-0.05847	-0.01710	0.00000	0.00000
91	C6	DYY	0.00000	0.06805	0.06494	0.00000	0.00000
92	C6	DZZ	0.00000	0.00266	-0.03797	0.00000	0.00000
93	C6	DXY	0.00000	-0.00211	-0.00711	0.00000	0.00000
94	C6	DXZ	0.31078	0.00000	0.00000	-0.00408	0.01403
95	C6	DYZ	-0.10445	0.00000	0.00000	0.14200	0.17351
96	C7	S	0.00000	-0.03367	0.00243	0.00000	0.00000
97	C7	S	0.00000	-0.47307	-0.02542	0.00000	0.00000
98	C7	PX	0.00000	0.02670	0.03286	0.00000	0.00000
99	C7	PY	0.00000	-0.02595	0.15003	0.00000	0.00000
100	C7	PZ	-0.08546	0.00000	0.00000	0.05583	0.00210
101	C7	S	0.00000	2.95027	-0.16454	0.00000	0.00000
102	C7	PX	0.00000	-1.97123	-0.72901	0.00000	0.00000
103	C7	PY	0.00000	1.21623	1.31634	0.00000	0.00000
104	C7	PZ	0.12576	0.00000	0.00000	0.01426	0.02608
105	C7	DXX	0.00000	0.02524	0.03164	0.00000	0.00000
106	C7	DYY	0.00000	-0.06441	-0.03207	0.00000	0.00000
107	C7	DZZ	0.00000	0.03761	-0.00651	0.00000	0.00000
108	C7	DXY	0.00000	0.03684	-0.05798	0.00000	0.00000
109	C7	DXZ	-0.17653	0.00000	0.00000	0.20333	0.16607
110	C7	DYZ	0.00947	0.00000	0.00000	-0.00263	0.30802
111	O1	S	0.00000	0.00788	0.01135	0.00000	0.00000
112	O1	S	0.00000	0.08318	0.32579	0.00000	0.00000
113	O1	PX	0.00000	-0.06796	-0.32039	0.00000	0.00000
114	O1	PY	0.00000	-0.11693	-0.02427	0.00000	0.00000
115	O1	PZ	0.03363	0.00000	0.00000	-0.00535	-0.02675
116	O1	S	0.00000	-0.39512	-0.80203	0.00000	0.00000
117	O1	PX	0.00000	0.04954	0.54989	0.00000	0.00000
118	O1	PY	0.00000	0.52694	-0.08493	0.00000	0.00000

119	O1	PZ	-0.08111	0.00000	0.00000	0.03999	0.01845
120	O1	DXX	0.00000	0.01944	-0.05517	0.00000	0.00000
121	O1	DYY	0.00000	0.03686	0.18331	0.00000	0.00000
122	O1	DZZ	0.00000	0.01127	0.17000	0.00000	0.00000
123	O1	DXY	0.00000	0.01406	0.09160	0.00000	0.00000
124	O1	DXZ	0.09819	0.00000	0.00000	0.22434	-0.06201
125	O1	DYZ	-0.01206	0.00000	0.00000	0.18480	-0.11423
126	H4	S	0.00000	-0.01906	0.01572	0.00000	0.00000
127	H4	S	0.00000	0.09988	0.14194	0.00000	0.00000
128	H4	PX	0.00000	-0.00440	0.02638	0.00000	0.00000
129	H4	PY	0.00000	-0.00847	0.04530	0.00000	0.00000
130	H4	PZ	0.02329	0.00000	0.00000	-0.03184	0.01175
131	N1	S	0.00000	0.00499	-0.00029	0.00000	0.00000
132	N1	S	0.00000	-0.05220	0.19890	0.00000	0.00000
133	N1	PX	0.00000	0.15540	-0.04241	0.00000	0.00000
134	N1	PY	0.00000	0.06462	0.18471	0.00000	0.00000
135	N1	PZ	-0.08639	0.00000	0.00000	0.02514	0.11935
136	N1	S	0.00000	0.21684	0.09867	0.00000	0.00000
137	N1	PX	0.00000	1.07664	0.75849	0.00000	0.00000
138	N1	PY	0.00000	-0.36650	-1.34838	0.00000	0.00000
139	N1	PZ	0.10906	0.00000	0.00000	0.03950	-0.21204
140	N1	DXX	0.00000	0.01755	0.07674	0.00000	0.00000
141	N1	DYY	0.00000	-0.03361	-0.00139	0.00000	0.00000
142	N1	DZZ	0.00000	-0.00920	-0.00362	0.00000	0.00000
143	N1	DXY	0.00000	-0.03906	0.01802	0.00000	0.00000
144	N1	DXZ	0.12709	0.00000	0.00000	-0.04521	0.08837
145	N1	DYZ	0.03649	0.00000	0.00000	-0.10084	-0.18932
146	H6	S	0.00000	0.44127	-0.27131	0.00000	0.00000
147	H6	S	0.00000	0.64761	-0.44334	0.00000	0.00000
148	H6	PX	0.00000	-0.01031	0.00784	0.00000	0.00000
149	H6	PY	0.00000	0.01662	0.00692	0.00000	0.00000
150	H6	PZ	0.02663	0.00000	0.00000	-0.09168	-0.07751
151	C8	S	0.00000	-0.00675	-0.01918	0.00000	0.00000
152	C8	S	0.00000	-0.25678	-0.39393	0.00000	0.00000
153	C8	PX	0.00000	-0.02738	-0.28421	0.00000	0.00000
154	C8	PY	0.00000	0.49280	-0.00613	0.00000	0.00000
155	C8	PZ	0.09840	0.00000	0.00000	-0.02193	-0.03054
156	C8	S	0.00000	1.66880	1.03196	0.00000	0.00000
157	C8	PX	0.00000	1.13347	2.67054	0.00000	0.00000
158	C8	PY	0.00000	-5.16351	-0.10548	0.00000	0.00000
159	C8	PZ	-0.25281	0.00000	0.00000	0.00271	0.05986
160	C8	DXX	0.00000	0.01707	-0.07091	0.00000	0.00000
161	C8	DYY	0.00000	0.00383	0.00527	0.00000	0.00000
162	C8	DZZ	0.00000	-0.02351	0.00752	0.00000	0.00000
163	C8	DXY	0.00000	-0.00380	-0.01113	0.00000	0.00000
164	C8	DXZ	-0.05024	0.00000	0.00000	-0.04037	-0.30991
165	C8	DYZ	0.17028	0.00000	0.00000	-0.17197	-0.29148
166	H8	S	0.00000	0.39283	0.27531	0.00000	0.00000
167	H8	S	0.00000	0.46221	0.29571	0.00000	0.00000
168	H8	PX	0.00000	0.04420	0.01949	0.00000	0.00000
169	H8	PY	0.00000	0.02648	0.00131	0.00000	0.00000
170	H8	PZ	-0.05269	0.00000	0.00000	0.09510	0.06850
171	C10	S	0.00000	0.02675	0.00991	0.00000	0.00000
172	C10	S	0.00000	0.48292	0.22643	0.00000	0.00000

173	C10	PX	0.00000	-0.10146	-0.04485	0.00000	0.00000
174	C10	PY	0.00000	-0.12374	0.01771	0.00000	0.00000
175	C10	PZ	0.03771	0.00000	0.00000	-0.03569	-0.07560
176	C10	S	0.00000	-5.21792	-1.18906	0.00000	0.00000
177	C10	PX	0.00000	1.00218	-0.99507	0.00000	0.00000
178	C10	PY	0.00000	-1.79957	-0.68970	0.00000	0.00000
179	C10	PZ	0.08093	0.00000	0.00000	0.00039	0.02784
180	C10	DXX	0.00000	0.11203	0.07041	0.00000	0.00000
181	C10	DYY	0.00000	-0.07848	-0.04028	0.00000	0.00000
182	C10	DZZ	0.00000	0.00462	-0.00129	0.00000	0.00000
183	C10	DXY	0.00000	0.09450	-0.05431	0.00000	0.00000
184	C10	DXZ	0.02290	0.00000	0.00000	-0.06703	-0.24496
185	C10	DYZ	-0.12798	0.00000	0.00000	0.10269	0.13597
186	H16	S	0.00000	-0.02979	0.22555	0.00000	0.00000
187	H16	S	0.00000	-0.09285	0.35553	0.00000	0.00000
188	H16	PX	0.00000	0.00215	0.01012	0.00000	0.00000
189	H16	PY	0.00000	0.03988	-0.01138	0.00000	0.00000
190	H16	PZ	0.03855	0.00000	0.00000	-0.04625	-0.12173
191	H18	S	0.00000	0.16163	-0.18783	0.00000	0.00000
192	H18	S	0.00000	0.32557	-0.26038	0.00000	0.00000
193	H18	PX	0.00000	0.01469	0.00827	0.00000	0.00000
194	H18	PY	0.00000	0.03037	0.02777	0.00000	0.00000
195	H18	PZ	0.03894	0.00000	0.00000	-0.01582	0.02604
196	C9	S	0.00000	0.01583	-0.07446	0.00000	0.00000
197	C9	S	0.00000	0.15677	-0.86602	0.00000	0.00000
198	C9	PX	0.00000	-0.00084	0.14417	0.00000	0.00000
199	C9	PY	0.00000	0.02899	0.12143	0.00000	0.00000
200	C9	PZ	-0.02747	0.00000	0.00000	-0.09547	0.03879
201	C9	S	0.00000	-0.65592	2.03324	0.00000	0.00000
202	C9	PX	0.00000	0.23361	-0.10311	0.00000	0.00000
203	C9	PY	0.00000	0.02708	-0.38281	0.00000	0.00000
204	C9	PZ	0.08071	0.00000	0.00000	0.07012	-0.03646
205	C9	DXX	0.00000	-0.00470	0.04141	0.00000	0.00000
206	C9	DYY	0.00000	0.01423	-0.09504	0.00000	0.00000
207	C9	DZZ	0.00000	-0.00133	-0.13518	0.00000	0.00000
208	C9	DXY	0.00000	-0.04078	-0.16760	0.00000	0.00000
209	C9	DXZ	-0.01109	0.00000	0.00000	-0.18024	0.08911
210	C9	DYZ	-0.08439	0.00000	0.00000	-0.31562	0.11805
211	H3	S	0.00000	0.05394	-0.17260	0.00000	0.00000
212	H3	S	0.00000	0.09573	-0.15368	0.00000	0.00000
213	H3	PX	0.00000	-0.01687	-0.06643	0.00000	0.00000
214	H3	PY	0.00000	-0.00688	-0.02551	0.00000	0.00000
215	H3	PZ	-0.03139	0.00000	0.00000	-0.12400	0.04508
216	H5	S	-0.03411	0.05138	-0.31806	-0.05220	0.01346
217	H5	S	0.10458	0.02931	-0.25321	0.05400	-0.00641
218	H5	PX	0.00671	0.00335	0.02968	0.04712	-0.02090
219	H5	PY	0.02557	-0.01017	-0.04046	0.11720	-0.04792
220	H5	PZ	-0.00093	0.00308	0.05033	0.01370	-0.00840
221	H7	S	0.03411	0.05138	-0.31806	0.05220	-0.01346
222	H7	S	-0.10458	0.02931	-0.25321	-0.05400	0.00641
223	H7	PX	-0.00671	0.00335	0.02968	-0.04712	0.02090
224	H7	PY	-0.02557	-0.01017	-0.04046	-0.11720	0.04792
225	H7	PZ	-0.00093	-0.00308	-0.05033	0.01370	-0.00840

MO:	121	122	123	124	125
Eigenvalues:	1.59404	1.61346	1.61640	1.62192	1.65269
(ev):	43.37592	43.90445	43.98446	44.13471	44.97201

		A	A	A	A	A	
1	H1	S	0.09575	0.00000	0.00000	0.19006	0.00000
2	H1	S	0.37753	0.00000	0.00000	0.33977	0.00000
3	H1	PX	0.00275	0.00000	0.00000	0.00030	0.00000
4	H1	PY	0.01825	0.00000	0.00000	0.02519	0.00000
5	H1	PZ	0.00000	0.08068	-0.03023	0.00000	0.05313
6	C1	S	0.00474	0.00000	0.00000	-0.02553	0.00000
7	C1	S	0.07641	0.00000	0.00000	-0.61363	0.00000
8	C1	PX	-0.00689	0.00000	0.00000	0.13378	0.00000
9	C1	PY	-0.15941	0.00000	0.00000	0.34206	0.00000
10	C1	PZ	0.00000	0.04663	0.00865	0.00000	0.04059
11	C1	S	0.81296	0.00000	0.00000	2.67700	0.00000
12	C1	PX	-1.32952	0.00000	0.00000	-2.02282	0.00000
13	C1	PY	1.06198	0.00000	0.00000	0.78028	0.00000
14	C1	PZ	0.00000	0.03317	-0.14884	0.00000	-0.02787
15	C1	DXX	0.02690	0.00000	0.00000	0.00844	0.00000
16	C1	DYY	-0.02672	0.00000	0.00000	-0.05480	0.00000
17	C1	DZZ	0.02604	0.00000	0.00000	0.01063	0.00000
18	C1	DXY	0.02899	0.00000	0.00000	-0.02796	0.00000
19	C1	DXZ	0.00000	0.12198	-0.03284	0.00000	0.10268
20	C1	DYZ	0.00000	0.11215	0.10835	0.00000	0.03693
21	C2	S	-0.03994	0.00000	0.00000	-0.01722	0.00000
22	C2	S	-0.42550	0.00000	0.00000	-0.24960	0.00000
23	C2	PX	0.11652	0.00000	0.00000	0.00965	0.00000
24	C2	PY	-0.26918	0.00000	0.00000	-0.08074	0.00000
25	C2	PZ	0.00000	0.00944	0.06114	0.00000	-0.13061
26	C2	S	3.98461	0.00000	0.00000	1.62680	0.00000
27	C2	PX	0.88766	0.00000	0.00000	1.75042	0.00000
28	C2	PY	-0.70818	0.00000	0.00000	-0.33118	0.00000
29	C2	PZ	0.00000	0.01936	-0.13113	0.00000	0.13479
30	C2	DXX	-0.07065	0.00000	0.00000	0.06191	0.00000
31	C2	DYY	0.02613	0.00000	0.00000	-0.07212	0.00000
32	C2	DZZ	0.06334	0.00000	0.00000	0.01756	0.00000
33	C2	DXY	-0.05533	0.00000	0.00000	-0.05481	0.00000
34	C2	DXZ	0.00000	0.08080	-0.12659	0.00000	0.31113
35	C2	DYZ	0.00000	-0.21229	-0.07953	0.00000	0.29282
36	C3	S	-0.02335	0.00000	0.00000	0.00334	0.00000
37	C3	S	-0.66182	0.00000	0.00000	-0.05597	0.00000
38	C3	PX	-0.12925	0.00000	0.00000	-0.20781	0.00000
39	C3	PY	0.14171	0.00000	0.00000	-0.02446	0.00000
40	C3	PZ	0.00000	0.00621	-0.07787	0.00000	-0.00718
41	C3	S	1.77081	0.00000	0.00000	-0.86062	0.00000
42	C3	PX	2.10930	0.00000	0.00000	-0.16274	0.00000
43	C3	PY	-0.80570	0.00000	0.00000	2.05898	0.00000
44	C3	PZ	0.00000	-0.09981	0.21609	0.00000	0.05309
45	C3	DXX	-0.10731	0.00000	0.00000	0.02896	0.00000
46	C3	DYY	0.00512	0.00000	0.00000	-0.05203	0.00000
47	C3	DZZ	0.03197	0.00000	0.00000	-0.00274	0.00000
48	C3	DXY	-0.07846	0.00000	0.00000	0.00088	0.00000
49	C3	DXZ	0.00000	0.19361	0.26701	0.00000	0.10823

50	C3	DYZ	0.00000	-0.25568	-0.14257	0.00000	-0.11419
51	C4	S	0.00550	0.00000	0.00000	0.02325	0.00000
52	C4	S	0.10796	0.00000	0.00000	0.57120	0.00000
53	C4	PX	-0.05979	0.00000	0.00000	0.17627	0.00000
54	C4	PY	-0.16301	0.00000	0.00000	0.00920	0.00000
55	C4	PZ	0.00000	0.02397	-0.04088	0.00000	0.02167
56	C4	S	-0.74268	0.00000	0.00000	-3.44493	0.00000
57	C4	PX	-0.79513	0.00000	0.00000	-2.11494	0.00000
58	C4	PY	1.59422	0.00000	0.00000	1.48722	0.00000
59	C4	PZ	0.00000	-0.05492	0.15044	0.00000	-0.08939
60	C4	DXX	-0.05759	0.00000	0.00000	0.02869	0.00000
61	C4	DYY	0.06716	0.00000	0.00000	-0.04689	0.00000
62	C4	DZZ	0.03492	0.00000	0.00000	0.02972	0.00000
63	C4	DXY	0.02864	0.00000	0.00000	0.04213	0.00000
64	C4	DXZ	0.00000	-0.18199	0.17558	0.00000	-0.05776
65	C4	DYZ	0.00000	-0.19898	0.01242	0.00000	-0.05699
66	C5	S	0.00593	0.00000	0.00000	-0.00790	0.00000
67	C5	S	0.29171	0.00000	0.00000	-0.27414	0.00000
68	C5	PX	-0.02978	0.00000	0.00000	0.03791	0.00000
69	C5	PY	-0.08931	0.00000	0.00000	0.23805	0.00000
70	C5	PZ	0.00000	-0.02999	0.02586	0.00000	-0.12164
71	C5	S	-1.23552	0.00000	0.00000	-0.26385	0.00000
72	C5	PX	0.14771	0.00000	0.00000	-0.08808	0.00000
73	C5	PY	0.08422	0.00000	0.00000	-1.53091	0.00000
74	C5	PZ	0.00000	0.07151	0.02509	0.00000	0.07037
75	C5	DXX	0.01089	0.00000	0.00000	0.01515	0.00000
76	C5	DYY	-0.08443	0.00000	0.00000	-0.02825	0.00000
77	C5	DZZ	0.08840	0.00000	0.00000	0.01831	0.00000
78	C5	DXY	-0.03279	0.00000	0.00000	-0.03576	0.00000
79	C5	DXZ	0.00000	0.27326	-0.17727	0.00000	0.20991
80	C5	DYZ	0.00000	0.11413	0.10400	0.00000	-0.42656
81	C6	S	-0.02462	0.00000	0.00000	0.01870	0.00000
82	C6	S	-0.01856	0.00000	0.00000	0.51618	0.00000
83	C6	PX	-0.33853	0.00000	0.00000	0.01425	0.00000
84	C6	PY	0.05950	0.00000	0.00000	0.39563	0.00000
85	C6	PZ	0.00000	0.02933	-0.06391	0.00000	0.04874
86	C6	S	-1.50151	0.00000	0.00000	-0.34211	0.00000
87	C6	PX	4.29752	0.00000	0.00000	0.69139	0.00000
88	C6	PY	-0.52547	0.00000	0.00000	-4.58544	0.00000
89	C6	PZ	0.00000	-0.02343	0.10147	0.00000	-0.19072
90	C6	DXX	-0.04510	0.00000	0.00000	0.05809	0.00000
91	C6	DYY	-0.13249	0.00000	0.00000	0.05911	0.00000
92	C6	DZZ	0.12138	0.00000	0.00000	-0.01036	0.00000
93	C6	DXY	-0.04779	0.00000	0.00000	-0.00634	0.00000
94	C6	DXZ	0.00000	-0.12372	-0.23039	0.00000	-0.04035
95	C6	DYZ	0.00000	0.00782	-0.23515	0.00000	-0.01556
96	C7	S	0.04294	0.00000	0.00000	0.01093	0.00000
97	C7	S	0.87913	0.00000	0.00000	0.15276	0.00000
98	C7	PX	-0.30296	0.00000	0.00000	-0.06227	0.00000
99	C7	PY	0.05853	0.00000	0.00000	0.18749	0.00000
100	C7	PZ	0.00000	-0.12939	-0.03763	0.00000	-0.06717
101	C7	S	-3.17298	0.00000	0.00000	-0.36802	0.00000
102	C7	PX	1.66306	0.00000	0.00000	-1.02146	0.00000
103	C7	PY	-1.08869	0.00000	0.00000	1.49627	0.00000

104	C7	PZ	0.00000	0.11411	-0.10983	0.00000	0.03266
105	C7	DXX	0.01359	0.00000	0.00000	0.08682	0.00000
106	C7	DYY	0.07803	0.00000	0.00000	-0.01212	0.00000
107	C7	DZZ	-0.02225	0.00000	0.00000	-0.02495	0.00000
108	C7	DXY	0.06458	0.00000	0.00000	-0.03009	0.00000
109	C7	DXZ	0.00000	-0.23926	-0.09780	0.00000	-0.16006
110	C7	DYZ	0.00000	0.21556	0.19637	0.00000	0.03836
111	O1	S	0.01245	0.00000	0.00000	-0.00651	0.00000
112	O1	S	0.24692	0.00000	0.00000	-0.32537	0.00000
113	O1	PX	-0.15803	0.00000	0.00000	0.05196	0.00000
114	O1	PY	-0.12095	0.00000	0.00000	0.22619	0.00000
115	O1	PZ	0.00000	0.08026	0.08117	0.00000	-0.09152
116	O1	S	-0.81533	0.00000	0.00000	0.40048	0.00000
117	O1	PX	0.65286	0.00000	0.00000	0.01762	0.00000
118	O1	PY	0.62486	0.00000	0.00000	-0.49346	0.00000
119	O1	PZ	0.00000	-0.09829	-0.18473	0.00000	0.21018
120	O1	DXX	0.00870	0.00000	0.00000	-0.08860	0.00000
121	O1	DYY	0.08699	0.00000	0.00000	-0.12674	0.00000
122	O1	DZZ	0.10222	0.00000	0.00000	-0.01333	0.00000
123	O1	DXY	0.04579	0.00000	0.00000	-0.04422	0.00000
124	O1	DXZ	0.00000	0.09742	0.11261	0.00000	-0.11148
125	O1	DYZ	0.00000	0.18084	-0.02053	0.00000	0.04013
126	H4	S	0.09353	0.00000	0.00000	0.27617	0.00000
127	H4	S	0.24432	0.00000	0.00000	0.36697	0.00000
128	H4	PX	0.01284	0.00000	0.00000	-0.01635	0.00000
129	H4	PY	0.02368	0.00000	0.00000	-0.00541	0.00000
130	H4	PZ	0.00000	-0.03392	0.10175	0.00000	-0.21909
131	N1	S	0.01768	0.00000	0.00000	-0.01095	0.00000
132	N1	S	0.22352	0.00000	0.00000	-0.16738	0.00000
133	N1	PX	0.28947	0.00000	0.00000	-0.05972	0.00000
134	N1	PY	-0.30668	0.00000	0.00000	-0.13101	0.00000
135	N1	PZ	0.00000	0.00957	0.01985	0.00000	-0.03010
136	N1	S	-0.72675	0.00000	0.00000	-0.00524	0.00000
137	N1	PX	-2.05956	0.00000	0.00000	1.10488	0.00000
138	N1	PY	1.97029	0.00000	0.00000	-1.52354	0.00000
139	N1	PZ	0.00000	-0.09672	-0.09268	0.00000	0.15308
140	N1	DXX	0.06950	0.00000	0.00000	0.03105	0.00000
141	N1	DYY	0.04567	0.00000	0.00000	-0.10394	0.00000
142	N1	DZZ	0.01829	0.00000	0.00000	-0.00233	0.00000
143	N1	DXY	-0.01297	0.00000	0.00000	-0.02197	0.00000
144	N1	DXZ	0.00000	0.13890	-0.22683	0.00000	-0.14300
145	N1	DYZ	0.00000	-0.03000	0.19902	0.00000	0.05750
146	H6	S	-0.08203	0.00000	0.00000	0.22272	0.00000
147	H6	S	-0.09791	0.00000	0.00000	0.41118	0.00000
148	H6	PX	-0.01508	0.00000	0.00000	-0.02603	0.00000
149	H6	PY	0.01849	0.00000	0.00000	0.00146	0.00000
150	H6	PZ	0.00000	0.00839	0.03933	0.00000	-0.17751
151	C8	S	-0.00598	0.00000	0.00000	0.00363	0.00000
152	C8	S	-0.33847	0.00000	0.00000	-0.10439	0.00000
153	C8	PX	-0.14843	0.00000	0.00000	-0.42052	0.00000
154	C8	PY	0.24590	0.00000	0.00000	-0.12760	0.00000
155	C8	PZ	0.00000	-0.00025	0.00206	0.00000	0.01487
156	C8	S	4.66409	0.00000	0.00000	-0.46778	0.00000
157	C8	PX	-0.48555	0.00000	0.00000	4.19037	0.00000

158	C8	PY	-2.42023	0.00000	0.00000	-0.61509	0.00000
159	C8	PZ	0.00000	0.05116	0.03948	0.00000	-0.05813
160	C8	DXX	0.13408	0.00000	0.00000	-0.03253	0.00000
161	C8	DYY	0.00970	0.00000	0.00000	0.00243	0.00000
162	C8	DZZ	-0.05847	0.00000	0.00000	-0.00483	0.00000
163	C8	DXY	-0.00296	0.00000	0.00000	0.02288	0.00000
164	C8	DXZ	0.00000	-0.18830	0.21489	0.00000	0.17922
165	C8	DYZ	0.00000	0.14818	-0.24245	0.00000	-0.00763
166	H8	S	-0.05948	0.00000	0.00000	0.28969	0.00000
167	H8	S	-0.37519	0.00000	0.00000	0.46272	0.00000
168	H8	PX	0.00688	0.00000	0.00000	0.03794	0.00000
169	H8	PY	0.00949	0.00000	0.00000	0.02801	0.00000
170	H8	PZ	0.00000	-0.11371	-0.09007	0.00000	-0.08871
171	C10	S	0.02357	0.00000	0.00000	0.00379	0.00000
172	C10	S	0.20734	0.00000	0.00000	-0.05387	0.00000
173	C10	PX	0.17708	0.00000	0.00000	0.04937	0.00000
174	C10	PY	-0.16403	0.00000	0.00000	-0.08448	0.00000
175	C10	PZ	0.00000	0.05374	-0.12503	0.00000	-0.01707
176	C10	S	-3.47738	0.00000	0.00000	-0.90100	0.00000
177	C10	PX	-0.13079	0.00000	0.00000	-2.01979	0.00000
178	C10	PY	-1.27698	0.00000	0.00000	-0.72432	0.00000
179	C10	PZ	0.00000	-0.04213	0.08305	0.00000	0.02400
180	C10	DXX	0.05661	0.00000	0.00000	0.06576	0.00000
181	C10	DYY	-0.10340	0.00000	0.00000	-0.05031	0.00000
182	C10	DZZ	0.02859	0.00000	0.00000	-0.01399	0.00000
183	C10	DXY	0.00768	0.00000	0.00000	-0.11250	0.00000
184	C10	DXZ	0.00000	-0.05821	0.07444	0.00000	0.17803
185	C10	DYZ	0.00000	-0.16112	0.29843	0.00000	0.08638
186	H16	S	0.20316	0.00000	0.00000	0.35243	0.00000
187	H16	S	0.24297	0.00000	0.00000	0.66018	0.00000
188	H16	PX	-0.03008	0.00000	0.00000	0.00646	0.00000
189	H16	PY	-0.00974	0.00000	0.00000	-0.02432	0.00000
190	H16	PZ	0.00000	0.00571	-0.01791	0.00000	0.06747
191	H18	S	0.02753	0.00000	0.00000	-0.36491	0.00000
192	H18	S	-0.05436	0.00000	0.00000	-0.61253	0.00000
193	H18	PX	-0.02509	0.00000	0.00000	-0.00506	0.00000
194	H18	PY	0.02110	0.00000	0.00000	0.03963	0.00000
195	H18	PZ	0.00000	0.06861	-0.11634	0.00000	-0.08782
196	C9	S	0.02099	0.00000	0.00000	-0.01785	0.00000
197	C9	S	0.24938	0.00000	0.00000	-0.19406	0.00000
198	C9	PX	0.07987	0.00000	0.00000	-0.02146	0.00000
199	C9	PY	-0.10217	0.00000	0.00000	0.10038	0.00000
200	C9	PZ	0.00000	-0.07901	-0.02089	0.00000	0.03135
201	C9	S	-0.99438	0.00000	0.00000	0.50418	0.00000
202	C9	PX	0.15071	0.00000	0.00000	-0.02249	0.00000
203	C9	PY	0.48180	0.00000	0.00000	-0.37956	0.00000
204	C9	PZ	0.00000	0.15109	0.10365	0.00000	-0.15807
205	C9	DXX	0.03950	0.00000	0.00000	-0.08100	0.00000
206	C9	DYY	-0.03588	0.00000	0.00000	0.00994	0.00000
207	C9	DZZ	0.00458	0.00000	0.00000	0.05416	0.00000
208	C9	DXY	-0.12616	0.00000	0.00000	0.10487	0.00000
209	C9	DXZ	0.00000	-0.12700	-0.04172	0.00000	0.04991
210	C9	DYZ	0.00000	-0.19626	-0.09076	0.00000	0.10099
211	H3	S	0.07140	0.00000	0.00000	-0.00130	0.00000

212	H3	S	-0.11404	0.00000	0.00000	0.14681	0.00000
213	H3	PX	-0.06477	0.00000	0.00000	0.07705	0.00000
214	H3	PY	0.00572	0.00000	0.00000	0.00484	0.00000
215	H3	PZ	0.00000	-0.07445	-0.02772	0.00000	0.02531
216	H5	S	0.12546	-0.04399	0.00366	-0.08564	-0.00742
217	H5	S	0.09300	0.10690	0.04996	-0.08509	-0.08160
218	H5	PX	0.01502	0.03259	0.01346	-0.03284	-0.01971
219	H5	PY	-0.00360	0.07551	0.02630	0.00023	-0.03387
220	H5	PZ	0.01961	0.01051	0.00471	-0.02299	-0.00702
221	H7	S	0.12546	0.04399	-0.00366	-0.08564	0.00742
222	H7	S	0.09300	-0.10690	-0.04996	-0.08509	0.08160
223	H7	PX	0.01502	-0.03259	-0.01346	-0.03284	0.01971
224	H7	PY	-0.00360	-0.07551	-0.02630	0.00023	0.03387
225	H7	PZ	-0.01961	0.01051	0.00471	0.02299	-0.00702

MO:	126	127	128	129	130
Eigenvalues:	1.66549	1.68081	1.68528	1.70352	1.71993
(ev):	45.32025	45.73720	45.85883	46.35520	46.80183

		A	A	A	A	A	
1	H1	S	0.16851	0.00000	0.55819	0.00000	0.00000
2	H1	S	0.18463	0.00000	1.07200	0.00000	0.00000
3	H1	PX	-0.01046	0.00000	0.02693	0.00000	0.00000
4	H1	PY	0.02803	0.00000	0.01841	0.00000	0.00000
5	H1	PZ	0.00000	-0.03610	0.00000	0.04791	-0.15354
6	C1	S	0.04540	0.00000	-0.00356	0.00000	0.00000
7	C1	S	0.76507	0.00000	-0.26109	0.00000	0.00000
8	C1	PX	-0.05190	0.00000	0.18168	0.00000	0.00000
9	C1	PY	-0.13805	0.00000	-0.00799	0.00000	0.00000
10	C1	PZ	0.00000	0.01762	0.00000	0.00043	-0.16004
11	C1	S	-5.05081	0.00000	-0.31330	0.00000	0.00000
12	C1	PX	0.41693	0.00000	-2.97723	0.00000	0.00000
13	C1	PY	1.27707	0.00000	0.62287	0.00000	0.00000
14	C1	PZ	0.00000	-0.15417	0.00000	0.04643	0.24269
15	C1	DXX	0.05354	0.00000	0.09130	0.00000	0.00000
16	C1	DYY	0.05468	0.00000	-0.10491	0.00000	0.00000
17	C1	DZZ	-0.06250	0.00000	0.02380	0.00000	0.00000
18	C1	DXY	0.07426	0.00000	0.04491	0.00000	0.00000
19	C1	DXZ	0.00000	0.00019	0.00000	-0.02568	-0.36026
20	C1	DYZ	0.00000	0.00305	0.00000	0.22613	0.06477
21	C2	S	0.02364	0.00000	-0.01561	0.00000	0.00000
22	C2	S	0.48565	0.00000	-0.43786	0.00000	0.00000
23	C2	PX	0.03204	0.00000	-0.19584	0.00000	0.00000
24	C2	PY	0.15841	0.00000	0.05151	0.00000	0.00000
25	C2	PZ	0.00000	-0.09710	0.00000	0.04184	-0.03846
26	C2	S	-2.29989	0.00000	1.56749	0.00000	0.00000
27	C2	PX	-1.62578	0.00000	1.99916	0.00000	0.00000
28	C2	PY	-0.66699	0.00000	1.16861	0.00000	0.00000
29	C2	PZ	0.00000	0.14598	0.00000	0.04918	0.00739
30	C2	DXX	-0.00907	0.00000	-0.04783	0.00000	0.00000
31	C2	DYY	0.01439	0.00000	-0.01606	0.00000	0.00000
32	C2	DZZ	-0.02447	0.00000	0.04487	0.00000	0.00000
33	C2	DXY	0.00505	0.00000	0.09884	0.00000	0.00000
34	C2	DXZ	0.00000	0.31183	0.00000	-0.05631	0.08238

35	C2	DYZ	0.00000	-0.12785	0.00000	-0.17700	-0.08315
36	C3	S	-0.00610	0.00000	0.01911	0.00000	0.00000
37	C3	S	-0.48581	0.00000	0.21190	0.00000	0.00000
38	C3	PX	-0.44044	0.00000	-0.45149	0.00000	0.00000
39	C3	PY	0.12484	0.00000	-0.23514	0.00000	0.00000
40	C3	PZ	0.00000	-0.02844	0.00000	-0.04338	0.05506
41	C3	S	2.01149	0.00000	-0.50347	0.00000	0.00000
42	C3	PX	4.31556	0.00000	3.72735	0.00000	0.00000
43	C3	PY	0.30181	0.00000	0.96192	0.00000	0.00000
44	C3	PZ	0.00000	0.19802	0.00000	0.11123	-0.13586
45	C3	DXX	-0.01375	0.00000	0.09158	0.00000	0.00000
46	C3	DYY	0.08572	0.00000	-0.03850	0.00000	0.00000
47	C3	DZZ	-0.08712	0.00000	-0.01424	0.00000	0.00000
48	C3	DXY	-0.01797	0.00000	-0.01645	0.00000	0.00000
49	C3	DXZ	0.00000	0.06161	0.00000	-0.28310	0.12367
50	C3	DYZ	0.00000	0.06696	0.00000	-0.19199	0.02329
51	C4	S	-0.04221	0.00000	0.00504	0.00000	0.00000
52	C4	S	-0.84244	0.00000	0.01445	0.00000	0.00000
53	C4	PX	-0.05393	0.00000	-0.29679	0.00000	0.00000
54	C4	PY	0.33044	0.00000	-0.08075	0.00000	0.00000
55	C4	PZ	0.00000	-0.02370	0.00000	-0.00872	-0.01564
56	C4	S	2.18340	0.00000	-0.74310	0.00000	0.00000
57	C4	PX	0.96231	0.00000	0.07850	0.00000	0.00000
58	C4	PY	-2.67242	0.00000	0.99082	0.00000	0.00000
59	C4	PZ	0.00000	0.14134	0.00000	-0.11106	-0.21071
60	C4	DXX	-0.01010	0.00000	-0.02502	0.00000	0.00000
61	C4	DYY	-0.07620	0.00000	0.03641	0.00000	0.00000
62	C4	DZZ	0.00891	0.00000	0.01933	0.00000	0.00000
63	C4	DXY	-0.03385	0.00000	0.04246	0.00000	0.00000
64	C4	DXZ	0.00000	0.23641	0.00000	-0.05608	0.20100
65	C4	DYZ	0.00000	0.23815	0.00000	-0.18295	-0.28085
66	C5	S	-0.00044	0.00000	0.01362	0.00000	0.00000
67	C5	S	-0.04449	0.00000	0.48267	0.00000	0.00000
68	C5	PX	-0.04661	0.00000	0.21643	0.00000	0.00000
69	C5	PY	0.00841	0.00000	-0.12449	0.00000	0.00000
70	C5	PZ	0.00000	0.06272	0.00000	0.05693	0.06988
71	C5	S	0.98274	0.00000	-1.87787	0.00000	0.00000
72	C5	PX	-0.09947	0.00000	-1.32521	0.00000	0.00000
73	C5	PY	-0.14455	0.00000	1.97502	0.00000	0.00000
74	C5	PZ	0.00000	-0.07582	0.00000	-0.03948	-0.01080
75	C5	DXX	-0.03972	0.00000	0.00679	0.00000	0.00000
76	C5	DYY	0.06818	0.00000	-0.05002	0.00000	0.00000
77	C5	DZZ	-0.04106	0.00000	0.05021	0.00000	0.00000
78	C5	DXY	0.02109	0.00000	0.05809	0.00000	0.00000
79	C5	DXZ	0.00000	-0.21220	0.00000	0.07592	-0.13301
80	C5	DYZ	0.00000	0.05872	0.00000	0.19930	0.00958
81	C6	S	-0.03509	0.00000	-0.00234	0.00000	0.00000
82	C6	S	-0.55143	0.00000	-0.02906	0.00000	0.00000
83	C6	PX	0.03515	0.00000	0.30693	0.00000	0.00000
84	C6	PY	-0.03055	0.00000	-0.19651	0.00000	0.00000
85	C6	PZ	0.00000	0.09108	0.00000	0.04003	0.00979
86	C6	S	4.30492	0.00000	2.09993	0.00000	0.00000
87	C6	PX	1.03298	0.00000	0.03805	0.00000	0.00000
88	C6	PY	1.92582	0.00000	0.59630	0.00000	0.00000

89	C6	PZ	0.00000	-0.27570	0.00000	-0.19614	0.02813
90	C6	DXX	0.01207	0.00000	0.02885	0.00000	0.00000
91	C6	DYY	0.00973	0.00000	-0.02396	0.00000	0.00000
92	C6	DZZ	-0.04125	0.00000	0.01520	0.00000	0.00000
93	C6	DXY	-0.00233	0.00000	0.08731	0.00000	0.00000
94	C6	DXZ	0.00000	-0.24472	0.00000	0.16066	-0.21843
95	C6	DYZ	0.00000	0.31873	0.00000	0.27281	-0.01027
96	C7	S	0.03038	0.00000	0.00455	0.00000	0.00000
97	C7	S	0.31190	0.00000	-0.11458	0.00000	0.00000
98	C7	PX	0.05111	0.00000	0.06413	0.00000	0.00000
99	C7	PY	0.05040	0.00000	-0.03923	0.00000	0.00000
100	C7	PZ	0.00000	-0.05267	0.00000	-0.00388	-0.04755
101	C7	S	-3.33786	0.00000	-1.63008	0.00000	0.00000
102	C7	PX	-1.12820	0.00000	-0.79721	0.00000	0.00000
103	C7	PY	-1.41535	0.00000	-0.98191	0.00000	0.00000
104	C7	PZ	0.00000	-0.00968	0.00000	0.02749	0.05590
105	C7	DXX	0.12773	0.00000	0.01494	0.00000	0.00000
106	C7	DYY	-0.06154	0.00000	-0.04505	0.00000	0.00000
107	C7	DZZ	-0.05582	0.00000	0.02754	0.00000	0.00000
108	C7	DXY	0.03187	0.00000	-0.03045	0.00000	0.00000
109	C7	DXZ	0.00000	-0.16577	0.00000	-0.02829	-0.09718
110	C7	DYZ	0.00000	-0.07806	0.00000	-0.03983	0.03474
111	O1	S	-0.00445	0.00000	0.00508	0.00000	0.00000
112	O1	S	-0.00541	0.00000	0.14400	0.00000	0.00000
113	O1	PX	0.27309	0.00000	-0.20443	0.00000	0.00000
114	O1	PY	-0.05340	0.00000	-0.08577	0.00000	0.00000
115	O1	PZ	0.00000	0.03963	0.00000	-0.04553	-0.14717
116	O1	S	0.62886	0.00000	-0.40346	0.00000	0.00000
117	O1	PX	-0.91614	0.00000	0.58216	0.00000	0.00000
118	O1	PY	-0.32952	0.00000	0.46321	0.00000	0.00000
119	O1	PZ	0.00000	-0.20498	0.00000	0.21113	0.48525
120	O1	DXX	0.14052	0.00000	-0.01589	0.00000	0.00000
121	O1	DYY	-0.01799	0.00000	0.07859	0.00000	0.00000
122	O1	DZZ	-0.13660	0.00000	0.06038	0.00000	0.00000
123	O1	DXY	-0.08382	0.00000	0.02354	0.00000	0.00000
124	O1	DXZ	0.00000	0.15044	0.00000	-0.13134	-0.24789
125	O1	DYZ	0.00000	-0.21699	0.00000	0.19028	0.23218
126	H4	S	0.01274	0.00000	-0.40492	0.00000	0.00000
127	H4	S	-0.10272	0.00000	-0.68887	0.00000	0.00000
128	H4	PX	-0.01679	0.00000	0.02244	0.00000	0.00000
129	H4	PY	-0.02763	0.00000	-0.00429	0.00000	0.00000
130	H4	PZ	0.00000	0.10626	0.00000	0.05104	0.07204
131	N1	S	-0.00144	0.00000	0.01859	0.00000	0.00000
132	N1	S	0.24132	0.00000	0.24913	0.00000	0.00000
133	N1	PX	0.08803	0.00000	0.08288	0.00000	0.00000
134	N1	PY	0.09550	0.00000	-0.01921	0.00000	0.00000
135	N1	PZ	0.00000	0.06906	0.00000	0.07580	0.00775
136	N1	S	0.26317	0.00000	-1.22721	0.00000	0.00000
137	N1	PX	-0.18513	0.00000	-0.47734	0.00000	0.00000
138	N1	PY	-0.10857	0.00000	-0.37986	0.00000	0.00000
139	N1	PZ	0.00000	0.09586	0.00000	0.18203	-0.08186
140	N1	DXX	0.06157	0.00000	0.02550	0.00000	0.00000
141	N1	DYY	0.02927	0.00000	0.05359	0.00000	0.00000
142	N1	DZZ	-0.01743	0.00000	0.03698	0.00000	0.00000

143	N1	DXY	-0.00381	0.00000	0.02339	0.00000	0.00000
144	N1	DXZ	0.00000	-0.07818	0.00000	-0.13478	0.00765
145	N1	DYZ	0.00000	-0.18977	0.00000	-0.23836	0.03466
146	H6	S	-0.20573	0.00000	0.44840	0.00000	0.00000
147	H6	S	-0.40230	0.00000	0.70990	0.00000	0.00000
148	H6	PX	0.01897	0.00000	-0.02913	0.00000	0.00000
149	H6	PY	0.01211	0.00000	-0.01835	0.00000	0.00000
150	H6	PZ	0.00000	-0.12707	0.00000	0.08013	-0.04197
151	C8	S	-0.01494	0.00000	-0.00553	0.00000	0.00000
152	C8	S	-0.45188	0.00000	-0.15027	0.00000	0.00000
153	C8	PX	-0.20067	0.00000	-0.07846	0.00000	0.00000
154	C8	PY	0.01900	0.00000	-0.25835	0.00000	0.00000
155	C8	PZ	0.00000	-0.01881	0.00000	0.00997	-0.01181
156	C8	S	1.51665	0.00000	-0.87062	0.00000	0.00000
157	C8	PX	0.88938	0.00000	-0.63612	0.00000	0.00000
158	C8	PY	-0.96385	0.00000	2.61431	0.00000	0.00000
159	C8	PZ	0.00000	0.06505	0.00000	-0.15390	0.09643
160	C8	DXX	-0.01248	0.00000	-0.06189	0.00000	0.00000
161	C8	DYY	0.02131	0.00000	-0.05819	0.00000	0.00000
162	C8	DZZ	-0.03501	0.00000	0.08308	0.00000	0.00000
163	C8	DXY	-0.01535	0.00000	-0.03544	0.00000	0.00000
164	C8	DXZ	0.00000	0.05771	0.00000	0.12164	-0.04495
165	C8	DYZ	0.00000	0.18734	0.00000	-0.11047	0.10135
166	H8	S	0.53355	0.00000	0.33972	0.00000	0.00000
167	H8	S	0.65196	0.00000	0.37525	0.00000	0.00000
168	H8	PX	0.02354	0.00000	0.02375	0.00000	0.00000
169	H8	PY	-0.03144	0.00000	-0.03759	0.00000	0.00000
170	H8	PZ	0.00000	-0.08865	0.00000	-0.00180	-0.05100
171	C10	S	0.01676	0.00000	-0.00979	0.00000	0.00000
172	C10	S	0.21621	0.00000	-0.03738	0.00000	0.00000
173	C10	PX	0.02475	0.00000	-0.02328	0.00000	0.00000
174	C10	PY	-0.01604	0.00000	0.13591	0.00000	0.00000
175	C10	PZ	0.00000	0.07767	0.00000	-0.02960	0.03710
176	C10	S	-1.71725	0.00000	2.25270	0.00000	0.00000
177	C10	PX	-0.42307	0.00000	-0.30762	0.00000	0.00000
178	C10	PY	-0.90127	0.00000	0.86479	0.00000	0.00000
179	C10	PZ	0.00000	-0.08985	0.00000	0.05705	-0.05958
180	C10	DXX	0.07442	0.00000	-0.06617	0.00000	0.00000
181	C10	DYY	-0.03550	0.00000	0.03945	0.00000	0.00000
182	C10	DZZ	-0.02961	0.00000	0.04984	0.00000	0.00000
183	C10	DXY	-0.01385	0.00000	-0.03195	0.00000	0.00000
184	C10	DXZ	0.00000	0.19505	0.00000	0.31519	-0.14786
185	C10	DYZ	0.00000	-0.14189	0.00000	0.17395	-0.13298
186	H16	S	0.15817	0.00000	0.01187	0.00000	0.00000
187	H16	S	0.14199	0.00000	0.05032	0.00000	0.00000
188	H16	PX	-0.00757	0.00000	0.00892	0.00000	0.00000
189	H16	PY	-0.00474	0.00000	-0.01647	0.00000	0.00000
190	H16	PZ	0.00000	0.11275	0.00000	0.13259	-0.05821
191	H18	S	-0.07303	0.00000	-0.04594	0.00000	0.00000
192	H18	S	-0.20072	0.00000	-0.03155	0.00000	0.00000
193	H18	PX	0.00233	0.00000	-0.00457	0.00000	0.00000
194	H18	PY	0.01726	0.00000	-0.00798	0.00000	0.00000
195	H18	PZ	0.00000	-0.02897	0.00000	-0.18301	0.10433
196	C9	S	0.00735	0.00000	0.01506	0.00000	0.00000

197	C9	S	0.11357	0.00000	0.17776	0.00000	0.00000
198	C9	PX	-0.10007	0.00000	0.07919	0.00000	0.00000
199	C9	PY	-0.07254	0.00000	-0.03207	0.00000	0.00000
200	C9	PZ	0.00000	-0.00636	0.00000	0.01313	0.07119
201	C9	S	0.37220	0.00000	-0.86014	0.00000	0.00000
202	C9	PX	-0.28168	0.00000	0.15951	0.00000	0.00000
203	C9	PY	0.00325	0.00000	0.34255	0.00000	0.00000
204	C9	PZ	0.00000	0.14747	0.00000	-0.16843	-0.44117
205	C9	DXX	-0.05233	0.00000	0.02921	0.00000	0.00000
206	C9	DYY	0.07704	0.00000	-0.03604	0.00000	0.00000
207	C9	DZZ	0.03090	0.00000	-0.00101	0.00000	0.00000
208	C9	DXY	0.18389	0.00000	-0.13171	0.00000	0.00000
209	C9	DXZ	0.00000	-0.01084	0.00000	0.03581	0.13988
210	C9	DYZ	0.00000	-0.08795	0.00000	0.11053	0.30611
211	H3	S	-0.05175	0.00000	0.03998	0.00000	0.00000
212	H3	S	-0.08665	0.00000	-0.03495	0.00000	0.00000
213	H3	PX	0.06707	0.00000	-0.06990	0.00000	0.00000
214	H3	PY	0.00859	0.00000	-0.00491	0.00000	0.00000
215	H3	PZ	0.00000	-0.01504	0.00000	0.02107	0.07685
216	H5	S	0.01148	0.03908	0.08372	-0.04149	-0.05000
217	H5	S	0.03361	0.05694	0.07838	-0.06063	-0.19823
218	H5	PX	-0.02342	0.01977	0.01623	-0.02939	-0.07776
219	H5	PY	0.03149	0.01998	-0.00234	-0.03413	-0.10237
220	H5	PZ	-0.03630	0.00513	0.01969	-0.00845	-0.02332
221	H7	S	0.01148	-0.03908	0.08372	0.04149	0.05000
222	H7	S	0.03361	-0.05694	0.07838	0.06063	0.19823
223	H7	PX	-0.02342	-0.01977	0.01623	0.02939	0.07776
224	H7	PY	0.03149	-0.01998	-0.00234	0.03413	0.10237
225	H7	PZ	0.03630	0.00513	-0.01969	-0.00845	-0.02332

MO:	131	132	133	134	135
Eigenvalues:	1.76128	1.77360	1.88956	1.93003	1.98351
(ev):	47.92702	48.26220	51.41768	52.51890	53.97413

		A	A	A	A	A	
1	H1	S	0.00000	-0.22188	-0.05629	0.13897	-0.18629
2	H1	S	0.00000	-0.04031	-0.00271	0.35563	-0.13177
3	H1	PX	0.00000	-0.02408	-0.00126	0.02052	-0.02359
4	H1	PY	0.00000	0.05217	-0.02240	-0.07853	-0.04362
5	H1	PZ	-0.05805	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.03289	-0.02192	0.01814	0.00359
7	C1	S	0.00000	0.53373	-0.09084	0.17671	0.14808
8	C1	PX	0.00000	-0.15607	-0.02254	0.09716	-0.00597
9	C1	PY	0.00000	-0.01057	-0.00245	-0.13244	-0.10437
10	C1	PZ	-0.04569	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-3.64290	1.49353	-2.64644	-0.09275
12	C1	PX	0.00000	0.81929	-0.64320	0.20772	0.36247
13	C1	PY	0.00000	2.76291	0.69742	-0.94982	0.32023
14	C1	PZ	0.08445	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.03574	0.04454	0.09123	0.07717
16	C1	DYY	0.00000	-0.00472	-0.16847	-0.08849	-0.07915
17	C1	DZZ	0.00000	-0.03859	0.17266	-0.02208	0.01672
18	C1	DXY	0.00000	-0.01500	-0.06618	-0.09555	0.01344
19	C1	DXZ	-0.08250	0.00000	0.00000	0.00000	0.00000

20	C1	DYZ	-0.08329	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.03044	-0.00171	0.00368	-0.00445
22	C2	S	0.00000	0.59337	0.22177	0.25140	0.00531
23	C2	PX	0.00000	0.18706	0.15622	0.12660	0.02977
24	C2	PY	0.00000	-0.02230	-0.11123	-0.19916	-0.01323
25	C2	PZ	-0.00571	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-3.69143	0.43162	-1.07691	-0.01978
27	C2	PX	0.00000	-2.45783	-0.03245	-0.65366	-0.69030
28	C2	PY	0.00000	-0.16981	-0.04949	-0.07354	-1.32415
29	C2	PZ	-0.05238	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	0.00718	-0.06570	-0.01459	-0.10720
31	C2	DYY	0.00000	0.02409	-0.02097	-0.04606	0.00422
32	C2	DZZ	0.00000	-0.01996	0.11811	0.07602	0.13308
33	C2	DXY	0.00000	-0.03249	0.09497	0.11436	0.12304
34	C2	DXZ	-0.02798	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02779	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.01418	0.02639	-0.00216	0.01425
37	C3	S	0.00000	-0.50427	0.49625	-0.22690	0.27599
38	C3	PX	0.00000	0.02003	0.06645	0.14335	-0.08072
39	C3	PY	0.00000	-0.58057	0.10281	-0.13267	0.08518
40	C3	PZ	0.02715	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	2.28403	-1.62373	0.40692	-3.04955
42	C3	PX	0.00000	-0.72130	1.02791	-1.23867	0.81201
43	C3	PY	0.00000	6.02401	0.41785	1.33322	0.46253
44	C3	PZ	-0.15073	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00365	0.17751	0.14714	-0.04868
46	C3	DYY	0.00000	-0.01494	-0.19919	-0.16832	-0.04062
47	C3	DZZ	0.00000	-0.03529	0.04374	0.02464	0.15126
48	C3	DXY	0.00000	-0.00401	-0.12725	-0.07468	-0.08073
49	C3	DXZ	0.19684	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.08427	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.03347	0.00786	-0.00321	-0.00817
52	C4	S	0.00000	0.38116	0.28106	-0.02786	-0.02676
53	C4	PX	0.00000	-0.02269	0.04175	-0.20224	-0.00371
54	C4	PY	0.00000	-0.22077	0.19773	-0.19734	0.05890
55	C4	PZ	0.00126	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-1.49259	-0.96965	0.17156	1.06810
57	C4	PX	0.00000	0.18445	-1.56105	3.11144	-0.54722
58	C4	PY	0.00000	2.79761	-0.03889	1.16493	-0.28304
59	C4	PZ	-0.02215	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	-0.02634	-0.15691	-0.01752	-0.09637
61	C4	DYY	0.00000	0.16439	0.03293	-0.01933	0.08496
62	C4	DZZ	0.00000	-0.09312	0.15904	0.00397	0.04270
63	C4	DXY	0.00000	0.04163	-0.05707	-0.18388	-0.04817
64	C4	DXZ	0.03880	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.02599	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.03049	0.00090	-0.02631	0.01226
67	C5	S	0.00000	-0.69620	0.05520	-0.19228	0.27626
68	C5	PX	0.00000	-0.17775	0.02268	0.13806	0.03579
69	C5	PY	0.00000	-0.00499	0.00569	0.20490	-0.08760
70	C5	PZ	0.00422	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	3.41289	-0.81334	2.84668	-0.05980
72	C5	PX	0.00000	2.19485	-0.22353	1.40949	-0.86003

73	C5	PY	0.00000	-1.91610	-0.34170	-1.07785	-0.03422
74	C5	PZ	0.00788	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.01065	-0.16352	-0.10235	-0.09808
76	C5	DYY	0.00000	-0.02365	0.02719	0.07880	0.07639
77	C5	DZZ	0.00000	-0.01875	0.15166	0.05899	0.02344
78	C5	DXY	0.00000	-0.04392	-0.03626	-0.03640	-0.04442
79	C5	DXZ	-0.04947	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.03016	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	0.00889	-0.00637	0.01703	-0.01113
82	C6	S	0.00000	0.13133	-0.08129	0.37500	0.07503
83	C6	PX	0.00000	0.10668	-0.13019	-0.11564	-0.15407
84	C6	PY	0.00000	-0.13964	0.01416	0.06943	-0.06381
85	C6	PZ	-0.01395	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	2.55040	3.06611	0.06141	-2.32265
87	C6	PX	0.00000	-1.41900	1.59398	-0.40578	1.87942
88	C6	PY	0.00000	-0.43439	-1.64632	-1.48185	3.44351
89	C6	PZ	0.19711	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.01789	-0.08010	-0.03907	-0.11486
91	C6	DYY	0.00000	0.07395	0.05107	0.06958	-0.15587
92	C6	DZZ	0.00000	-0.05527	0.03367	-0.01169	0.36897
93	C6	DXY	0.00000	0.00543	0.21519	0.21334	0.03021
94	C6	DXZ	-0.02585	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.12630	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	-0.00183	0.00516	0.00753	-0.01957
97	C7	S	0.00000	-0.03278	-0.00418	-0.02518	-0.42367
98	C7	PX	0.00000	-0.02545	-0.06062	0.00617	0.02888
99	C7	PY	0.00000	0.20734	0.00397	0.12948	-0.13085
100	C7	PZ	0.06320	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	1.84004	0.12453	0.12734	2.29331
102	C7	PX	0.00000	-1.00912	0.61204	0.20288	-2.37140
103	C7	PY	0.00000	0.83387	-0.57614	0.52383	0.47385
104	C7	PZ	-0.09727	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.00153	-0.19977	-0.12991	-0.01452
106	C7	DYY	0.00000	0.01722	0.12954	0.10064	-0.07995
107	C7	DZZ	0.00000	-0.00930	0.04890	0.02801	0.17577
108	C7	DXY	0.00000	-0.08174	0.04831	0.01508	-0.08384
109	C7	DXZ	0.21815	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.23940	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00643	-0.01387	0.05872	0.00388
112	O1	S	0.00000	-0.07366	-0.19921	0.63385	0.06668
113	O1	PX	0.00000	-0.18809	-0.05709	0.28583	-0.00811
114	O1	PY	0.00000	-0.19489	-0.10585	0.12861	-0.06196
115	O1	PZ	-0.01401	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	0.01197	0.73270	-2.50599	-0.13326
117	O1	PX	0.00000	1.07112	0.46518	-1.42096	0.14093
118	O1	PY	0.00000	1.29298	0.41311	-0.39967	0.34937
119	O1	PZ	0.04381	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.05212	-0.11032	0.30815	-0.00230
121	O1	DYY	0.00000	-0.01601	-0.05131	0.19746	0.04480
122	O1	DZZ	0.00000	-0.03125	0.01898	-0.00357	-0.01032
123	O1	DXY	0.00000	-0.05866	-0.12233	0.21600	-0.03159
124	O1	DXZ	-0.01948	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.01043	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	0.31521	0.08919	0.17391	-0.14830

127	H4	S	0.00000	0.67989	0.09722	0.44026	-0.18647
128	H4	PX	0.00000	-0.01491	0.02615	-0.01315	0.02725
129	H4	PY	0.00000	0.03838	0.02626	-0.00318	-0.00783
130	H4	PZ	0.00790	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	0.00334	0.08153	0.01435	-0.08700
132	N1	S	0.00000	-0.05745	1.01957	0.02745	-1.29721
133	N1	PX	0.00000	-0.14029	0.08259	-0.01491	0.09267
134	N1	PY	0.00000	0.00435	-0.01891	-0.04172	-0.06824
135	N1	PZ	-0.09482	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	-0.62349	-5.42373	-1.06153	7.19966
137	N1	PX	0.00000	0.74918	-1.67930	0.10905	0.85801
138	N1	PY	0.00000	-1.30852	-0.78215	-0.91176	1.81129
139	N1	PZ	-0.13483	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.07873	0.11246	-0.12805	-0.28168
141	N1	DYY	0.00000	0.00570	0.19158	0.04244	-0.28698
142	N1	DZZ	0.00000	0.03865	0.04713	0.07627	0.22550
143	N1	DXY	0.00000	-0.00808	-0.15139	-0.18723	0.05185
144	N1	DXZ	0.34769	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.03428	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00000	-0.21413	-0.01203	-0.09914	-0.24106
147	H6	S	0.00000	-0.57029	-0.05666	-0.10741	-0.33979
148	H6	PX	0.00000	0.01490	0.01372	0.04012	0.04903
149	H6	PY	0.00000	0.01168	-0.01983	-0.05398	-0.07644
150	H6	PZ	-0.00256	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.00923	0.01302	0.00995	0.01921
152	C8	S	0.00000	-0.04892	0.08659	0.07350	0.43761
153	C8	PX	0.00000	-0.12627	0.01219	-0.07883	-0.10871
154	C8	PY	0.00000	-0.20279	-0.05250	-0.14021	0.08020
155	C8	PZ	-0.02715	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	-1.86436	0.61847	-0.98674	-2.57796
157	C8	PX	0.00000	0.78446	-2.30724	0.55344	1.62453
158	C8	PY	0.00000	3.13767	1.68899	2.09835	-2.50495
159	C8	PZ	0.17372	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.07652	0.13469	0.07620	-0.10235
161	C8	DYY	0.00000	-0.04528	-0.13814	-0.12413	-0.06844
162	C8	DZZ	0.00000	0.07355	0.00035	0.01714	0.21241
163	C8	DXY	0.00000	0.01891	0.03006	0.09160	-0.02451
164	C8	DXZ	-0.30860	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.03477	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	0.11888	0.04624	0.11878	0.31817
167	H8	S	0.00000	0.24079	-0.33573	-0.12629	0.67148
168	H8	PX	0.00000	0.01919	0.03037	0.03051	0.04189
169	H8	PY	0.00000	-0.01629	-0.00591	0.01143	-0.05524
170	H8	PZ	0.09793	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	-0.01546	-0.00620	-0.01234	0.00275
172	C10	S	0.00000	0.01979	0.05492	0.01938	-0.10203
173	C10	PX	0.00000	-0.05213	-0.03393	-0.03790	0.01581
174	C10	PY	0.00000	0.22061	0.14619	0.18794	-0.06390
175	C10	PZ	0.02564	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	2.70893	1.36583	1.80492	-1.17880
177	C10	PX	0.00000	-0.77495	0.79893	-0.53947	-0.59157
178	C10	PY	0.00000	0.90481	0.67882	0.55267	-0.42071
179	C10	PZ	-0.06982	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.03425	-0.04796	0.00627	-0.00411

181	C10	DYY	0.00000	0.03119	0.00008	-0.00618	-0.03633
182	C10	DZZ	0.00000	0.03742	0.08358	0.04972	0.09115
183	C10	DXY	0.00000	-0.05058	0.03391	-0.01601	-0.00587
184	C10	DXZ	0.47851	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00589	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.01316	-0.15200	-0.00830	0.13135
187	H16	S	0.00000	0.19742	-0.26120	0.14066	0.25365
188	H16	PX	0.00000	0.01569	0.00439	0.01889	0.02447
189	H16	PY	0.00000	-0.01086	0.00431	0.01824	0.01577
190	H16	PZ	0.27469	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	-0.12383	0.14620	-0.10019	-0.10901
192	H18	S	0.00000	-0.17685	0.25908	-0.14385	-0.14189
193	H18	PX	0.00000	-0.00230	-0.02470	-0.01459	-0.00597
194	H18	PY	0.00000	-0.00518	0.00065	0.00984	0.01488
195	H18	PZ	-0.23021	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.07625	-0.00830	0.00494	-0.00081
197	C9	S	0.00000	0.87661	-0.11980	-0.04626	-0.02934
198	C9	PX	0.00000	0.12214	0.04698	-0.17689	0.01374
199	C9	PY	0.00000	-0.15464	0.10156	-0.10865	0.00838
200	C9	PZ	0.00890	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	-3.17215	-0.20040	1.34302	-0.05517
202	C9	PX	0.00000	0.56601	0.36763	-0.63082	0.13601
203	C9	PY	0.00000	1.10981	-0.39377	0.27851	-0.09599
204	C9	PZ	-0.04374	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	-0.10657	-0.30974	0.35305	-0.12446
206	C9	DYY	0.00000	0.03237	0.12065	-0.05743	0.06220
207	C9	DZZ	0.00000	0.13439	0.18067	-0.24220	0.06449
208	C9	DXY	0.00000	-0.06075	0.15690	-0.00508	0.07596
209	C9	DXZ	0.01711	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.03353	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.18945	0.05406	-0.18872	0.01158
212	H3	S	0.00000	-0.08306	0.24360	-0.34527	0.05169
213	H3	PX	0.00000	-0.01489	0.16396	-0.07963	0.08242
214	H3	PY	0.00000	0.01917	0.00987	-0.00484	0.00799
215	H3	PZ	0.01026	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00206	0.35679	-0.04896	0.01931	-0.00624
217	H5	S	-0.02007	0.30600	-0.08960	-0.10861	-0.04371
218	H5	PX	-0.00839	-0.03465	-0.10387	0.08944	-0.04895
219	H5	PY	-0.01047	0.02545	-0.03075	0.00183	-0.01598
220	H5	PZ	-0.00272	-0.02144	-0.05465	0.03906	-0.02522
221	H7	S	0.00206	0.35679	-0.04896	0.01931	-0.00624
222	H7	S	0.02007	0.30600	-0.08960	-0.10861	-0.04371
223	H7	PX	0.00839	-0.03465	-0.10387	0.08944	-0.04895
224	H7	PY	0.01047	0.02545	-0.03075	0.00183	-0.01598
225	H7	PZ	-0.00272	0.02144	0.05465	-0.03906	0.02522

M0:	136	137	138	139	140
Eigenvalues:	2.03285	2.07072	2.10565	2.10726	2.12833
(ev):	55.31678	56.34722	57.29768	57.34162	57.91471

		A	A	A	A	A	
1	H1	S	-0.03448	-0.00721	0.17825	0.00000	0.23073
2	H1	S	0.08424	0.38995	0.13455	0.00000	0.47675
3	H1	PX	0.02129	-0.01379	0.09304	0.00000	0.02346

4	H1	PY	0.01617	0.01124	-0.07421	0.00000	0.03635
5	H1	PZ	0.00000	0.00000	0.00000	-0.24925	0.00000
6	C1	S	-0.01942	-0.01913	-0.01747	0.00000	-0.01097
7	C1	S	-0.24978	-0.23415	-0.04903	0.00000	-0.51555
8	C1	PX	-0.01437	-0.02442	-0.07614	0.00000	0.18270
9	C1	PY	-0.04443	0.11912	0.08463	0.00000	0.13625
10	C1	PZ	0.00000	0.00000	0.00000	0.00206	0.00000
11	C1	S	0.56215	0.63208	2.12566	0.00000	0.89898
12	C1	PX	-0.53362	-1.32361	-1.03065	0.00000	-1.73184
13	C1	PY	0.55078	0.59393	0.10710	0.00000	0.15503
14	C1	PZ	0.00000	0.00000	0.00000	0.54326	0.00000
15	C1	DXX	0.03150	0.05553	-0.05695	0.00000	0.02851
16	C1	DYY	0.09710	0.06638	0.00226	0.00000	0.09033
17	C1	DZZ	-0.09148	-0.02696	0.05990	0.00000	-0.18561
18	C1	DXY	-0.00610	0.17987	-0.15152	0.00000	-0.15165
19	C1	DXZ	0.00000	0.00000	0.00000	-0.31069	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.42950	0.00000
21	C2	S	-0.01365	0.01165	-0.01535	0.00000	0.00634
22	C2	S	0.04959	0.50570	-0.23220	0.00000	0.12467
23	C2	PX	0.07250	0.22370	0.02937	0.00000	0.06567
24	C2	PY	-0.02608	-0.00310	-0.04059	0.00000	-0.14202
25	C2	PZ	0.00000	0.00000	0.00000	0.01620	0.00000
26	C2	S	0.83916	-0.77106	1.09378	0.00000	-0.55301
27	C2	PX	-0.55355	-1.17286	0.75032	0.00000	-0.49157
28	C2	PY	-1.35388	-1.69391	-0.52256	0.00000	-1.05235
29	C2	PZ	0.00000	0.00000	0.00000	-0.13725	0.00000
30	C2	DXX	-0.06816	0.00318	-0.07924	0.00000	-0.21487
31	C2	DYY	0.08812	-0.08685	0.05457	0.00000	0.13514
32	C2	DZZ	-0.05563	0.10579	0.09327	0.00000	0.03228
33	C2	DXY	0.06123	-0.12544	-0.16307	0.00000	0.00472
34	C2	DXZ	0.00000	0.00000	0.00000	-0.08891	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.14446	0.00000
36	C3	S	0.03410	0.05226	0.01674	0.00000	0.03701
37	C3	S	0.20335	0.70247	0.24908	0.00000	0.23368
38	C3	PX	0.04510	-0.23067	0.02949	0.00000	0.08096
39	C3	PY	0.09415	-0.13942	-0.09311	0.00000	-0.14688
40	C3	PZ	0.00000	0.00000	0.00000	-0.04023	0.00000
41	C3	S	-4.34098	-6.41876	-1.98770	0.00000	-5.23912
42	C3	PX	2.04117	2.62263	0.23932	0.00000	1.02869
43	C3	PY	0.95943	3.30769	0.52916	0.00000	3.33352
44	C3	PZ	0.00000	0.00000	0.00000	-0.85225	0.00000
45	C3	DXX	0.23600	-0.06188	0.08297	0.00000	0.03713
46	C3	DYY	-0.03397	-0.02975	-0.09744	0.00000	0.05690
47	C3	DZZ	-0.26662	-0.00725	0.04716	0.00000	-0.18925
48	C3	DXY	0.07952	-0.18937	0.08991	0.00000	0.19302
49	C3	DXZ	0.00000	0.00000	0.00000	-0.01238	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.04772	0.00000
51	C4	S	0.00392	0.01356	0.00386	0.00000	0.01169
52	C4	S	-0.05992	-0.03159	-0.27160	0.00000	0.21100
53	C4	PX	-0.13273	0.14943	0.20262	0.00000	-0.05012
54	C4	PY	0.03681	-0.00319	0.08662	0.00000	-0.02290
55	C4	PZ	0.00000	0.00000	0.00000	0.00743	0.00000
56	C4	S	-1.57040	-2.57958	0.99230	0.00000	-1.05173
57	C4	PX	-0.10874	-0.60283	-2.27189	0.00000	-0.18199

58	C4	PY	-0.98423	0.65645	2.07045	0.00000	2.62256
59	C4	PZ	0.00000	0.00000	0.00000	-0.23692	0.00000
60	C4	DXX	0.05621	0.08204	0.21792	0.00000	0.05418
61	C4	DYY	-0.00396	-0.01121	-0.01206	0.00000	0.04858
62	C4	DZZ	-0.09088	-0.07921	-0.25609	0.00000	-0.17682
63	C4	DXY	0.06085	0.25109	0.13333	0.00000	-0.17212
64	C4	DXZ	0.00000	0.00000	0.00000	-0.22570	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.04719	0.00000
66	C5	S	-0.00346	-0.01136	0.02266	0.00000	-0.01030
67	C5	S	-0.09338	-0.33730	0.08408	0.00000	-0.13239
68	C5	PX	-0.02960	-0.14071	-0.13890	0.00000	0.09555
69	C5	PY	-0.02784	-0.01203	-0.11831	0.00000	0.07490
70	C5	PZ	0.00000	0.00000	0.00000	-0.03768	0.00000
71	C5	S	1.07778	2.35907	-1.61752	0.00000	1.68230
72	C5	PX	-0.31146	0.82408	-0.61103	0.00000	0.33090
73	C5	PY	0.40231	-1.33629	-0.57910	0.00000	-1.51124
74	C5	PZ	0.00000	0.00000	0.00000	0.04699	0.00000
75	C5	DXX	0.02595	0.18740	0.26238	0.00000	-0.10495
76	C5	DYY	0.09224	-0.12665	-0.16645	0.00000	0.10356
77	C5	DZZ	-0.16361	-0.02398	-0.13518	0.00000	-0.00695
78	C5	DXY	-0.00292	-0.00927	0.15535	0.00000	0.11165
79	C5	DXZ	0.00000	0.00000	0.00000	-0.07117	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.01026	0.00000
81	C6	S	-0.01956	-0.03695	0.01610	0.00000	-0.02773
82	C6	S	-0.46839	-0.31063	-0.07208	0.00000	-0.41972
83	C6	PX	-0.29634	-0.01067	-0.03963	0.00000	-0.14666
84	C6	PY	0.02175	0.07796	-0.08085	0.00000	0.05143
85	C6	PZ	0.00000	0.00000	0.00000	0.00468	0.00000
86	C6	S	0.74896	4.92261	-0.85754	0.00000	2.94850
87	C6	PX	3.47371	3.80549	1.35323	0.00000	2.93571
88	C6	PY	1.81077	-1.04675	0.15515	0.00000	-0.61196
89	C6	PZ	0.00000	0.00000	0.00000	0.45460	0.00000
90	C6	DXX	0.17530	-0.16320	0.02764	0.00000	0.23644
91	C6	DYY	-0.10381	0.02439	-0.09072	0.00000	-0.13939
92	C6	DZZ	-0.08069	0.19921	0.04222	0.00000	-0.01182
93	C6	DXY	0.15134	-0.01514	0.00561	0.00000	0.02107
94	C6	DXZ	0.00000	0.00000	0.00000	0.23247	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.10797	0.00000
96	C7	S	-0.02561	-0.03306	-0.00325	0.00000	-0.04075
97	C7	S	-0.61724	-0.46556	-0.23577	0.00000	-0.16601
98	C7	PX	0.17831	-0.00891	0.03287	0.00000	-0.15200
99	C7	PY	0.02746	-0.11014	0.11935	0.00000	-0.04144
100	C7	PZ	0.00000	0.00000	0.00000	-0.02748	0.00000
101	C7	S	2.85837	5.31405	1.25287	0.00000	5.11123
102	C7	PX	-2.63996	-3.14134	-0.59520	0.00000	-2.57323
103	C7	PY	-0.42153	-0.34975	-0.10347	0.00000	0.24508
104	C7	PZ	0.00000	0.00000	0.00000	0.59243	0.00000
105	C7	DXX	0.02752	-0.12835	-0.05873	0.00000	0.13748
106	C7	DYY	0.11769	0.01172	0.07021	0.00000	-0.17717
107	C7	DZZ	-0.12555	0.16343	0.03745	0.00000	0.14348
108	C7	DXY	0.13079	-0.20453	0.16985	0.00000	-0.14731
109	C7	DXZ	0.00000	0.00000	0.00000	-0.43207	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.19020	0.00000
111	O1	S	-0.05763	-0.00178	0.04418	0.00000	0.03133

112	O1	S	-0.78193	-0.17534	0.74869	0.00000	0.43789
113	O1	PX	-0.09522	0.00449	-0.14016	0.00000	-0.01551
114	O1	PY	0.08103	0.23142	-0.11974	0.00000	-0.17182
115	O1	PZ	0.00000	0.00000	0.00000	0.00973	0.00000
116	O1	S	2.74907	0.29491	-2.71966	0.00000	-1.88109
117	O1	PX	0.49055	-0.12603	0.54307	0.00000	0.11576
118	O1	PY	-0.49113	-0.74541	0.91635	0.00000	0.91641
119	O1	PZ	0.00000	0.00000	0.00000	-0.00855	0.00000
120	O1	DXX	-0.32759	0.05998	0.39227	0.00000	0.10067
121	O1	DYY	-0.25084	-0.06651	0.29019	0.00000	0.17800
122	O1	DZZ	0.01768	-0.06624	-0.19134	0.00000	-0.01601
123	O1	DXY	0.02611	-0.10222	-0.23070	0.00000	0.13118
124	O1	DXZ	0.00000	0.00000	0.00000	-0.15048	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.15309	0.00000
126	H4	S	-0.25746	0.09322	0.18628	0.00000	0.22275
127	H4	S	-0.25951	0.38222	0.06122	0.00000	0.26451
128	H4	PX	0.04730	-0.07815	-0.13265	0.00000	-0.01627
129	H4	PY	0.00397	-0.06226	-0.05955	0.00000	0.06567
130	H4	PZ	0.00000	0.00000	0.00000	0.03748	0.00000
131	N1	S	-0.03781	0.05386	-0.01068	0.00000	0.01365
132	N1	S	-0.49112	0.56409	-0.10941	0.00000	0.13969
133	N1	PX	0.08456	-0.01806	0.08891	0.00000	-0.02956
134	N1	PY	-0.01982	-0.06892	-0.00829	0.00000	0.02635
135	N1	PZ	0.00000	0.00000	0.00000	0.03211	0.00000
136	N1	S	2.71623	-3.21965	0.64585	0.00000	-0.96737
137	N1	PX	-0.37964	-1.21221	-0.36573	0.00000	-0.47553
138	N1	PY	1.26511	0.01602	0.47881	0.00000	0.31147
139	N1	PZ	0.00000	0.00000	0.00000	-0.04398	0.00000
140	N1	DXX	-0.10198	0.12334	-0.09700	0.00000	0.22217
141	N1	DYY	-0.06362	0.02542	-0.01897	0.00000	-0.09688
142	N1	DZZ	-0.01327	0.02734	0.10784	0.00000	-0.07688
143	N1	DXY	-0.24342	-0.02922	-0.07525	0.00000	-0.03767
144	N1	DXZ	0.00000	0.00000	0.00000	0.09051	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.20354	0.00000
146	H6	S	-0.21959	-0.16069	0.17855	0.00000	0.04915
147	H6	S	-0.37741	-0.50846	0.05504	0.00000	-0.25545
148	H6	PX	0.02269	0.00485	-0.07138	0.00000	-0.02751
149	H6	PY	-0.05362	-0.02451	-0.02898	0.00000	-0.06372
150	H6	PZ	0.00000	0.00000	0.00000	0.00742	0.00000
151	C8	S	0.02196	0.02079	0.01376	0.00000	0.00844
152	C8	S	0.11055	0.59617	0.09381	0.00000	0.24401
153	C8	PX	-0.03287	0.02380	-0.05848	0.00000	0.07374
154	C8	PY	-0.09972	0.21029	-0.09768	0.00000	0.16669
155	C8	PZ	0.00000	0.00000	0.00000	-0.01769	0.00000
156	C8	S	-1.59171	-1.40113	-0.61659	0.00000	-0.81212
157	C8	PX	-0.34136	-2.39707	-0.27558	0.00000	-1.20472
158	C8	PY	-2.19811	-2.75568	-0.10204	0.00000	-3.17120
159	C8	PZ	0.00000	0.00000	0.00000	-0.39478	0.00000
160	C8	DXX	0.24502	0.14046	0.07842	0.00000	0.04411
161	C8	DYY	-0.04858	-0.18139	-0.05080	0.00000	-0.00696
162	C8	DZZ	-0.26958	0.08222	-0.03080	0.00000	-0.06965
163	C8	DXY	0.10922	-0.14347	0.18549	0.00000	-0.34206
164	C8	DXZ	0.00000	0.00000	0.00000	-0.12092	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	-0.08632	0.00000

166	H8	S	0.27341	0.26092	0.07871	0.00000	-0.03590
167	H8	S	0.72590	0.66012	0.07460	0.00000	0.60466
168	H8	PX	0.05971	0.04874	0.05117	0.00000	0.01455
169	H8	PY	0.05328	-0.15815	0.13337	0.00000	-0.04120
170	H8	PZ	0.00000	0.00000	0.00000	-0.25810	0.00000
171	C10	S	-0.00968	0.00742	-0.00345	0.00000	0.00374
172	C10	S	-0.09720	0.01645	0.00606	0.00000	-0.11704
173	C10	PX	0.02566	-0.06013	0.02663	0.00000	-0.03224
174	C10	PY	-0.04340	-0.03203	0.05673	0.00000	-0.20323
175	C10	PZ	0.00000	0.00000	0.00000	-0.00895	0.00000
176	C10	S	-0.82189	-1.27583	0.18309	0.00000	-1.75730
177	C10	PX	0.30374	1.49318	0.11266	0.00000	0.86807
178	C10	PY	-0.42899	-0.18857	0.02126	0.00000	-0.44100
179	C10	PZ	0.00000	0.00000	0.00000	0.17644	0.00000
180	C10	DXX	0.18124	-0.02434	0.10830	0.00000	-0.07608
181	C10	DYY	-0.03297	-0.03282	-0.08347	0.00000	0.10982
182	C10	DZZ	-0.16646	0.10168	0.00001	0.00000	-0.08044
183	C10	DXY	0.03032	0.15130	-0.07213	0.00000	0.22473
184	C10	DXZ	0.00000	0.00000	0.00000	-0.05276	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.21613	0.00000
186	H16	S	-0.16312	-0.11662	-0.16277	0.00000	0.09435
187	H16	S	-0.08668	-0.46007	0.01547	0.00000	-0.31654
188	H16	PX	-0.02594	0.02848	-0.03840	0.00000	0.05477
189	H16	PY	0.05332	0.01223	0.03832	0.00000	-0.02553
190	H16	PZ	0.00000	0.00000	0.00000	-0.05409	0.00000
191	H18	S	-0.07205	0.14321	0.05328	0.00000	-0.05727
192	H18	S	0.01140	0.47442	-0.00808	0.00000	0.31061
193	H18	PX	-0.02974	-0.02161	-0.06524	0.00000	0.07039
194	H18	PY	0.06063	0.05749	0.02486	0.00000	0.04550
195	H18	PZ	0.00000	0.00000	0.00000	-0.07067	0.00000
196	C9	S	0.02235	-0.00710	-0.02380	0.00000	0.00776
197	C9	S	0.26556	-0.01795	-0.28826	0.00000	0.03869
198	C9	PX	0.08222	-0.04296	0.04885	0.00000	0.03835
199	C9	PY	0.01108	-0.00436	0.05331	0.00000	-0.02238
200	C9	PZ	0.00000	0.00000	0.00000	0.00622	0.00000
201	C9	S	-1.24455	0.32265	0.55968	0.00000	-0.21714
202	C9	PX	0.22658	-0.26653	0.03223	0.00000	0.13574
203	C9	PY	0.27810	0.14373	-0.20047	0.00000	-0.01304
204	C9	PZ	0.00000	0.00000	0.00000	0.12362	0.00000
205	C9	DXX	0.02964	0.15804	-0.13671	0.00000	-0.05399
206	C9	DYY	-0.09019	-0.06322	0.14065	0.00000	0.01224
207	C9	DZZ	0.06480	-0.09212	-0.04586	0.00000	0.01953
208	C9	DXY	-0.13743	-0.11995	0.04306	0.00000	0.13047
209	C9	DXZ	0.00000	0.00000	0.00000	0.02521	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.05684	0.00000
211	H3	S	0.13263	-0.08223	-0.13510	0.00000	0.08020
212	H3	S	0.06284	-0.08895	0.03811	0.00000	-0.01309
213	H3	PX	-0.08092	-0.15055	0.01286	0.00000	0.12924
214	H3	PY	0.01139	-0.02649	-0.04476	0.00000	0.03725
215	H3	PZ	0.00000	0.00000	0.00000	0.02424	0.00000
216	H5	S	0.08440	0.00085	-0.03417	0.06195	0.02934
217	H5	S	0.17209	0.03433	-0.13043	0.03865	-0.05227
218	H5	PX	0.03023	0.07611	-0.02956	0.07033	-0.05022
219	H5	PY	0.03074	0.03617	-0.01901	0.07033	-0.01467

220	H5	PZ	0.02305	0.03512	-0.02572	-0.00068	-0.02844
221	H7	S	0.08440	0.00085	-0.03417	-0.06195	0.02934
222	H7	S	0.17209	0.03433	-0.13043	-0.03865	-0.05227
223	H7	PX	0.03023	0.07611	-0.02956	-0.07033	-0.05022
224	H7	PY	0.03074	0.03617	-0.01901	-0.07033	-0.01467
225	H7	PZ	-0.02305	-0.03512	0.02572	-0.00068	0.02844

MO:	141	142	143	144	145
Eigenvalues:	2.16374	2.16713	2.17488	2.17972	2.21319
(ev):	58.87839	58.97055	59.18163	59.31313	60.22393

			A	A	A	A	A
1	H1	S	0.17763	0.00000	0.22691	-0.32980	0.00000
2	H1	S	-0.51849	0.00000	0.29965	-0.06370	0.00000
3	H1	PX	0.08963	0.00000	0.05662	-0.03069	0.00000
4	H1	PY	0.01433	0.00000	0.00184	-0.12010	0.00000
5	H1	PZ	0.00000	-0.17654	0.00000	0.00000	-0.07086
6	C1	S	0.01484	0.00000	0.00385	-0.00212	0.00000
7	C1	S	0.21476	0.00000	-0.26185	0.13677	0.00000
8	C1	PX	-0.07084	0.00000	0.09117	0.04394	0.00000
9	C1	PY	-0.14740	0.00000	0.03492	-0.28627	0.00000
10	C1	PZ	0.00000	0.01409	0.00000	0.00000	0.02604
11	C1	S	-1.00866	0.00000	-1.32729	-0.22142	0.00000
12	C1	PX	1.18872	0.00000	-0.78791	0.56419	0.00000
13	C1	PY	0.12823	0.00000	0.32984	0.45213	0.00000
14	C1	PZ	0.00000	0.29955	0.00000	0.00000	0.09289
15	C1	DXX	-0.25805	0.00000	-0.03253	0.22211	0.00000
16	C1	DYY	0.16253	0.00000	0.07574	-0.18841	0.00000
17	C1	DZZ	0.14687	0.00000	-0.01151	-0.04794	0.00000
18	C1	DXY	-0.12071	0.00000	-0.14835	0.01066	0.00000
19	C1	DXZ	0.00000	-0.33103	0.00000	0.00000	-0.15910
20	C1	DYZ	0.00000	0.20695	0.00000	0.00000	0.16736
21	C2	S	0.00370	0.00000	0.02714	0.00961	0.00000
22	C2	S	0.09322	0.00000	0.41730	-0.10509	0.00000
23	C2	PX	0.10347	0.00000	0.10261	-0.07807	0.00000
24	C2	PY	-0.02725	0.00000	-0.02777	0.04794	0.00000
25	C2	PZ	0.00000	0.04100	0.00000	0.00000	-0.01664
26	C2	S	0.23103	0.00000	-1.61310	-0.84827	0.00000
27	C2	PX	-0.06229	0.00000	-1.79777	0.13401	0.00000
28	C2	PY	0.99189	0.00000	-1.27371	0.19627	0.00000
29	C2	PZ	0.00000	0.15897	0.00000	0.00000	-0.17268
30	C2	DXX	-0.19397	0.00000	-0.00375	-0.20007	0.00000
31	C2	DYY	0.14294	0.00000	-0.01651	0.19980	0.00000
32	C2	DZZ	0.10767	0.00000	-0.03507	-0.00844	0.00000
33	C2	DXY	-0.01936	0.00000	-0.09052	-0.25694	0.00000
34	C2	DXZ	0.00000	0.28900	0.00000	0.00000	-0.15069
35	C2	DYZ	0.00000	-0.30696	0.00000	0.00000	0.02768
36	C3	S	-0.00463	0.00000	0.03487	-0.01246	0.00000
37	C3	S	-0.44673	0.00000	0.71360	-0.10667	0.00000
38	C3	PX	0.10126	0.00000	-0.10456	-0.03832	0.00000
39	C3	PY	0.08747	0.00000	-0.32422	0.17174	0.00000
40	C3	PZ	0.00000	0.00993	0.00000	0.00000	0.00895
41	C3	S	3.79486	0.00000	-5.27719	0.82740	0.00000
42	C3	PX	-0.69916	0.00000	1.85011	-0.59696	0.00000

43	C3	PY	-2.16063	0.00000	3.59313	-0.51620	0.00000
44	C3	PZ	0.00000	0.11195	0.00000	0.00000	0.04388
45	C3	DXX	0.01136	0.00000	-0.02602	0.22995	0.00000
46	C3	DYY	-0.02284	0.00000	-0.01939	-0.16297	0.00000
47	C3	DZZ	0.07022	0.00000	0.06162	-0.04916	0.00000
48	C3	DXY	0.08066	0.00000	0.17239	-0.25588	0.00000
49	C3	DXZ	0.00000	-0.28929	0.00000	0.00000	0.06338
50	C3	DYZ	0.00000	-0.13679	0.00000	0.00000	-0.09794
51	C4	S	0.01042	0.00000	0.02244	0.00291	0.00000
52	C4	S	-0.19777	0.00000	0.17250	-0.04731	0.00000
53	C4	PX	-0.00379	0.00000	-0.13322	0.08780	0.00000
54	C4	PY	0.12520	0.00000	0.05093	-0.00884	0.00000
55	C4	PZ	0.00000	-0.10475	0.00000	0.00000	-0.03043
56	C4	S	-0.02677	0.00000	-2.36528	-0.04804	0.00000
57	C4	PX	0.28051	0.00000	1.49114	0.25397	0.00000
58	C4	PY	-2.97318	0.00000	0.18486	-0.33591	0.00000
59	C4	PZ	0.00000	-0.54353	0.00000	0.00000	-0.18606
60	C4	DXX	0.26443	0.00000	0.02136	-0.01744	0.00000
61	C4	DYY	-0.42375	0.00000	-0.09287	0.02216	0.00000
62	C4	DZZ	0.25839	0.00000	0.04449	-0.01457	0.00000
63	C4	DXY	-0.03349	0.00000	-0.15617	-0.12697	0.00000
64	C4	DXZ	0.00000	0.07951	0.00000	0.00000	-0.07170
65	C4	DYZ	0.00000	0.13231	0.00000	0.00000	0.01659
66	C5	S	0.01714	0.00000	-0.02271	-0.00426	0.00000
67	C5	S	-0.13016	0.00000	-0.27802	-0.03478	0.00000
68	C5	PX	-0.11943	0.00000	0.01866	0.14271	0.00000
69	C5	PY	0.03135	0.00000	0.00522	0.10864	0.00000
70	C5	PZ	0.00000	0.03086	0.00000	0.00000	-0.00134
71	C5	S	-1.02198	0.00000	3.49724	0.22159	0.00000
72	C5	PX	0.14250	0.00000	1.31114	0.07908	0.00000
73	C5	PY	1.07829	0.00000	-0.90316	-0.31857	0.00000
74	C5	PZ	0.00000	0.23641	0.00000	0.00000	0.14979
75	C5	DXX	-0.05968	0.00000	-0.06693	-0.06352	0.00000
76	C5	DYY	-0.04655	0.00000	0.04410	-0.02657	0.00000
77	C5	DZZ	0.11449	0.00000	0.12104	0.12685	0.00000
78	C5	DXY	0.25713	0.00000	0.05784	0.25466	0.00000
79	C5	DXZ	0.00000	0.41017	0.00000	0.00000	0.02564
80	C5	DYZ	0.00000	0.11767	0.00000	0.00000	-0.08237
81	C6	S	0.02447	0.00000	-0.02474	0.00591	0.00000
82	C6	S	0.18714	0.00000	-0.50177	-0.22561	0.00000
83	C6	PX	0.04851	0.00000	-0.10652	0.04783	0.00000
84	C6	PY	-0.07072	0.00000	0.03800	-0.10119	0.00000
85	C6	PZ	0.00000	-0.09362	0.00000	0.00000	0.02908
86	C6	S	-1.19706	0.00000	4.45622	-0.65287	0.00000
87	C6	PX	-1.61570	0.00000	2.66825	-1.09255	0.00000
88	C6	PY	0.25322	0.00000	0.11165	0.52167	0.00000
89	C6	PZ	0.00000	-0.40499	0.00000	0.00000	0.15008
90	C6	DXX	0.06972	0.00000	-0.09656	0.16566	0.00000
91	C6	DYY	-0.08363	0.00000	-0.02176	-0.07466	0.00000
92	C6	DZZ	0.03430	0.00000	0.17476	-0.11118	0.00000
93	C6	DXY	0.14674	0.00000	-0.15124	-0.16340	0.00000
94	C6	DXZ	0.00000	0.04169	0.00000	0.00000	-0.10773
95	C6	DYZ	0.00000	-0.17887	0.00000	0.00000	0.04298
96	C7	S	0.02848	0.00000	-0.02117	-0.00915	0.00000

97	C7	S	0.47412	0.00000	-0.47359	-0.15256	0.00000
98	C7	PX	-0.11969	0.00000	0.04166	-0.01231	0.00000
99	C7	PY	-0.01109	0.00000	0.12634	-0.20331	0.00000
100	C7	PZ	0.00000	0.01462	0.00000	0.00000	-0.01663
101	C7	S	-3.93981	0.00000	5.14135	0.51475	0.00000
102	C7	PX	2.23350	0.00000	-3.02092	-0.48979	0.00000
103	C7	PY	0.00720	0.00000	-0.43066	0.30554	0.00000
104	C7	PZ	0.00000	0.01013	0.00000	0.00000	-0.25570
105	C7	DXX	-0.06315	0.00000	0.14233	-0.25933	0.00000
106	C7	DYY	-0.04217	0.00000	-0.15894	0.26877	0.00000
107	C7	DZZ	0.13452	0.00000	0.10701	-0.00328	0.00000
108	C7	DXY	-0.00835	0.00000	0.14342	0.00149	0.00000
109	C7	DXZ	0.00000	-0.02430	0.00000	0.00000	0.21424
110	C7	DYZ	0.00000	-0.10053	0.00000	0.00000	0.18096
111	O1	S	-0.05934	0.00000	-0.01379	-0.00725	0.00000
112	O1	S	-0.52991	0.00000	-0.26741	-0.20666	0.00000
113	O1	PX	0.01077	0.00000	0.05576	0.05061	0.00000
114	O1	PY	-0.11179	0.00000	-0.03679	0.02060	0.00000
115	O1	PZ	0.00000	-0.08389	0.00000	0.00000	0.09096
116	O1	S	2.70098	0.00000	0.86170	0.61075	0.00000
117	O1	PX	-0.05230	0.00000	-0.29551	-0.14704	0.00000
118	O1	PY	-0.83815	0.00000	-0.25116	-0.17709	0.00000
119	O1	PZ	0.00000	0.22127	0.00000	0.00000	-0.16057
120	O1	DXX	-0.10089	0.00000	-0.12177	-0.07677	0.00000
121	O1	DYY	-0.33040	0.00000	-0.12943	-0.07470	0.00000
122	O1	DZZ	0.11255	0.00000	0.10508	0.03579	0.00000
123	O1	DXY	-0.09137	0.00000	0.19415	0.08414	0.00000
124	O1	DXZ	0.00000	-0.00187	0.00000	0.00000	-0.52813
125	O1	DYZ	0.00000	-0.36607	0.00000	0.00000	-0.21113
126	H4	S	0.17321	0.00000	0.11985	0.29457	0.00000
127	H4	S	-0.21268	0.00000	0.28493	-0.00979	0.00000
128	H4	PX	-0.07109	0.00000	-0.02154	-0.06172	0.00000
129	H4	PY	0.03957	0.00000	0.05855	0.09498	0.00000
130	H4	PZ	0.00000	-0.10687	0.00000	0.00000	-0.07675
131	N1	S	-0.00349	0.00000	0.00888	-0.00812	0.00000
132	N1	S	-0.05711	0.00000	0.51193	-0.21174	0.00000
133	N1	PX	0.03919	0.00000	0.23807	-0.11218	0.00000
134	N1	PY	0.12407	0.00000	-0.06707	0.04059	0.00000
135	N1	PZ	0.00000	-0.11003	0.00000	0.00000	0.07413
136	N1	S	0.59194	0.00000	-1.45956	0.99564	0.00000
137	N1	PX	0.32650	0.00000	-0.78165	0.56799	0.00000
138	N1	PY	-0.51741	0.00000	0.23623	0.23036	0.00000
139	N1	PZ	0.00000	0.28544	0.00000	0.00000	-0.24860
140	N1	DXX	-0.09924	0.00000	-0.00750	0.16556	0.00000
141	N1	DYY	-0.02999	0.00000	0.01792	-0.10296	0.00000
142	N1	DZZ	0.14484	0.00000	0.13842	-0.05182	0.00000
143	N1	DXY	-0.11653	0.00000	0.14994	0.31141	0.00000
144	N1	DXZ	0.00000	0.18983	0.00000	0.00000	-0.28725
145	N1	DYZ	0.00000	0.28185	0.00000	0.00000	-0.05206
146	H6	S	0.18983	0.00000	-0.22078	0.34358	0.00000
147	H6	S	-0.00190	0.00000	-0.61456	0.02509	0.00000
148	H6	PX	-0.06259	0.00000	0.02284	-0.12534	0.00000
149	H6	PY	-0.06219	0.00000	0.01236	0.03426	0.00000
150	H6	PZ	0.00000	-0.10628	0.00000	0.00000	0.10425

151	C8	S	0.00379	0.00000	0.02205	-0.00043	0.00000
152	C8	S	-0.04681	0.00000	0.36320	-0.05460	0.00000
153	C8	PX	-0.02965	0.00000	-0.08546	-0.01301	0.00000
154	C8	PY	0.01129	0.00000	0.16877	-0.04643	0.00000
155	C8	PZ	0.00000	-0.03450	0.00000	0.00000	0.06904
156	C8	S	0.77233	0.00000	-1.36579	-0.20244	0.00000
157	C8	PX	1.23507	0.00000	-1.43423	0.08582	0.00000
158	C8	PY	1.81042	0.00000	-2.73687	-0.88397	0.00000
159	C8	PZ	0.00000	-0.16952	0.00000	0.00000	0.43555
160	C8	DXX	-0.07491	0.00000	-0.22323	-0.00242	0.00000
161	C8	DYY	-0.11212	0.00000	0.12854	0.02936	0.00000
162	C8	DZZ	0.23945	0.00000	0.11878	-0.01715	0.00000
163	C8	DXY	-0.05580	0.00000	0.17703	-0.00036	0.00000
164	C8	DXZ	0.00000	-0.02334	0.00000	0.00000	0.07708
165	C8	DYZ	0.00000	0.01056	0.00000	0.00000	-0.00379
166	H8	S	-0.05865	0.00000	0.06336	0.30185	0.00000
167	H8	S	-0.51416	0.00000	0.69522	0.03204	0.00000
168	H8	PX	-0.00399	0.00000	0.00994	0.09913	0.00000
169	H8	PY	-0.02126	0.00000	0.09958	-0.08923	0.00000
170	H8	PZ	0.00000	0.02632	0.00000	0.00000	0.14593
171	C10	S	0.00897	0.00000	0.01024	0.00183	0.00000
172	C10	S	0.13512	0.00000	-0.01885	-0.05316	0.00000
173	C10	PX	-0.02188	0.00000	0.03180	0.00887	0.00000
174	C10	PY	0.13202	0.00000	-0.08934	-0.08401	0.00000
175	C10	PZ	0.00000	0.00221	0.00000	0.00000	-0.01138
176	C10	S	0.67635	0.00000	-1.44600	-0.57304	0.00000
177	C10	PX	-0.93708	0.00000	1.24851	0.31112	0.00000
178	C10	PY	0.14443	0.00000	-0.18040	-0.12077	0.00000
179	C10	PZ	0.00000	0.10143	0.00000	0.00000	-0.23894
180	C10	DXX	-0.15772	0.00000	0.00151	0.05696	0.00000
181	C10	DYY	0.01829	0.00000	-0.07928	-0.04139	0.00000
182	C10	DZZ	0.22137	0.00000	0.08431	-0.02182	0.00000
183	C10	DXY	0.05301	0.00000	-0.26734	-0.04772	0.00000
184	C10	DXZ	0.00000	-0.02138	0.00000	0.00000	0.06118
185	C10	DYZ	0.00000	0.14884	0.00000	0.00000	-0.31038
186	H16	S	0.30279	0.00000	-0.29484	-0.12333	0.00000
187	H16	S	0.24931	0.00000	-0.28172	-0.02941	0.00000
188	H16	PX	0.08459	0.00000	-0.13786	-0.02236	0.00000
189	H16	PY	-0.00947	0.00000	-0.09866	0.01717	0.00000
190	H16	PZ	0.00000	-0.03630	0.00000	0.00000	0.09577
191	H18	S	-0.11194	0.00000	0.47404	0.08268	0.00000
192	H18	S	-0.23997	0.00000	0.27457	0.10213	0.00000
193	H18	PX	0.06139	0.00000	-0.14559	-0.02598	0.00000
194	H18	PY	-0.05656	0.00000	-0.02542	0.00880	0.00000
195	H18	PZ	0.00000	-0.06147	0.00000	0.00000	0.12699
196	C9	S	-0.00530	0.00000	0.01647	0.01416	0.00000
197	C9	S	-0.02777	0.00000	0.13743	0.11371	0.00000
198	C9	PX	0.02996	0.00000	0.00936	-0.01604	0.00000
199	C9	PY	0.06966	0.00000	-0.00548	-0.03595	0.00000
200	C9	PZ	0.00000	-0.00001	0.00000	0.00000	0.03746
201	C9	S	-0.06514	0.00000	-0.33730	-0.22133	0.00000
202	C9	PX	-0.04888	0.00000	-0.03045	-0.02016	0.00000
203	C9	PY	-0.11415	0.00000	0.11941	0.20463	0.00000
204	C9	PZ	0.00000	0.06083	0.00000	0.00000	0.29296

205	C9	DXX	0.00558	0.00000	0.09298	0.06281	0.00000
206	C9	DYY	-0.01701	0.00000	-0.07786	-0.03070	0.00000
207	C9	DZZ	0.00920	0.00000	-0.00279	-0.00408	0.00000
208	C9	DXY	-0.10949	0.00000	0.02555	0.01527	0.00000
209	C9	DXZ	0.00000	0.11252	0.00000	0.00000	0.09306
210	C9	DYZ	0.00000	-0.05278	0.00000	0.00000	-0.20117
211	H3	S	-0.01692	0.00000	0.08275	0.02397	0.00000
212	H3	S	0.10566	0.00000	-0.03386	-0.07637	0.00000
213	H3	PX	-0.14990	0.00000	0.01713	0.01220	0.00000
214	H3	PY	-0.04498	0.00000	0.03449	0.02302	0.00000
215	H3	PZ	0.00000	-0.00093	0.00000	0.00000	-0.02264
216	H5	S	-0.03317	0.09517	0.04111	0.06799	0.20963
217	H5	S	0.09288	-0.02413	0.05001	0.00466	-0.00844
218	H5	PX	0.06999	0.03451	0.02447	0.01792	0.25349
219	H5	PY	0.01970	0.00748	0.00527	0.00755	0.16822
220	H5	PZ	0.02756	-0.02004	0.00943	0.00873	0.01942
221	H7	S	-0.03317	-0.09517	0.04111	0.06799	-0.20963
222	H7	S	0.09288	0.02413	0.05001	0.00466	0.00844
223	H7	PX	0.06999	-0.03451	0.02447	0.01792	-0.25349
224	H7	PY	0.01970	-0.00748	0.00527	0.00755	-0.16822
225	H7	PZ	-0.02756	-0.02004	-0.00943	-0.00873	0.01942

MO:	146	147	148	149	150
Eigenvalues:	2.22326	2.23489	2.28694	2.28708	2.29163
(ev):	60.49797	60.81459	62.23095	62.23476	62.35851

			A	A	A	A	A
1	H1	S	0.00000	-0.14262	0.05545	0.00000	-0.32355
2	H1	S	0.00000	0.10920	0.02209	0.00000	-0.15533
3	H1	PX	0.00000	0.00743	0.02900	0.00000	-0.17584
4	H1	PY	0.00000	-0.04910	-0.08020	0.00000	0.10110
5	H1	PZ	-0.10012	0.00000	0.00000	-0.17317	0.00000
6	C1	S	0.00000	-0.01564	-0.01127	0.00000	-0.00923
7	C1	S	0.00000	0.08324	-0.11613	0.00000	-0.17923
8	C1	PX	0.00000	-0.07662	0.05182	0.00000	0.01184
9	C1	PY	0.00000	-0.01172	-0.09587	0.00000	0.12565
10	C1	PZ	-0.04574	0.00000	0.00000	0.04721	0.00000
11	C1	S	0.00000	1.23753	0.09068	0.00000	0.62291
12	C1	PX	0.00000	-0.32440	-0.02964	0.00000	0.77007
13	C1	PY	0.00000	0.41149	-0.73678	0.00000	-1.12088
14	C1	PZ	0.37905	0.00000	0.00000	0.21300	0.00000
15	C1	DXX	0.00000	0.11449	0.04976	0.00000	0.14000
16	C1	DYY	0.00000	-0.12222	0.04634	0.00000	0.08658
17	C1	DZZ	0.00000	0.03181	-0.11426	0.00000	-0.29991
18	C1	DXY	0.00000	-0.01598	-0.09458	0.00000	0.31565
19	C1	DXZ	-0.16008	0.00000	0.00000	-0.12043	0.00000
20	C1	DYZ	-0.01069	0.00000	0.00000	-0.17838	0.00000
21	C2	S	0.00000	-0.01021	-0.01557	0.00000	0.01791
22	C2	S	0.00000	0.02991	-0.02704	0.00000	0.20309
23	C2	PX	0.00000	0.02400	0.05183	0.00000	0.05392
24	C2	PY	0.00000	-0.04283	0.11349	0.00000	0.03087
25	C2	PZ	-0.00270	0.00000	0.00000	0.05408	0.00000
26	C2	S	0.00000	0.02461	1.46213	0.00000	-0.58117
27	C2	PX	0.00000	0.27605	0.54060	0.00000	0.19349

28	C2	PY	0.00000	0.13986	-0.35456	0.00000	0.55505
29	C2	PZ	-0.60043	0.00000	0.00000	0.30111	0.00000
30	C2	DXX	0.00000	-0.11521	0.18901	0.00000	-0.32451
31	C2	DYY	0.00000	0.11906	-0.09810	0.00000	0.04077
32	C2	DZZ	0.00000	-0.03716	-0.04459	0.00000	0.40468
33	C2	DXY	0.00000	0.15704	-0.22375	0.00000	-0.06573
34	C2	DXZ	-0.37202	0.00000	0.00000	0.20171	0.00000
35	C2	DYZ	-0.09878	0.00000	0.00000	0.12251	0.00000
36	C3	S	0.00000	-0.00385	-0.00558	0.00000	-0.00981
37	C3	S	0.00000	0.01130	-0.10471	0.00000	-0.30696
38	C3	PX	0.00000	0.10261	-0.04779	0.00000	0.25933
39	C3	PY	0.00000	0.13823	0.17075	0.00000	-0.02023
40	C3	PZ	0.02248	0.00000	0.00000	-0.06661	0.00000
41	C3	S	0.00000	-0.31730	0.69871	0.00000	0.63687
42	C3	PX	0.00000	-0.22680	-0.08602	0.00000	-1.27629
43	C3	PY	0.00000	-0.26922	-1.68604	0.00000	-1.26735
44	C3	PZ	-0.38881	0.00000	0.00000	-0.10073	0.00000
45	C3	DXX	0.00000	0.18989	0.06226	0.00000	-0.09192
46	C3	DYY	0.00000	-0.15143	-0.08921	0.00000	0.20949
47	C3	DZZ	0.00000	-0.02753	0.02492	0.00000	-0.16339
48	C3	DXY	0.00000	-0.00935	0.07548	0.00000	-0.02873
49	C3	DXZ	0.11844	0.00000	0.00000	-0.04162	0.00000
50	C3	DYZ	0.02549	0.00000	0.00000	-0.24228	0.00000
51	C4	S	0.00000	-0.01272	-0.01064	0.00000	-0.01157
52	C4	S	0.00000	-0.14827	-0.29194	0.00000	-0.06457
53	C4	PX	0.00000	-0.03507	0.03600	0.00000	0.15596
54	C4	PY	0.00000	-0.02753	0.20076	0.00000	-0.01163
55	C4	PZ	-0.03058	0.00000	0.00000	-0.01952	0.00000
56	C4	S	0.00000	-0.30986	0.44543	0.00000	1.61324
57	C4	PX	0.00000	-1.10601	1.07104	0.00000	0.01006
58	C4	PY	0.00000	0.55712	-0.71487	0.00000	-0.24502
59	C4	PZ	-0.57581	0.00000	0.00000	-0.04072	0.00000
60	C4	DXX	0.00000	-0.00175	-0.02875	0.00000	-0.11008
61	C4	DYY	0.00000	0.16341	0.19599	0.00000	0.16438
62	C4	DZZ	0.00000	-0.20820	-0.28547	0.00000	0.00202
63	C4	DXY	0.00000	0.13209	-0.00216	0.00000	0.09184
64	C4	DXZ	0.19865	0.00000	0.00000	-0.21192	0.00000
65	C4	DYZ	0.05764	0.00000	0.00000	0.04857	0.00000
66	C5	S	0.00000	-0.00483	-0.01189	0.00000	0.02199
67	C5	S	0.00000	-0.27282	0.01389	0.00000	0.31286
68	C5	PX	0.00000	-0.06786	0.02057	0.00000	0.13724
69	C5	PY	0.00000	0.16745	-0.08260	0.00000	0.00507
70	C5	PZ	0.01363	0.00000	0.00000	-0.03900	0.00000
71	C5	S	0.00000	-0.34653	0.38336	0.00000	-1.13048
72	C5	PX	0.00000	-0.14358	0.14150	0.00000	-0.56951
73	C5	PY	0.00000	-0.70230	1.05220	0.00000	0.29609
74	C5	PZ	0.61032	0.00000	0.00000	-0.23353	0.00000
75	C5	DXX	0.00000	-0.01733	0.34243	0.00000	-0.06001
76	C5	DYY	0.00000	0.11661	-0.16752	0.00000	-0.12644
77	C5	DZZ	0.00000	-0.19297	-0.15833	0.00000	0.21443
78	C5	DXY	0.00000	-0.09927	-0.07877	0.00000	0.11292
79	C5	DXZ	0.33381	0.00000	0.00000	0.01329	0.00000
80	C5	DYZ	-0.22428	0.00000	0.00000	0.25059	0.00000
81	C6	S	0.00000	-0.00822	0.00963	0.00000	0.01492

82	C6	S	0.00000	-0.09486	-0.06074	0.00000	0.18128
83	C6	PX	0.00000	-0.14946	0.00417	0.00000	0.16987
84	C6	PY	0.00000	0.14807	-0.02822	0.00000	0.09276
85	C6	PZ	0.03261	0.00000	0.00000	-0.02195	0.00000
86	C6	S	0.00000	0.44052	-0.86673	0.00000	-1.31187
87	C6	PX	0.00000	0.29657	0.35912	0.00000	-1.33146
88	C6	PY	0.00000	-1.03465	-0.59231	0.00000	0.59692
89	C6	PZ	0.55354	0.00000	0.00000	-0.12485	0.00000
90	C6	DXX	0.00000	0.13158	-0.03655	0.00000	0.08737
91	C6	DYY	0.00000	-0.08033	-0.01462	0.00000	-0.16385
92	C6	DZZ	0.00000	-0.02727	-0.05126	0.00000	0.07726
93	C6	DXY	0.00000	0.13688	-0.00497	0.00000	0.08181
94	C6	DXZ	-0.07557	0.00000	0.00000	0.30208	0.00000
95	C6	DYZ	0.10995	0.00000	0.00000	-0.02602	0.00000
96	C7	S	0.00000	-0.00552	0.01671	0.00000	-0.00647
97	C7	S	0.00000	-0.00599	0.21415	0.00000	-0.24068
98	C7	PX	0.00000	-0.06307	-0.07705	0.00000	0.19865
99	C7	PY	0.00000	-0.13142	0.07705	0.00000	0.03032
100	C7	PZ	-0.00198	0.00000	0.00000	-0.03157	0.00000
101	C7	S	0.00000	0.67845	-1.81043	0.00000	-0.37445
102	C7	PX	0.00000	-0.47447	1.01594	0.00000	0.24962
103	C7	PY	0.00000	0.20844	-0.19031	0.00000	0.21167
104	C7	PZ	0.06569	0.00000	0.00000	-0.18427	0.00000
105	C7	DXX	0.00000	0.07335	-0.10877	0.00000	0.15703
106	C7	DYY	0.00000	-0.00417	0.10476	0.00000	-0.11339
107	C7	DZZ	0.00000	-0.03304	0.06131	0.00000	-0.16364
108	C7	DXY	0.00000	0.09858	0.04856	0.00000	-0.02590
109	C7	DXZ	-0.01253	0.00000	0.00000	0.17405	0.00000
110	C7	DYZ	0.13680	0.00000	0.00000	0.38342	0.00000
111	O1	S	0.00000	-0.00087	0.00592	0.00000	0.01867
112	O1	S	0.00000	-0.17456	-0.16914	0.00000	0.16099
113	O1	PX	0.00000	-0.07638	-0.01933	0.00000	0.08736
114	O1	PY	0.00000	0.18982	-0.00852	0.00000	0.08114
115	O1	PZ	-0.14290	0.00000	0.00000	-0.07038	0.00000
116	O1	S	0.00000	0.17012	0.36439	0.00000	-0.70638
117	O1	PX	0.00000	0.34458	-0.09333	0.00000	-0.34453
118	O1	PY	0.00000	-0.18218	0.15829	0.00000	0.00598
119	O1	PZ	0.35488	0.00000	0.00000	0.13747	0.00000
120	O1	DXX	0.00000	0.08385	-0.21205	0.00000	-0.01294
121	O1	DYY	0.00000	0.01881	0.02111	0.00000	0.04634
122	O1	DZZ	0.00000	-0.19774	0.09725	0.00000	0.05424
123	O1	DXY	0.00000	-0.20744	0.34796	0.00000	0.02648
124	O1	DXZ	0.38158	0.00000	0.00000	0.26644	0.00000
125	O1	DYZ	-0.20639	0.00000	0.00000	-0.01321	0.00000
126	H4	S	0.00000	-0.04077	-0.25563	0.00000	0.13418
127	H4	S	0.00000	0.21070	-0.18691	0.00000	-0.22905
128	H4	PX	0.00000	0.05707	-0.05829	0.00000	-0.06410
129	H4	PY	0.00000	-0.03109	-0.10870	0.00000	0.01214
130	H4	PZ	-0.30750	0.00000	0.00000	0.17430	0.00000
131	N1	S	0.00000	-0.00261	0.00184	0.00000	-0.01192
132	N1	S	0.00000	0.11416	-0.00346	0.00000	0.07831
133	N1	PX	0.00000	0.10745	-0.01187	0.00000	0.16143
134	N1	PY	0.00000	-0.00027	0.06176	0.00000	0.17205
135	N1	PZ	0.08147	0.00000	0.00000	0.04574	0.00000

136	N1	S	0.00000	-0.19365	0.14197	0.00000	0.62420
137	N1	PX	0.00000	0.23397	0.07848	0.00000	0.06391
138	N1	PY	0.00000	-0.22015	-0.27617	0.00000	-0.09102
139	N1	PZ	-0.28508	0.00000	0.00000	-0.09803	0.00000
140	N1	DXX	0.00000	0.10466	-0.12484	0.00000	-0.13111
141	N1	DYY	0.00000	-0.02221	0.06576	0.00000	0.09370
142	N1	DZZ	0.00000	-0.01896	0.08005	0.00000	0.08051
143	N1	DXY	0.00000	0.08447	-0.14249	0.00000	-0.24711
144	N1	DXZ	-0.16591	0.00000	0.00000	-0.27708	0.00000
145	N1	DYZ	-0.22851	0.00000	0.00000	0.14154	0.00000
146	H6	S	0.00000	0.06676	-0.05414	0.00000	0.37777
147	H6	S	0.00000	0.10865	0.05190	0.00000	0.04620
148	H6	PX	0.00000	0.02643	-0.04708	0.00000	-0.13825
149	H6	PY	0.00000	-0.09897	0.10092	0.00000	-0.03079
150	H6	PZ	0.31567	0.00000	0.00000	-0.19892	0.00000
151	C8	S	0.00000	0.01236	0.02005	0.00000	0.00093
152	C8	S	0.00000	-0.18351	0.05039	0.00000	-0.04822
153	C8	PX	0.00000	-0.09911	-0.08694	0.00000	0.09224
154	C8	PY	0.00000	0.27013	0.09022	0.00000	0.04629
155	C8	PZ	0.03569	0.00000	0.00000	0.08933	0.00000
156	C8	S	0.00000	-0.06457	0.20905	0.00000	-0.04628
157	C8	PX	0.00000	0.58701	0.80044	0.00000	0.26896
158	C8	PY	0.00000	-1.99822	0.02995	0.00000	0.58477
159	C8	PZ	0.13333	0.00000	0.00000	0.43544	0.00000
160	C8	DXX	0.00000	-0.26843	0.03895	0.00000	-0.03501
161	C8	DYY	0.00000	0.20651	-0.13312	0.00000	0.01877
162	C8	DZZ	0.00000	-0.02009	0.15449	0.00000	0.00379
163	C8	DXY	0.00000	-0.10297	0.05700	0.00000	0.15612
164	C8	DXZ	-0.01594	0.00000	0.00000	0.18346	0.00000
165	C8	DYZ	-0.03582	0.00000	0.00000	-0.03745	0.00000
166	H8	S	0.00000	0.01534	0.04206	0.00000	-0.15275
167	H8	S	0.00000	0.12594	-0.29576	0.00000	0.02778
168	H8	PX	0.00000	0.00516	0.03844	0.00000	-0.10481
169	H8	PY	0.00000	-0.00766	-0.04340	0.00000	-0.01071
170	H8	PZ	-0.02374	0.00000	0.00000	0.15561	0.00000
171	C10	S	0.00000	0.00967	0.02038	0.00000	0.00144
172	C10	S	0.00000	-0.04722	0.21398	0.00000	0.07172
173	C10	PX	0.00000	0.02769	0.02086	0.00000	-0.03776
174	C10	PY	0.00000	-0.14991	0.12029	0.00000	0.07034
175	C10	PZ	-0.00790	0.00000	0.00000	-0.02986	0.00000
176	C10	S	0.00000	-1.57495	-0.55195	0.00000	0.31208
177	C10	PX	0.00000	0.03730	-0.61483	0.00000	-0.00989
178	C10	PY	0.00000	-0.00865	-0.14183	0.00000	0.20492
179	C10	PZ	-0.08641	0.00000	0.00000	-0.26461	0.00000
180	C10	DXX	0.00000	-0.39387	-0.25250	0.00000	-0.04440
181	C10	DYY	0.00000	0.24288	0.01467	0.00000	-0.02289
182	C10	DZZ	0.00000	0.16786	0.38877	0.00000	0.10693
183	C10	DXY	0.00000	-0.20136	0.05644	0.00000	-0.14908
184	C10	DXZ	0.01857	0.00000	0.00000	0.06973	0.00000
185	C10	DYZ	-0.12634	0.00000	0.00000	-0.32850	0.00000
186	H16	S	0.00000	0.25310	0.35354	0.00000	-0.02913
187	H16	S	0.00000	0.04068	0.19553	0.00000	0.01448
188	H16	PX	0.00000	-0.01216	0.13923	0.00000	-0.05190
189	H16	PY	0.00000	-0.28081	-0.01383	0.00000	-0.09046

190	H16	PZ	0.04198	0.00000	0.00000	0.10888	0.00000
191	H18	S	0.00000	0.32680	0.02719	0.00000	0.15364
192	H18	S	0.00000	0.03711	-0.17355	0.00000	-0.01726
193	H18	PX	0.00000	0.06668	0.12033	0.00000	-0.06208
194	H18	PY	0.00000	-0.23026	-0.18226	0.00000	-0.05516
195	H18	PZ	0.05313	0.00000	0.00000	0.18007	0.00000
196	C9	S	0.00000	0.00322	0.00616	0.00000	-0.01362
197	C9	S	0.00000	0.01309	0.02957	0.00000	-0.04230
198	C9	PX	0.00000	0.01703	0.04176	0.00000	-0.09452
199	C9	PY	0.00000	0.01301	0.01643	0.00000	-0.03352
200	C9	PZ	-0.03611	0.00000	0.00000	-0.01701	0.00000
201	C9	S	0.00000	-0.20096	-0.19854	0.00000	0.53428
202	C9	PX	0.00000	-0.00741	0.06689	0.00000	-0.05241
203	C9	PY	0.00000	0.22057	-0.22671	0.00000	-0.26607
204	C9	PZ	-0.12269	0.00000	0.00000	-0.13082	0.00000
205	C9	DXX	0.00000	0.01321	0.08145	0.00000	0.01664
206	C9	DYY	0.00000	0.05813	-0.18403	0.00000	-0.08522
207	C9	DZZ	0.00000	-0.06211	0.10129	0.00000	0.05658
208	C9	DXY	0.00000	-0.07499	0.12355	0.00000	0.03186
209	C9	DXZ	0.06043	0.00000	0.00000	-0.05714	0.00000
210	C9	DYZ	0.08081	0.00000	0.00000	0.09321	0.00000
211	H3	S	0.00000	-0.08852	0.24417	0.00000	0.06265
212	H3	S	0.00000	-0.02414	0.02218	0.00000	0.00261
213	H3	PX	0.00000	-0.12255	0.20387	0.00000	0.04465
214	H3	PY	0.00000	-0.04177	0.14033	0.00000	0.03897
215	H3	PZ	0.01672	0.00000	0.00000	0.08726	0.00000
216	H5	S	-0.04518	0.07523	-0.05001	-0.10269	-0.10195
217	H5	S	-0.00978	0.00703	0.03150	0.02199	-0.03996
218	H5	PX	-0.15578	0.04413	-0.05476	-0.14918	-0.03883
219	H5	PY	-0.10848	0.04504	-0.01555	-0.02798	0.00730
220	H5	PZ	-0.05101	0.00688	-0.00682	-0.03433	0.00314
221	H7	S	0.04518	0.07523	-0.05001	0.10269	-0.10195
222	H7	S	0.00978	0.00703	0.03150	-0.02199	-0.03996
223	H7	PX	0.15578	0.04413	-0.05476	0.14918	-0.03883
224	H7	PY	0.10848	0.04504	-0.01555	0.02798	0.00730
225	H7	PZ	-0.05101	-0.00688	0.00682	-0.03433	-0.00314

MO:	151	152	153	154	155
Eigenvalues:	2.31790	2.32310	2.34457	2.34735	2.35830
(ev):	63.07317	63.21490	63.79889	63.87459	64.17265

			A	A	A	A	A
1	H1	S	-0.10218	0.00000	-0.04429	0.15793	0.00000
2	H1	S	-0.05713	0.00000	-0.05055	0.04742	0.00000
3	H1	PX	-0.03593	0.00000	-0.02036	0.03362	0.00000
4	H1	PY	0.00104	0.00000	0.00266	-0.03762	0.00000
5	H1	PZ	0.00000	0.01196	0.00000	0.00000	0.10022
6	C1	S	-0.01126	0.00000	0.01630	-0.00818	0.00000
7	C1	S	-0.09348	0.00000	0.30023	-0.14682	0.00000
8	C1	PX	0.04051	0.00000	-0.16126	0.00947	0.00000
9	C1	PY	-0.01030	0.00000	0.13040	-0.00369	0.00000
10	C1	PZ	0.00000	0.02198	0.00000	0.00000	-0.00188
11	C1	S	1.06292	0.00000	-2.09647	0.45790	0.00000
12	C1	PX	0.14116	0.00000	0.68630	-0.35288	0.00000

13	C1	PY	-0.42762	0.00000	0.12908	-0.86313	0.00000
14	C1	PZ	0.00000	-0.09559	0.00000	0.00000	-0.14130
15	C1	DXX	0.00667	0.00000	0.13099	-0.04157	0.00000
16	C1	DYY	0.06462	0.00000	-0.09748	0.09182	0.00000
17	C1	DZZ	-0.13955	0.00000	0.01468	-0.05834	0.00000
18	C1	DXY	0.08181	0.00000	-0.08337	-0.03060	0.00000
19	C1	DXZ	0.00000	0.03043	0.00000	0.00000	0.05965
20	C1	DYZ	0.00000	0.04740	0.00000	0.00000	-0.04512
21	C2	S	-0.02246	0.00000	0.01662	-0.01739	0.00000
22	C2	S	-0.38735	0.00000	0.27070	-0.20345	0.00000
23	C2	PX	-0.12490	0.00000	0.01627	-0.03188	0.00000
24	C2	PY	-0.08303	0.00000	0.16912	-0.11372	0.00000
25	C2	PZ	0.00000	-0.01003	0.00000	0.00000	0.01162
26	C2	S	1.07827	0.00000	-1.22323	0.48053	0.00000
27	C2	PX	1.34448	0.00000	-0.56250	0.29786	0.00000
28	C2	PY	1.15707	0.00000	-0.62651	-0.02070	0.00000
29	C2	PZ	0.00000	-0.01861	0.00000	0.00000	0.06138
30	C2	DXX	-0.13714	0.00000	-0.10269	0.10378	0.00000
31	C2	DYY	0.25548	0.00000	0.05018	0.06160	0.00000
32	C2	DZZ	-0.19259	0.00000	0.08446	-0.23037	0.00000
33	C2	DXY	0.13216	0.00000	-0.11690	0.00798	0.00000
34	C2	DXZ	0.00000	-0.01331	0.00000	0.00000	0.01922
35	C2	DYZ	0.00000	-0.02544	0.00000	0.00000	0.05879
36	C3	S	-0.01042	0.00000	0.00985	-0.00356	0.00000
37	C3	S	-0.22571	0.00000	0.12268	-0.13996	0.00000
38	C3	PX	-0.01797	0.00000	0.14780	-0.05489	0.00000
39	C3	PY	0.17636	0.00000	-0.13586	0.08516	0.00000
40	C3	PZ	0.00000	0.00086	0.00000	0.00000	-0.01781
41	C3	S	3.21289	0.00000	0.67411	-1.36979	0.00000
42	C3	PX	-0.65456	0.00000	0.23230	-0.54183	0.00000
43	C3	PY	-2.53555	0.00000	0.98940	-0.03694	0.00000
44	C3	PZ	0.00000	0.09392	0.00000	0.00000	0.07759
45	C3	DXX	-0.16036	0.00000	0.05850	0.00835	0.00000
46	C3	DYY	0.02649	0.00000	-0.10878	0.04205	0.00000
47	C3	DZZ	0.11817	0.00000	0.17438	-0.15187	0.00000
48	C3	DXY	0.07713	0.00000	0.22726	-0.05501	0.00000
49	C3	DXZ	0.00000	-0.00296	0.00000	0.00000	0.06194
50	C3	DYZ	0.00000	0.02331	0.00000	0.00000	0.04422
51	C4	S	-0.02974	0.00000	-0.00278	0.00500	0.00000
52	C4	S	-0.22169	0.00000	-0.21590	0.06718	0.00000
53	C4	PX	0.01206	0.00000	-0.17415	-0.06744	0.00000
54	C4	PY	0.02050	0.00000	0.03219	-0.07813	0.00000
55	C4	PZ	0.00000	0.00388	0.00000	0.00000	0.03028
56	C4	S	1.07872	0.00000	0.45565	-0.21355	0.00000
57	C4	PX	-0.60658	0.00000	1.18946	1.15878	0.00000
58	C4	PY	-0.54962	0.00000	-0.18739	1.06320	0.00000
59	C4	PZ	0.00000	0.03984	0.00000	0.00000	0.05086
60	C4	DXX	0.04904	0.00000	-0.26377	0.04764	0.00000
61	C4	DYY	0.17046	0.00000	0.22940	-0.12615	0.00000
62	C4	DZZ	-0.25109	0.00000	0.01934	0.01751	0.00000
63	C4	DXY	0.01077	0.00000	0.11859	-0.01135	0.00000
64	C4	DXZ	0.00000	0.03461	0.00000	0.00000	-0.03599
65	C4	DYZ	0.00000	0.03010	0.00000	0.00000	-0.20498
66	C5	S	-0.01252	0.00000	-0.00377	-0.01859	0.00000

67	C5	S	-0.26033	0.00000	-0.07360	-0.19217	0.00000
68	C5	PX	-0.01211	0.00000	0.12450	0.03808	0.00000
69	C5	PY	0.23405	0.00000	0.09811	0.08683	0.00000
70	C5	PZ	0.00000	0.00854	0.00000	0.00000	-0.03112
71	C5	S	-1.58327	0.00000	1.52175	1.12825	0.00000
72	C5	PX	-0.58638	0.00000	0.18979	0.53560	0.00000
73	C5	PY	0.04998	0.00000	-0.36855	-0.35242	0.00000
74	C5	PZ	0.00000	0.01903	0.00000	0.00000	-0.07280
75	C5	DXX	-0.08394	0.00000	0.02371	0.06377	0.00000
76	C5	DYY	0.28009	0.00000	-0.05171	0.06139	0.00000
77	C5	DZZ	-0.36440	0.00000	0.07954	-0.16078	0.00000
78	C5	DXY	-0.03784	0.00000	-0.14043	0.06170	0.00000
79	C5	DXZ	0.00000	-0.00439	0.00000	0.00000	-0.02507
80	C5	DYZ	0.00000	-0.03198	0.00000	0.00000	0.04386
81	C6	S	0.01376	0.00000	0.01108	-0.01328	0.00000
82	C6	S	0.41536	0.00000	-0.13070	-0.07756	0.00000
83	C6	PX	0.05031	0.00000	-0.05637	-0.03339	0.00000
84	C6	PY	0.17692	0.00000	-0.07515	0.02689	0.00000
85	C6	PZ	0.00000	0.00264	0.00000	0.00000	0.01269
86	C6	S	-0.78433	0.00000	0.72518	0.10033	0.00000
87	C6	PX	-1.39364	0.00000	0.28489	0.33720	0.00000
88	C6	PY	-1.86918	0.00000	0.51621	-1.00103	0.00000
89	C6	PZ	0.00000	-0.03131	0.00000	0.00000	-0.03428
90	C6	DXX	0.10175	0.00000	0.17521	-0.00282	0.00000
91	C6	DYY	-0.17204	0.00000	-0.23954	0.12020	0.00000
92	C6	DZZ	0.00051	0.00000	0.09373	-0.16980	0.00000
93	C6	DXY	-0.03739	0.00000	-0.07084	0.00894	0.00000
94	C6	DXZ	0.00000	-0.05410	0.00000	0.00000	0.05298
95	C6	DYZ	0.00000	-0.00372	0.00000	0.00000	0.00665
96	C7	S	0.03211	0.00000	0.01722	-0.01054	0.00000
97	C7	S	0.58603	0.00000	0.35061	-0.13599	0.00000
98	C7	PX	-0.14056	0.00000	-0.16288	0.02449	0.00000
99	C7	PY	0.07779	0.00000	0.14505	-0.04390	0.00000
100	C7	PZ	0.00000	0.00449	0.00000	0.00000	-0.00018
101	C7	S	-3.84203	0.00000	-0.47942	1.28469	0.00000
102	C7	PX	2.58942	0.00000	0.57121	-0.73433	0.00000
103	C7	PY	-0.23949	0.00000	-0.65146	0.61989	0.00000
104	C7	PZ	0.00000	-0.01658	0.00000	0.00000	-0.02140
105	C7	DXX	-0.14162	0.00000	0.00572	-0.06494	0.00000
106	C7	DYY	0.00688	0.00000	-0.15349	0.10456	0.00000
107	C7	DZZ	0.11406	0.00000	0.23478	-0.02854	0.00000
108	C7	DXY	-0.04677	0.00000	0.22207	-0.16586	0.00000
109	C7	DXZ	0.00000	-0.00116	0.00000	0.00000	0.01274
110	C7	DYZ	0.00000	-0.05984	0.00000	0.00000	-0.00684
111	O1	S	-0.00280	0.00000	-0.00275	-0.01397	0.00000
112	O1	S	-0.25887	0.00000	0.07557	0.61348	0.00000
113	O1	PX	-0.11076	0.00000	0.31045	0.37728	0.00000
114	O1	PY	0.04654	0.00000	0.31528	0.03086	0.00000
115	O1	PZ	0.00000	0.00693	0.00000	0.00000	0.05642
116	O1	S	0.50485	0.00000	-0.05018	-1.11766	0.00000
117	O1	PX	0.23377	0.00000	-0.64166	-0.57186	0.00000
118	O1	PY	-0.01879	0.00000	-0.41989	0.18136	0.00000
119	O1	PZ	0.00000	-0.02636	0.00000	0.00000	-0.11273
120	O1	DXX	-0.02395	0.00000	-0.09414	-0.10911	0.00000

121	O1	DYY	-0.01851	0.00000	0.03699	0.14464	0.00000
122	O1	DZZ	-0.11244	0.00000	0.06020	0.15705	0.00000
123	O1	DXY	-0.01187	0.00000	-0.06784	0.01876	0.00000
124	O1	DXZ	0.00000	-0.04139	0.00000	0.00000	0.06200
125	O1	DYZ	0.00000	0.02594	0.00000	0.00000	-0.03097
126	H4	S	-0.10196	0.00000	-0.08177	0.04808	0.00000
127	H4	S	0.01557	0.00000	0.06534	0.11186	0.00000
128	H4	PX	0.16823	0.00000	0.02467	0.04986	0.00000
129	H4	PY	0.05708	0.00000	-0.02999	0.04640	0.00000
130	H4	PZ	0.00000	-0.03128	0.00000	0.00000	0.10371
131	N1	S	0.02177	0.00000	0.00190	0.00132	0.00000
132	N1	S	0.57437	0.00000	0.31053	-0.13652	0.00000
133	N1	PX	0.04172	0.00000	0.05169	-0.04223	0.00000
134	N1	PY	0.23104	0.00000	0.13955	-0.05326	0.00000
135	N1	PZ	0.00000	-0.00840	0.00000	0.00000	0.00075
136	N1	S	-2.38375	0.00000	-0.58595	0.04343	0.00000
137	N1	PX	-0.16259	0.00000	-0.25211	0.25308	0.00000
138	N1	PY	-1.14137	0.00000	-0.06237	-0.23542	0.00000
139	N1	PZ	0.00000	0.02270	0.00000	0.00000	0.01872
140	N1	DXX	0.03242	0.00000	0.07568	-0.03698	0.00000
141	N1	DYY	0.02155	0.00000	-0.05044	0.00425	0.00000
142	N1	DZZ	0.07143	0.00000	0.07749	-0.01058	0.00000
143	N1	DXY	0.04264	0.00000	0.05747	-0.01108	0.00000
144	N1	DXZ	0.00000	0.02908	0.00000	0.00000	0.01375
145	N1	DYZ	0.00000	-0.00266	0.00000	0.00000	-0.01187
146	H6	S	0.23511	0.00000	0.07771	-0.07137	0.00000
147	H6	S	0.44772	0.00000	-0.21672	0.11513	0.00000
148	H6	PX	0.03705	0.00000	-0.07329	0.05674	0.00000
149	H6	PY	-0.16931	0.00000	0.05666	-0.06508	0.00000
150	H6	PZ	0.00000	0.02330	0.00000	0.00000	-0.04036
151	C8	S	0.00749	0.00000	0.00287	0.01109	0.00000
152	C8	S	0.20854	0.00000	-0.00947	0.19701	0.00000
153	C8	PX	0.07629	0.00000	-0.01863	0.00852	0.00000
154	C8	PY	-0.12343	0.00000	-0.14076	0.12295	0.00000
155	C8	PZ	0.00000	-0.00986	0.00000	0.00000	-0.00103
156	C8	S	1.57230	0.00000	0.14324	-0.34317	0.00000
157	C8	PX	0.29353	0.00000	-0.40376	0.39495	0.00000
158	C8	PY	1.55837	0.00000	0.96670	-1.49622	0.00000
159	C8	PZ	0.00000	-0.03771	0.00000	0.00000	-0.01102
160	C8	DXX	-0.00515	0.00000	-0.13286	0.07324	0.00000
161	C8	DYY	-0.17474	0.00000	0.01752	-0.07051	0.00000
162	C8	DZZ	0.34784	0.00000	0.12141	0.04991	0.00000
163	C8	DXY	0.08431	0.00000	-0.02021	0.00094	0.00000
164	C8	DXZ	0.00000	-0.01874	0.00000	0.00000	0.03440
165	C8	DYZ	0.00000	0.00865	0.00000	0.00000	0.00798
166	H8	S	-0.07470	0.00000	-0.02469	0.07404	0.00000
167	H8	S	-0.71213	0.00000	-0.22346	0.17377	0.00000
168	H8	PX	-0.01515	0.00000	0.03116	0.01929	0.00000
169	H8	PY	-0.05780	0.00000	0.13554	-0.12114	0.00000
170	H8	PZ	0.00000	-0.00509	0.00000	0.00000	-0.00941
171	C10	S	0.01982	0.00000	-0.00678	0.01684	0.00000
172	C10	S	0.19679	0.00000	-0.04410	0.09109	0.00000
173	C10	PX	-0.05462	0.00000	0.06253	-0.06789	0.00000
174	C10	PY	0.11728	0.00000	0.03369	-0.03206	0.00000

175	C10	PZ	0.00000	0.00361	0.00000	0.00000	-0.00006
176	C10	S	0.29022	0.00000	0.81678	-1.26180	0.00000
177	C10	PX	0.05485	0.00000	-0.33654	0.47886	0.00000
178	C10	PY	-0.30405	0.00000	0.00116	-0.26769	0.00000
179	C10	PZ	0.00000	0.02729	0.00000	0.00000	0.00704
180	C10	DXX	0.20362	0.00000	0.07762	-0.04016	0.00000
181	C10	DYY	-0.31723	0.00000	0.01916	-0.10843	0.00000
182	C10	DZZ	0.17917	0.00000	-0.16779	0.24602	0.00000
183	C10	DXY	-0.01297	0.00000	0.15023	-0.11245	0.00000
184	C10	DXZ	0.00000	-0.00672	0.00000	0.00000	0.00075
185	C10	DYZ	0.00000	0.03352	0.00000	0.00000	0.00695
186	H16	S	-0.13365	0.00000	0.02344	-0.03386	0.00000
187	H16	S	-0.03408	0.00000	0.04732	-0.09885	0.00000
188	H16	PX	-0.05297	0.00000	0.07387	-0.06578	0.00000
189	H16	PY	0.08918	0.00000	0.23994	-0.19189	0.00000
190	H16	PZ	0.00000	-0.01132	0.00000	0.00000	-0.00967
191	H18	S	0.03789	0.00000	-0.22880	0.24160	0.00000
192	H18	S	-0.08537	0.00000	-0.14806	0.14982	0.00000
193	H18	PX	-0.17326	0.00000	0.12941	-0.15888	0.00000
194	H18	PY	0.17039	0.00000	0.01860	0.03098	0.00000
195	H18	PZ	0.00000	-0.02147	0.00000	0.00000	0.00436
196	C9	S	-0.00134	0.00000	0.00848	0.00199	0.00000
197	C9	S	-0.02778	0.00000	0.20376	0.15817	0.00000
198	C9	PX	0.05071	0.00000	-0.18831	-0.18337	0.00000
199	C9	PY	0.03998	0.00000	-0.09415	-0.09963	0.00000
200	C9	PZ	0.00000	0.01380	0.00000	0.00000	-0.11625
201	C9	S	-0.16944	0.00000	0.15926	0.20921	0.00000
202	C9	PX	-0.01050	0.00000	0.12820	0.36969	0.00000
203	C9	PY	-0.15471	0.00000	0.27924	0.17886	0.00000
204	C9	PZ	0.00000	-0.04469	0.00000	0.00000	0.61065
205	C9	DXX	0.06164	0.00000	-0.12340	-0.31077	0.00000
206	C9	DYY	-0.02682	0.00000	-0.05852	-0.02135	0.00000
207	C9	DZZ	-0.03265	0.00000	0.17717	0.28026	0.00000
208	C9	DXY	0.09132	0.00000	-0.28075	-0.37895	0.00000
209	C9	DXZ	0.00000	-0.05582	0.00000	0.00000	0.51986
210	C9	DYZ	0.00000	0.01657	0.00000	0.00000	-0.29111
211	H3	S	0.08501	0.00000	-0.07361	-0.09880	0.00000
212	H3	S	0.07049	0.00000	-0.11819	-0.05713	0.00000
213	H3	PX	0.02271	0.00000	-0.16083	-0.05122	0.00000
214	H3	PY	0.03922	0.00000	-0.03629	-0.07011	0.00000
215	H3	PZ	0.00000	0.59478	0.00000	0.00000	-0.22409
216	H5	S	0.03086	-0.03442	-0.11672	-0.20813	0.46738
217	H5	S	0.01625	-0.00744	0.02332	0.00008	-0.02118
218	H5	PX	0.04155	-0.21764	-0.11720	-0.22788	-0.14042
219	H5	PY	0.04497	0.45744	0.01645	-0.10570	-0.06778
220	H5	PZ	-0.00746	-0.25048	0.02935	0.02715	-0.39593
221	H7	S	0.03086	0.03442	-0.11672	-0.20813	-0.46738
222	H7	S	0.01625	0.00744	0.02332	0.00008	0.02118
223	H7	PX	0.04155	0.21764	-0.11720	-0.22788	0.14042
224	H7	PY	0.04497	-0.45744	0.01645	-0.10570	0.06778
225	H7	PZ	0.00746	-0.25048	-0.02935	-0.02715	-0.39593

MO:	156	157	158	159	160
Eigenvalues:	2.38941	2.40058	2.43816	2.44064	2.45653

(ev): 65.01916 65.32302 66.34566 66.41335 66.84554

		A	A	A	A	A	
1	H1	S	0.09481	0.00035	0.03272	0.00000	-0.05830
2	H1	S	-0.21783	0.21816	0.14406	0.00000	0.06162
3	H1	PX	0.03142	-0.04213	0.02906	0.00000	0.01828
4	H1	PY	0.07018	0.17535	0.01756	0.00000	-0.12263
5	H1	PZ	0.00000	0.00000	0.00000	-0.12102	0.00000
6	C1	S	0.01703	0.00844	-0.00909	0.00000	0.00637
7	C1	S	0.30134	-0.04085	-0.03642	0.00000	0.06574
8	C1	PX	-0.12504	-0.06456	0.00589	0.00000	0.03995
9	C1	PY	0.07102	0.24832	-0.05105	0.00000	-0.20223
10	C1	PZ	0.00000	0.00000	0.00000	-0.01161	0.00000
11	C1	S	-1.07822	0.18418	1.12917	0.00000	-1.91109
12	C1	PX	0.78632	-0.35856	-0.52643	0.00000	0.42978
13	C1	PY	-0.38170	-0.04304	0.18597	0.00000	0.86380
14	C1	PZ	0.00000	0.00000	0.00000	0.02794	0.00000
15	C1	DXX	-0.12035	-0.08534	0.01065	0.00000	-0.00714
16	C1	DYY	0.02037	0.03658	-0.07054	0.00000	0.06577
17	C1	DZZ	0.16973	0.09508	0.09385	0.00000	-0.08838
18	C1	DXY	-0.05393	0.12860	-0.06723	0.00000	0.05869
19	C1	DXZ	0.00000	0.00000	0.00000	0.02139	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.04625	0.00000
21	C2	S	0.01124	-0.00003	-0.01181	0.00000	0.00884
22	C2	S	0.25078	-0.13698	0.07408	0.00000	0.18390
23	C2	PX	0.03707	-0.11679	0.09122	0.00000	0.04939
24	C2	PY	0.26840	0.09188	-0.00196	0.00000	-0.04293
25	C2	PZ	0.00000	0.00000	0.00000	0.02795	0.00000
26	C2	S	-0.51880	-0.45052	0.92115	0.00000	-0.63745
27	C2	PX	-0.31468	-0.09825	0.40083	0.00000	-0.53552
28	C2	PY	-0.20981	-1.54381	-0.14041	0.00000	0.78883
29	C2	PZ	0.00000	0.00000	0.00000	-0.01259	0.00000
30	C2	DXX	0.00972	0.04790	0.04982	0.00000	-0.13510
31	C2	DYY	-0.04485	0.05928	0.00024	0.00000	0.06050
32	C2	DZZ	0.13670	-0.16247	-0.01741	0.00000	0.09339
33	C2	DXY	-0.04392	-0.13052	-0.05580	0.00000	0.01988
34	C2	DXZ	0.00000	0.00000	0.00000	0.04027	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	-0.00185	0.00000
36	C3	S	0.00469	0.01227	-0.02384	0.00000	0.00589
37	C3	S	-0.31355	0.06327	-0.28354	0.00000	0.05112
38	C3	PX	0.15094	-0.00962	0.15879	0.00000	-0.09793
39	C3	PY	0.07245	-0.06839	0.22257	0.00000	-0.13512
40	C3	PZ	0.00000	0.00000	0.00000	-0.00282	0.00000
41	C3	S	0.95837	-2.99933	-0.21182	0.00000	2.21198
42	C3	PX	-0.94251	0.68442	-0.60440	0.00000	0.66195
43	C3	PY	-0.19998	1.84762	-0.58018	0.00000	0.27333
44	C3	PZ	0.00000	0.00000	0.00000	0.01599	0.00000
45	C3	DXX	0.08050	-0.01149	0.30751	0.00000	-0.16703
46	C3	DYY	-0.08331	0.11692	-0.04917	0.00000	-0.02044
47	C3	DZZ	0.02568	-0.17433	-0.31782	0.00000	0.24972
48	C3	DXY	0.12307	0.20306	-0.02590	0.00000	-0.08869
49	C3	DXZ	0.00000	0.00000	0.00000	0.56676	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.06921	0.00000
51	C4	S	0.01073	0.01651	0.00359	0.00000	-0.00904

52	C4	S	0.04282	0.38718	0.02154	0.00000	-0.30255
53	C4	PX	-0.03009	-0.03557	0.02929	0.00000	0.06647
54	C4	PY	0.02638	-0.19413	-0.02905	0.00000	0.00897
55	C4	PZ	0.00000	0.00000	0.00000	-0.01891	0.00000
56	C4	S	0.43702	-0.48616	-0.96809	0.00000	-0.47297
57	C4	PX	0.73147	-0.32308	-0.25251	0.00000	1.05813
58	C4	PY	-0.38874	1.31697	0.44540	0.00000	-1.25858
59	C4	PZ	0.00000	0.00000	0.00000	-0.04623	0.00000
60	C4	DXX	-0.15388	-0.23940	-0.05959	0.00000	0.10054
61	C4	DYY	0.05285	0.02121	0.02958	0.00000	-0.01132
62	C4	DZZ	0.13869	0.27398	-0.03968	0.00000	-0.11344
63	C4	DXY	0.11820	0.04142	0.04804	0.00000	-0.00040
64	C4	DXZ	0.00000	0.00000	0.00000	0.12491	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.00526	0.00000
66	C5	S	0.00694	-0.00139	-0.00323	0.00000	-0.01552
67	C5	S	0.03623	0.10513	-0.03346	0.00000	-0.26459
68	C5	PX	0.05433	0.15906	0.02858	0.00000	-0.04707
69	C5	PY	-0.02001	0.03416	0.02957	0.00000	0.05579
70	C5	PZ	0.00000	0.00000	0.00000	0.00971	0.00000
71	C5	S	0.51715	1.20447	0.02791	0.00000	0.63062
72	C5	PX	0.10495	-0.51296	0.17583	0.00000	0.77376
73	C5	PY	0.54187	-1.09203	0.05318	0.00000	0.52582
74	C5	PZ	0.00000	0.00000	0.00000	0.02322	0.00000
75	C5	DXX	0.13572	-0.13196	0.13649	0.00000	0.15350
76	C5	DYY	-0.20124	0.06554	-0.12554	0.00000	0.01395
77	C5	DZZ	0.09595	0.10259	-0.00161	0.00000	-0.19114
78	C5	DXY	-0.22809	-0.10089	-0.02768	0.00000	0.05689
79	C5	DXZ	0.00000	0.00000	0.00000	0.11741	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.08793	0.00000
81	C6	S	0.00840	-0.00969	-0.01959	0.00000	0.01848
82	C6	S	0.00439	-0.44862	-0.31780	0.00000	0.38608
83	C6	PX	-0.05334	-0.10559	-0.16456	0.00000	0.18398
84	C6	PY	-0.19628	-0.05603	0.00448	0.00000	0.03894
85	C6	PZ	0.00000	0.00000	0.00000	0.04173	0.00000
86	C6	S	-0.53147	0.66740	0.21243	0.00000	0.45605
87	C6	PX	-0.71583	2.08146	0.70291	0.00000	-1.13378
88	C6	PY	0.58411	0.82097	-1.37951	0.00000	0.23708
89	C6	PZ	0.00000	0.00000	0.00000	0.05089	0.00000
90	C6	DXX	0.24426	0.22016	0.05107	0.00000	-0.11141
91	C6	DYY	-0.09473	-0.15995	0.14784	0.00000	-0.08733
92	C6	DZZ	-0.10972	-0.05686	-0.27577	0.00000	0.23852
93	C6	DXY	0.11473	-0.23159	0.21286	0.00000	0.02447
94	C6	DXZ	0.00000	0.00000	0.00000	0.36576	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.15473	0.00000
96	C7	S	0.00610	-0.01717	-0.00752	0.00000	0.01294
97	C7	S	0.41562	-0.32048	-0.02983	0.00000	0.15315
98	C7	PX	-0.17164	0.02537	-0.06510	0.00000	0.02703
99	C7	PY	-0.04680	0.17244	-0.18221	0.00000	0.01877
100	C7	PZ	0.00000	0.00000	0.00000	-0.10895	0.00000
101	C7	S	-0.79357	3.14890	0.26718	0.00000	-1.70317
102	C7	PX	0.58509	-1.86693	-0.07945	0.00000	0.78899
103	C7	PY	0.44057	-0.26775	0.86506	0.00000	-0.53780
104	C7	PZ	0.00000	0.00000	0.00000	-0.15760	0.00000
105	C7	DXX	-0.08828	-0.07506	0.20864	0.00000	-0.04379

106	C7	DYY	0.01291	0.15155	-0.16805	0.00000	-0.00171
107	C7	DZZ	0.15141	0.04664	-0.10574	0.00000	0.00087
108	C7	DXY	-0.06498	0.06728	-0.14138	0.00000	0.06261
109	C7	DXZ	0.00000	0.00000	0.00000	0.13396	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.02608	0.00000
111	O1	S	0.01581	0.02044	0.00144	0.00000	-0.02373
112	O1	S	0.00574	0.18244	-0.05715	0.00000	-0.23389
113	O1	PX	-0.03249	-0.02353	-0.02228	0.00000	0.11374
114	O1	PY	0.02480	0.06506	0.06338	0.00000	0.06735
115	O1	PZ	0.00000	0.00000	0.00000	0.00051	0.00000
116	O1	S	-0.20415	-1.02254	0.05518	0.00000	1.27596
117	O1	PX	-0.18928	-0.10830	0.12079	0.00000	-0.22246
118	O1	PY	-0.09681	-0.09129	-0.15758	0.00000	-0.56155
119	O1	PZ	0.00000	0.00000	0.00000	0.02209	0.00000
120	O1	DXX	-0.01223	0.05856	-0.07727	0.00000	-0.28883
121	O1	DYY	0.00797	0.05614	0.04037	0.00000	-0.04447
122	O1	DZZ	0.05270	-0.00226	0.02830	0.00000	0.20244
123	O1	DXY	0.06629	-0.09943	0.02935	0.00000	0.20730
124	O1	DXZ	0.00000	0.00000	0.00000	-0.04325	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.02217	0.00000
126	H4	S	-0.21082	-0.03210	-0.01475	0.00000	-0.05076
127	H4	S	-0.07995	0.07797	0.04902	0.00000	0.03320
128	H4	PX	-0.02925	0.11790	-0.04601	0.00000	-0.00302
129	H4	PY	-0.13310	0.10125	-0.04838	0.00000	-0.03049
130	H4	PZ	0.00000	0.00000	0.00000	0.00321	0.00000
131	N1	S	-0.00232	-0.00897	-0.01581	0.00000	0.01611
132	N1	S	-0.23318	-0.12379	0.11485	0.00000	0.22752
133	N1	PX	-0.13892	-0.02734	0.26801	0.00000	-0.05979
134	N1	PY	0.13043	0.14784	-0.21365	0.00000	0.07461
135	N1	PZ	0.00000	0.00000	0.00000	0.01330	0.00000
136	N1	S	0.79491	1.03923	0.20705	0.00000	-1.27918
137	N1	PX	0.55070	-0.13288	0.20790	0.00000	-0.28335
138	N1	PY	-0.41101	0.55065	-0.30540	0.00000	-0.23582
139	N1	PZ	0.00000	0.00000	0.00000	0.17593	0.00000
140	N1	DXX	0.10283	0.02177	-0.12689	0.00000	0.03170
141	N1	DYY	-0.15531	-0.02669	0.03618	0.00000	0.00752
142	N1	DZZ	0.03192	0.05183	0.07001	0.00000	-0.01532
143	N1	DXY	-0.02446	-0.04618	0.05610	0.00000	-0.02840
144	N1	DXZ	0.00000	0.00000	0.00000	0.34232	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.14855	0.00000
146	H6	S	-0.01251	-0.08009	0.00118	0.00000	0.08980
147	H6	S	-0.08165	-0.16292	0.06385	0.00000	-0.09380
148	H6	PX	-0.08275	-0.00530	-0.03979	0.00000	-0.01544
149	H6	PY	0.13653	0.07387	0.05525	0.00000	-0.12439
150	H6	PZ	0.00000	0.00000	0.00000	0.04384	0.00000
151	C8	S	-0.00126	0.02281	0.01948	0.00000	-0.02055
152	C8	S	-0.09737	0.15477	0.43259	0.00000	-0.28627
153	C8	PX	0.08071	-0.01130	-0.02367	0.00000	-0.01833
154	C8	PY	-0.03741	0.00402	0.03854	0.00000	-0.00541
155	C8	PZ	0.00000	0.00000	0.00000	-0.05773	0.00000
156	C8	S	-0.06127	-1.05960	0.37359	0.00000	0.22129
157	C8	PX	0.26035	-0.53811	1.58983	0.00000	-0.74809
158	C8	PY	0.65555	-1.81187	-2.19754	0.00000	2.36074
159	C8	PZ	0.00000	0.00000	0.00000	-0.16848	0.00000

160	C8	DXX	0.02110	0.17929	-0.45050	0.00000	0.07653
161	C8	DYY	-0.08652	-0.13563	0.20296	0.00000	-0.02367
162	C8	DZZ	0.05568	0.00483	0.36922	0.00000	-0.15776
163	C8	DXY	-0.27009	0.11851	0.02839	0.00000	-0.03837
164	C8	DXZ	0.00000	0.00000	0.00000	0.51862	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.32612	0.00000
166	H8	S	0.06562	0.16258	-0.15635	0.00000	0.01796
167	H8	S	-0.17200	0.36963	0.11113	0.00000	-0.17993
168	H8	PX	0.05540	0.09461	-0.12671	0.00000	-0.00096
169	H8	PY	0.01905	0.00881	-0.28404	0.00000	0.10418
170	H8	PZ	0.00000	0.00000	0.00000	0.25018	0.00000
171	C10	S	-0.00483	0.02584	0.01184	0.00000	-0.02460
172	C10	S	-0.03402	0.20190	-0.11931	0.00000	-0.05710
173	C10	PX	-0.16443	0.02134	0.06990	0.00000	-0.02239
174	C10	PY	-0.01160	0.04507	-0.20682	0.00000	0.11929
175	C10	PZ	0.00000	0.00000	0.00000	0.06204	0.00000
176	C10	S	0.53622	-1.37332	-1.85123	0.00000	2.00166
177	C10	PX	0.59310	0.31222	-0.34474	0.00000	-0.10250
178	C10	PY	0.30379	-0.35682	-1.03828	0.00000	0.82085
179	C10	PZ	0.00000	0.00000	0.00000	0.17028	0.00000
180	C10	DXX	0.06394	-0.12778	0.16538	0.00000	-0.03441
181	C10	DYY	-0.01754	-0.10331	-0.19816	0.00000	0.20142
182	C10	DZZ	-0.06429	0.39984	-0.04878	0.00000	-0.23548
183	C10	DXY	-0.13138	0.04575	0.02837	0.00000	-0.02701
184	C10	DXZ	0.00000	0.00000	0.00000	0.02513	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.19542	0.00000
186	H16	S	-0.19776	0.13421	-0.00202	0.00000	-0.05472
187	H16	S	-0.26291	-0.05349	0.19170	0.00000	-0.03486
188	H16	PX	-0.22292	0.11924	0.00011	0.00000	-0.03497
189	H16	PY	-0.39609	0.03015	0.27055	0.00000	-0.07656
190	H16	PZ	0.00000	0.00000	0.00000	-0.31455	0.00000
191	H18	S	0.13731	0.15252	-0.07654	0.00000	-0.07523
192	H18	S	0.25179	0.07221	-0.24889	0.00000	0.03963
193	H18	PX	-0.35134	0.06141	0.02510	0.00000	0.02869
194	H18	PY	0.30865	-0.16142	0.06474	0.00000	0.00580
195	H18	PZ	0.00000	0.00000	0.00000	-0.02630	0.00000
196	C9	S	-0.00556	-0.00686	0.00316	0.00000	0.01617
197	C9	S	-0.03321	0.00423	0.05180	0.00000	0.27610
198	C9	PX	-0.01877	-0.04964	0.02198	0.00000	0.00677
199	C9	PY	-0.01013	-0.11695	-0.09029	0.00000	-0.23219
200	C9	PZ	0.00000	0.00000	0.00000	0.01334	0.00000
201	C9	S	0.24905	0.32951	-0.11071	0.00000	-0.38970
202	C9	PX	-0.18020	-0.32140	-0.15099	0.00000	-0.26864
203	C9	PY	-0.07691	0.33238	0.39473	0.00000	0.91779
204	C9	PZ	0.00000	0.00000	0.00000	-0.04535	0.00000
205	C9	DXX	0.10333	0.02775	-0.01844	0.00000	-0.08176
206	C9	DYY	-0.00698	0.29677	0.20070	0.00000	0.31460
207	C9	DZZ	-0.08460	-0.31725	-0.18175	0.00000	-0.25431
208	C9	DXY	0.08435	0.03233	-0.05016	0.00000	-0.19068
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00004	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.01259	0.00000
211	H3	S	-0.00202	-0.30782	-0.20525	0.00000	-0.36237
212	H3	S	-0.01799	-0.07592	-0.07585	0.00000	-0.21861
213	H3	PX	0.08397	0.11738	0.16011	0.00000	0.36155

214	H3	PY	0.01967	-0.15475	-0.10128	0.00000	-0.18464
215	H3	PZ	0.00000	0.00000	0.00000	0.02377	0.00000
216	H5	S	0.00834	0.17021	0.14048	-0.00598	0.23379
217	H5	S	0.00232	-0.05393	0.01218	-0.02128	0.10750
218	H5	PX	0.02971	0.09292	0.03829	0.03694	0.03172
219	H5	PY	-0.02290	-0.10824	-0.12001	0.02163	-0.26928
220	H5	PZ	-0.00645	-0.02264	-0.01463	0.02715	-0.01456
221	H7	S	0.00834	0.17021	0.14048	0.00598	0.23379
222	H7	S	0.00232	-0.05393	0.01218	0.02128	0.10750
223	H7	PX	0.02971	0.09292	0.03829	-0.03694	0.03172
224	H7	PY	-0.02290	-0.10824	-0.12001	-0.02163	-0.26928
225	H7	PZ	0.00645	0.02264	0.01463	0.02715	0.01456

MO:	161	162	163	164	165
Eigenvalues:	2.47655	2.52504	2.52866	2.55727	2.60320
(ev):	67.39045	68.70988	68.80824	69.58695	70.83661

		A	A	A	A	A	
1	H1	S	-0.22887	0.00000	-0.04773	0.00000	0.00000
2	H1	S	0.35499	0.00000	-0.13486	0.00000	0.00000
3	H1	PX	-0.04542	0.00000	0.06107	0.00000	0.00000
4	H1	PY	-0.15085	0.00000	-0.07586	0.00000	0.00000
5	H1	PZ	0.00000	0.20268	0.00000	0.08744	0.39747
6	C1	S	-0.02280	0.00000	-0.03047	0.00000	0.00000
7	C1	S	-0.32963	0.00000	-0.28429	0.00000	0.00000
8	C1	PX	0.16686	0.00000	0.11427	0.00000	0.00000
9	C1	PY	-0.06254	0.00000	-0.04012	0.00000	0.00000
10	C1	PZ	0.00000	-0.10372	0.00000	-0.01461	-0.08272
11	C1	S	0.99711	0.00000	1.06038	0.00000	0.00000
12	C1	PX	-1.08684	0.00000	0.17386	0.00000	0.00000
13	C1	PY	2.06581	0.00000	-0.15947	0.00000	0.00000
14	C1	PZ	0.00000	-0.11696	0.00000	-0.05549	-0.08933
15	C1	DXX	0.33022	0.00000	-0.06944	0.00000	0.00000
16	C1	DYY	-0.22764	0.00000	0.31237	0.00000	0.00000
17	C1	DZZ	-0.25733	0.00000	-0.33667	0.00000	0.00000
18	C1	DXY	-0.18658	0.00000	-0.08820	0.00000	0.00000
19	C1	DXZ	0.00000	0.09135	0.00000	0.12032	-0.17079
20	C1	DYZ	0.00000	-0.06880	0.00000	-0.39383	0.17788
21	C2	S	-0.00641	0.00000	0.03898	0.00000	0.00000
22	C2	S	-0.21994	0.00000	0.22832	0.00000	0.00000
23	C2	PX	-0.02158	0.00000	-0.04471	0.00000	0.00000
24	C2	PY	-0.07756	0.00000	0.20810	0.00000	0.00000
25	C2	PZ	0.00000	0.04920	0.00000	-0.07694	0.02667
26	C2	S	0.96023	0.00000	-0.62612	0.00000	0.00000
27	C2	PX	0.55078	0.00000	-0.20068	0.00000	0.00000
28	C2	PY	-0.74291	0.00000	0.98883	0.00000	0.00000
29	C2	PZ	0.00000	0.04217	0.00000	-0.12235	0.08008
30	C2	DXX	0.20630	0.00000	-0.12578	0.00000	0.00000
31	C2	DYY	-0.21220	0.00000	-0.25932	0.00000	0.00000
32	C2	DZZ	-0.04030	0.00000	0.46240	0.00000	0.00000
33	C2	DXY	-0.12501	0.00000	0.34527	0.00000	0.00000
34	C2	DXZ	0.00000	0.12731	0.00000	0.11642	-0.02792
35	C2	DYZ	0.00000	-0.18486	0.00000	-0.42074	0.28290
36	C3	S	-0.01287	0.00000	-0.02466	0.00000	0.00000

37	C3	S	0.08110	0.00000	-0.39194	0.00000	0.00000
38	C3	PX	-0.06316	0.00000	-0.03569	0.00000	0.00000
39	C3	PY	0.19895	0.00000	-0.09690	0.00000	0.00000
40	C3	PZ	0.00000	-0.04729	0.00000	-0.10575	-0.02621
41	C3	S	1.20097	0.00000	1.90953	0.00000	0.00000
42	C3	PX	1.54774	0.00000	-1.68096	0.00000	0.00000
43	C3	PY	0.10095	0.00000	-1.01049	0.00000	0.00000
44	C3	PZ	0.00000	-0.13042	0.00000	-0.02929	-0.02509
45	C3	DXX	-0.05817	0.00000	0.04848	0.00000	0.00000
46	C3	DYY	0.09784	0.00000	0.04994	0.00000	0.00000
47	C3	DZZ	0.01505	0.00000	-0.17585	0.00000	0.00000
48	C3	DXY	0.13558	0.00000	0.02321	0.00000	0.00000
49	C3	DXZ	0.00000	0.10660	0.00000	-0.35610	-0.06833
50	C3	DYZ	0.00000	0.40444	0.00000	-0.03035	0.39190
51	C4	S	-0.02319	0.00000	-0.02217	0.00000	0.00000
52	C4	S	-0.29418	0.00000	-0.04971	0.00000	0.00000
53	C4	PX	-0.11435	0.00000	-0.18047	0.00000	0.00000
54	C4	PY	0.09193	0.00000	0.04436	0.00000	0.00000
55	C4	PZ	0.00000	0.01628	0.00000	0.11641	-0.11536
56	C4	S	-0.86762	0.00000	0.37019	0.00000	0.00000
57	C4	PX	-1.82595	0.00000	-0.47532	0.00000	0.00000
58	C4	PY	-0.44849	0.00000	-0.52860	0.00000	0.00000
59	C4	PZ	0.00000	0.06574	0.00000	0.10584	-0.05784
60	C4	DXX	-0.00620	0.00000	0.26047	0.00000	0.00000
61	C4	DYY	0.13810	0.00000	-0.09772	0.00000	0.00000
62	C4	DZZ	-0.22344	0.00000	-0.17816	0.00000	0.00000
63	C4	DXY	-0.27319	0.00000	-0.07456	0.00000	0.00000
64	C4	DXZ	0.00000	0.41164	0.00000	0.19770	-0.03632
65	C4	DYZ	0.00000	-0.02034	0.00000	0.05777	-0.29592
66	C5	S	0.01022	0.00000	0.02716	0.00000	0.00000
67	C5	S	0.40102	0.00000	0.13521	0.00000	0.00000
68	C5	PX	-0.01983	0.00000	-0.13916	0.00000	0.00000
69	C5	PY	-0.19532	0.00000	-0.17951	0.00000	0.00000
70	C5	PZ	0.00000	0.06074	0.00000	0.08918	-0.05872
71	C5	S	-1.27394	0.00000	-1.35455	0.00000	0.00000
72	C5	PX	-0.94238	0.00000	-0.15270	0.00000	0.00000
73	C5	PY	-0.03241	0.00000	0.75812	0.00000	0.00000
74	C5	PZ	0.00000	0.03684	0.00000	0.13801	-0.10935
75	C5	DXX	-0.14688	0.00000	-0.19138	0.00000	0.00000
76	C5	DYY	0.08047	0.00000	-0.00632	0.00000	0.00000
77	C5	DZZ	0.15108	0.00000	0.17889	0.00000	0.00000
78	C5	DXY	0.12432	0.00000	-0.28522	0.00000	0.00000
79	C5	DXZ	0.00000	0.16251	0.00000	-0.21251	0.18611
80	C5	DYZ	0.00000	0.08886	0.00000	-0.29550	0.15539
81	C6	S	-0.00333	0.00000	0.00293	0.00000	0.00000
82	C6	S	0.02922	0.00000	0.20191	0.00000	0.00000
83	C6	PX	0.07060	0.00000	-0.21441	0.00000	0.00000
84	C6	PY	-0.07342	0.00000	0.29605	0.00000	0.00000
85	C6	PZ	0.00000	-0.02927	0.00000	-0.12667	0.01039
86	C6	S	0.08527	0.00000	-1.00430	0.00000	0.00000
87	C6	PX	1.05718	0.00000	-2.28000	0.00000	0.00000
88	C6	PY	-0.21031	0.00000	-0.23906	0.00000	0.00000
89	C6	PZ	0.00000	-0.02914	0.00000	-0.13601	-0.00668
90	C6	DXX	-0.10854	0.00000	0.11096	0.00000	0.00000

91	C6	DYY	0.09815	0.00000	-0.10595	0.00000	0.00000
92	C6	DZZ	-0.05656	0.00000	0.02571	0.00000	0.00000
93	C6	DXY	-0.06099	0.00000	-0.10533	0.00000	0.00000
94	C6	DXZ	0.00000	0.43547	0.00000	0.04373	0.03636
95	C6	DYZ	0.00000	0.02910	0.00000	0.22791	0.13783
96	C7	S	0.00658	0.00000	-0.00506	0.00000	0.00000
97	C7	S	0.20306	0.00000	-0.03295	0.00000	0.00000
98	C7	PX	-0.10863	0.00000	0.03251	0.00000	0.00000
99	C7	PY	-0.01114	0.00000	-0.02667	0.00000	0.00000
100	C7	PZ	0.00000	0.09233	0.00000	-0.00566	0.05180
101	C7	S	-1.32938	0.00000	-0.28190	0.00000	0.00000
102	C7	PX	0.48940	0.00000	0.53680	0.00000	0.00000
103	C7	PY	-0.56262	0.00000	0.48994	0.00000	0.00000
104	C7	PZ	0.00000	0.19321	0.00000	-0.00315	0.07848
105	C7	DXX	0.16516	0.00000	-0.17988	0.00000	0.00000
106	C7	DYY	-0.13062	0.00000	0.20100	0.00000	0.00000
107	C7	DZZ	-0.04354	0.00000	-0.02570	0.00000	0.00000
108	C7	DXY	0.02151	0.00000	-0.04346	0.00000	0.00000
109	C7	DXZ	0.00000	0.04047	0.00000	-0.03491	0.04313
110	C7	DYZ	0.00000	0.18290	0.00000	0.45816	0.33908
111	O1	S	-0.03313	0.00000	-0.02528	0.00000	0.00000
112	O1	S	-0.53600	0.00000	-0.13079	0.00000	0.00000
113	O1	PX	-0.02436	0.00000	-0.01224	0.00000	0.00000
114	O1	PY	0.14068	0.00000	-0.05959	0.00000	0.00000
115	O1	PZ	0.00000	0.02867	0.00000	0.04056	-0.05212
116	O1	S	1.82151	0.00000	0.80921	0.00000	0.00000
117	O1	PX	0.76931	0.00000	0.49352	0.00000	0.00000
118	O1	PY	-0.19577	0.00000	0.18051	0.00000	0.00000
119	O1	PZ	0.00000	-0.04309	0.00000	-0.14585	0.25349
120	O1	DXX	0.00684	0.00000	0.05638	0.00000	0.00000
121	O1	DYY	-0.10844	0.00000	-0.08542	0.00000	0.00000
122	O1	DZZ	-0.14361	0.00000	-0.06108	0.00000	0.00000
123	O1	DXY	-0.15397	0.00000	0.02565	0.00000	0.00000
124	O1	DXZ	0.00000	-0.10827	0.00000	-0.08706	0.11688
125	O1	DYZ	0.00000	0.07793	0.00000	0.19753	-0.33232
126	H4	S	0.08016	0.00000	-0.13618	0.00000	0.00000
127	H4	S	-0.16141	0.00000	-0.06095	0.00000	0.00000
128	H4	PX	-0.13418	0.00000	-0.11102	0.00000	0.00000
129	H4	PY	0.01151	0.00000	-0.26517	0.00000	0.00000
130	H4	PZ	0.00000	-0.06770	0.00000	-0.17834	0.21575
131	N1	S	0.00427	0.00000	-0.01113	0.00000	0.00000
132	N1	S	-0.04610	0.00000	-0.08386	0.00000	0.00000
133	N1	PX	-0.08174	0.00000	-0.01939	0.00000	0.00000
134	N1	PY	-0.00387	0.00000	0.13165	0.00000	0.00000
135	N1	PZ	0.00000	-0.00254	0.00000	0.00770	0.01029
136	N1	S	-0.19944	0.00000	0.50397	0.00000	0.00000
137	N1	PX	-0.21413	0.00000	0.85290	0.00000	0.00000
138	N1	PY	-0.07922	0.00000	-0.29268	0.00000	0.00000
139	N1	PZ	0.00000	0.11460	0.00000	0.14221	-0.02267
140	N1	DXX	-0.12618	0.00000	0.27637	0.00000	0.00000
141	N1	DYY	0.03884	0.00000	-0.00569	0.00000	0.00000
142	N1	DZZ	0.02431	0.00000	-0.21496	0.00000	0.00000
143	N1	DXY	-0.18239	0.00000	0.28071	0.00000	0.00000
144	N1	DXZ	0.00000	0.11420	0.00000	-0.04472	-0.21065

145	N1	DYZ	0.00000	0.09051	0.00000	0.37126	0.14771
146	H6	S	-0.10261	0.00000	0.03911	0.00000	0.00000
147	H6	S	0.05667	0.00000	0.10814	0.00000	0.00000
148	H6	PX	0.01202	0.00000	-0.02510	0.00000	0.00000
149	H6	PY	0.16976	0.00000	0.14562	0.00000	0.00000
150	H6	PZ	0.00000	-0.01707	0.00000	0.22778	-0.00391
151	C8	S	0.00588	0.00000	-0.00009	0.00000	0.00000
152	C8	S	0.05876	0.00000	-0.11477	0.00000	0.00000
153	C8	PX	-0.03282	0.00000	0.15281	0.00000	0.00000
154	C8	PY	-0.05345	0.00000	-0.11493	0.00000	0.00000
155	C8	PZ	0.00000	0.02921	0.00000	0.03106	0.05251
156	C8	S	0.30157	0.00000	0.35812	0.00000	0.00000
157	C8	PX	-0.08506	0.00000	0.59970	0.00000	0.00000
158	C8	PY	0.23865	0.00000	-0.15360	0.00000	0.00000
159	C8	PZ	0.00000	-0.00223	0.00000	-0.01828	-0.03460
160	C8	DXX	0.12154	0.00000	-0.04891	0.00000	0.00000
161	C8	DYY	-0.13134	0.00000	0.05296	0.00000	0.00000
162	C8	DZZ	0.06544	0.00000	0.06281	0.00000	0.00000
163	C8	DXY	-0.11713	0.00000	0.08795	0.00000	0.00000
164	C8	DXZ	0.00000	0.18143	0.00000	0.07784	-0.10444
165	C8	DYZ	0.00000	-0.32286	0.00000	0.28137	0.30520
166	H8	S	-0.12275	0.00000	0.04081	0.00000	0.00000
167	H8	S	-0.01515	0.00000	-0.23795	0.00000	0.00000
168	H8	PX	-0.06466	0.00000	0.08123	0.00000	0.00000
169	H8	PY	0.05689	0.00000	0.00368	0.00000	0.00000
170	H8	PZ	0.00000	-0.44615	0.00000	0.15159	-0.17404
171	C10	S	0.01249	0.00000	0.01514	0.00000	0.00000
172	C10	S	0.12165	0.00000	0.07723	0.00000	0.00000
173	C10	PX	-0.03926	0.00000	-0.00499	0.00000	0.00000
174	C10	PY	0.05076	0.00000	-0.05013	0.00000	0.00000
175	C10	PZ	0.00000	-0.10159	0.00000	0.06440	0.10242
176	C10	S	-0.12407	0.00000	-0.55218	0.00000	0.00000
177	C10	PX	0.12518	0.00000	-0.07906	0.00000	0.00000
178	C10	PY	-0.13856	0.00000	-0.28611	0.00000	0.00000
179	C10	PZ	0.00000	-0.16313	0.00000	0.09814	0.14977
180	C10	DXX	-0.02820	0.00000	0.05733	0.00000	0.00000
181	C10	DYY	-0.07320	0.00000	-0.17575	0.00000	0.00000
182	C10	DZZ	0.15770	0.00000	0.15881	0.00000	0.00000
183	C10	DXY	0.10034	0.00000	-0.08802	0.00000	0.00000
184	C10	DXZ	0.00000	0.03829	0.00000	0.02338	0.00453
185	C10	DYZ	0.00000	-0.10893	0.00000	0.05550	-0.01943
186	H16	S	0.08362	0.00000	-0.03273	0.00000	0.00000
187	H16	S	-0.14356	0.00000	0.11290	0.00000	0.00000
188	H16	PX	-0.02601	0.00000	0.03284	0.00000	0.00000
189	H16	PY	-0.18871	0.00000	0.16849	0.00000	0.00000
190	H16	PZ	0.00000	0.24786	0.00000	-0.22432	-0.31538
191	H18	S	-0.00697	0.00000	0.08941	0.00000	0.00000
192	H18	S	0.05973	0.00000	-0.09598	0.00000	0.00000
193	H18	PX	-0.14273	0.00000	0.02530	0.00000	0.00000
194	H18	PY	0.16272	0.00000	-0.11685	0.00000	0.00000
195	H18	PZ	0.00000	0.31628	0.00000	-0.13005	-0.31650
196	C9	S	0.02489	0.00000	0.00610	0.00000	0.00000
197	C9	S	0.08755	0.00000	-0.04681	0.00000	0.00000
198	C9	PX	0.17154	0.00000	0.15952	0.00000	0.00000

199	C9	PY	-0.01904	0.00000	0.04090	0.00000	0.00000
200	C9	PZ	0.00000	0.00972	0.00000	-0.00857	0.01087
201	C9	S	-0.93982	0.00000	-0.46616	0.00000	0.00000
202	C9	PX	0.22460	0.00000	0.24329	0.00000	0.00000
203	C9	PY	0.57957	0.00000	0.08501	0.00000	0.00000
204	C9	PZ	0.00000	-0.04116	0.00000	0.09678	-0.23394
205	C9	DXX	-0.24458	0.00000	-0.20052	0.00000	0.00000
206	C9	DYY	0.29528	0.00000	0.11471	0.00000	0.00000
207	C9	DZZ	-0.04343	0.00000	0.04259	0.00000	0.00000
208	C9	DXY	-0.15204	0.00000	-0.10600	0.00000	0.00000
209	C9	DXZ	0.00000	0.03697	0.00000	0.00857	0.05574
210	C9	DYZ	0.00000	0.01229	0.00000	-0.02264	0.04609
211	H3	S	-0.19344	0.00000	-0.04263	0.00000	0.00000
212	H3	S	0.01556	0.00000	0.08985	0.00000	0.00000
213	H3	PX	-0.19985	0.00000	-0.07625	0.00000	0.00000
214	H3	PY	-0.16480	0.00000	-0.08351	0.00000	0.00000
215	H3	PZ	0.00000	0.03309	0.00000	-0.05598	0.15545
216	H5	S	0.19872	0.00828	0.02556	0.03507	-0.04690
217	H5	S	0.01156	-0.03278	0.02097	0.01084	-0.06438
218	H5	PX	0.05879	0.08230	-0.01623	0.00290	0.07258
219	H5	PY	0.06176	0.04914	-0.01132	0.01160	0.00930
220	H5	PZ	-0.02333	0.02661	-0.01770	-0.03492	0.08202
221	H7	S	0.19872	-0.00828	0.02556	-0.03507	0.04690
222	H7	S	0.01156	0.03278	0.02097	-0.01084	0.06438
223	H7	PX	0.05879	-0.08230	-0.01623	-0.00290	-0.07258
224	H7	PY	0.06176	-0.04914	-0.01132	-0.01160	-0.00930
225	H7	PZ	0.02333	0.02661	0.01770	-0.03492	0.08202

MO:	166	167	168	169	170
Eigenvalues:	2.63875	2.64334	2.68250	2.68802	2.72102
(ev):	71.80413	71.92893	72.99470	73.14466	74.04273

		A	A	A	A	A	
1	H1	S	-0.14924	0.00000	0.13262	0.00000	0.08486
2	H1	S	0.17018	0.00000	-0.17897	0.00000	-0.03949
3	H1	PX	-0.22235	0.00000	0.07119	0.00000	-0.05745
4	H1	PY	0.10714	0.00000	0.09716	0.00000	0.12680
5	H1	PZ	0.00000	0.30492	0.00000	-0.20333	0.00000
6	C1	S	-0.05104	0.00000	0.01956	0.00000	0.01887
7	C1	S	-0.32063	0.00000	-0.05381	0.00000	0.26443
8	C1	PX	-0.07723	0.00000	0.20744	0.00000	-0.03397
9	C1	PY	-0.07012	0.00000	-0.05720	0.00000	-0.02389
10	C1	PZ	0.00000	-0.02799	0.00000	0.06528	0.00000
11	C1	S	2.23251	0.00000	-0.25222	0.00000	-2.07409
12	C1	PX	-0.41051	0.00000	0.21248	0.00000	0.32965
13	C1	PY	-1.13182	0.00000	-0.11854	0.00000	0.41615
14	C1	PZ	0.00000	-0.07293	0.00000	0.09315	0.00000
15	C1	DXX	0.11500	0.00000	-0.18753	0.00000	0.03457
16	C1	DYY	0.23038	0.00000	-0.03232	0.00000	-0.15114
17	C1	DZZ	-0.48682	0.00000	0.23781	0.00000	0.08642
18	C1	DXY	0.19343	0.00000	-0.04993	0.00000	-0.16300
19	C1	DXZ	0.00000	-0.06832	0.00000	-0.08473	0.00000
20	C1	DYZ	0.00000	-0.22905	0.00000	0.40437	0.00000
21	C2	S	-0.02761	0.00000	-0.00403	0.00000	0.01439

22	C2	S	-0.47040	0.00000	-0.04239	0.00000	0.20073
23	C2	PX	-0.02065	0.00000	-0.01392	0.00000	-0.05085
24	C2	PY	-0.12064	0.00000	-0.04710	0.00000	-0.00999
25	C2	PZ	0.00000	-0.08702	0.00000	-0.08332	0.00000
26	C2	S	2.87479	0.00000	-0.18298	0.00000	-0.28693
27	C2	PX	1.81558	0.00000	0.22120	0.00000	-0.82916
28	C2	PY	0.09791	0.00000	-1.06185	0.00000	0.20218
29	C2	PZ	0.00000	-0.03660	0.00000	-0.08153	0.00000
30	C2	DXX	0.22666	0.00000	0.02224	0.00000	-0.13828
31	C2	DYY	-0.12347	0.00000	0.02439	0.00000	0.05089
32	C2	DZZ	-0.06869	0.00000	-0.05921	0.00000	0.16050
33	C2	DXY	-0.03014	0.00000	-0.19854	0.00000	-0.02590
34	C2	DXZ	0.00000	0.11545	0.00000	0.11734	0.00000
35	C2	DYZ	0.00000	-0.16367	0.00000	0.25426	0.00000
36	C3	S	0.00604	0.00000	0.01822	0.00000	0.03949
37	C3	S	-0.07608	0.00000	-0.01198	0.00000	0.25846
38	C3	PX	0.15784	0.00000	-0.06463	0.00000	0.03302
39	C3	PY	-0.26264	0.00000	0.25896	0.00000	0.00405
40	C3	PZ	0.00000	-0.01566	0.00000	0.04704	0.00000
41	C3	S	0.76007	0.00000	-1.06009	0.00000	-1.36385
42	C3	PX	-0.40299	0.00000	-0.95095	0.00000	0.63969
43	C3	PY	-2.26361	0.00000	0.65178	0.00000	1.79494
44	C3	PZ	0.00000	0.11125	0.00000	-0.04323	0.00000
45	C3	DXX	0.10363	0.00000	-0.17813	0.00000	-0.17806
46	C3	DYY	-0.05430	0.00000	-0.02132	0.00000	-0.06800
47	C3	DZZ	-0.00619	0.00000	0.09975	0.00000	0.33377
48	C3	DXY	-0.04476	0.00000	0.08159	0.00000	0.06575
49	C3	DXZ	0.00000	-0.03936	0.00000	-0.12205	0.00000
50	C3	DYZ	0.00000	-0.23928	0.00000	0.18733	0.00000
51	C4	S	0.00142	0.00000	-0.01332	0.00000	0.02317
52	C4	S	0.03633	0.00000	0.12678	0.00000	-0.04243
53	C4	PX	0.03573	0.00000	0.04412	0.00000	0.06990
54	C4	PY	0.18418	0.00000	-0.11876	0.00000	0.17040
55	C4	PZ	0.00000	-0.05000	0.00000	-0.03134	0.00000
56	C4	S	0.64653	0.00000	0.42131	0.00000	-0.47972
57	C4	PX	-0.44929	0.00000	0.09368	0.00000	1.20172
58	C4	PY	-0.02893	0.00000	0.28271	0.00000	-0.23529
59	C4	PZ	0.00000	-0.04868	0.00000	-0.00704	0.00000
60	C4	DXX	0.01234	0.00000	0.02515	0.00000	-0.25754
61	C4	DYY	-0.08401	0.00000	0.10946	0.00000	0.11950
62	C4	DZZ	0.11043	0.00000	-0.16939	0.00000	0.14605
63	C4	DXY	-0.04195	0.00000	-0.24880	0.00000	-0.13697
64	C4	DXZ	0.00000	-0.12393	0.00000	-0.35484	0.00000
65	C4	DYZ	0.00000	-0.53306	0.00000	0.24893	0.00000
66	C5	S	-0.00460	0.00000	-0.01163	0.00000	-0.02598
67	C5	S	0.28918	0.00000	-0.06498	0.00000	-0.05358
68	C5	PX	0.04655	0.00000	0.03314	0.00000	0.15723
69	C5	PY	-0.10567	0.00000	-0.02859	0.00000	-0.00918
70	C5	PZ	0.00000	-0.01345	0.00000	-0.08504	0.00000
71	C5	S	-1.60770	0.00000	0.96497	0.00000	1.13819
72	C5	PX	-0.82156	0.00000	-0.25632	0.00000	0.88849
73	C5	PY	0.78574	0.00000	-0.62294	0.00000	0.52199
74	C5	PZ	0.00000	-0.03629	0.00000	-0.02757	0.00000
75	C5	DXX	0.05608	0.00000	-0.06824	0.00000	0.28108

76	C5	DYY	0.00490	0.00000	0.16053	0.00000	-0.09308
77	C5	DZZ	-0.14136	0.00000	-0.06919	0.00000	-0.21549
78	C5	DXY	0.09306	0.00000	-0.10830	0.00000	0.05134
79	C5	DXZ	0.00000	-0.12295	0.00000	-0.00584	0.00000
80	C5	DYZ	0.00000	-0.33174	0.00000	-0.08729	0.00000
81	C6	S	-0.01313	0.00000	0.04470	0.00000	-0.04961
82	C6	S	0.05998	0.00000	0.33639	0.00000	-0.40267
83	C6	PX	-0.11010	0.00000	0.14018	0.00000	0.02945
84	C6	PY	-0.00566	0.00000	-0.13534	0.00000	0.22317
85	C6	PZ	0.00000	-0.02941	0.00000	-0.07389	0.00000
86	C6	S	-1.28132	0.00000	-1.04821	0.00000	1.57637
87	C6	PX	0.76188	0.00000	0.27191	0.00000	0.69872
88	C6	PY	-1.99094	0.00000	-0.26928	0.00000	0.63275
89	C6	PZ	0.00000	-0.08734	0.00000	-0.07413	0.00000
90	C6	DXX	-0.02752	0.00000	0.10272	0.00000	0.05399
91	C6	DYY	0.16585	0.00000	-0.28534	0.00000	0.13785
92	C6	DZZ	-0.29431	0.00000	0.22338	0.00000	-0.23484
93	C6	DXY	0.12397	0.00000	-0.02418	0.00000	0.07684
94	C6	DXZ	0.00000	-0.10512	0.00000	-0.20947	0.00000
95	C6	DYZ	0.00000	0.02227	0.00000	0.39000	0.00000
96	C7	S	0.07218	0.00000	0.00282	0.00000	0.04096
97	C7	S	0.57880	0.00000	0.05584	0.00000	0.17731
98	C7	PX	0.08099	0.00000	0.04343	0.00000	-0.04673
99	C7	PY	-0.08561	0.00000	0.23815	0.00000	0.27367
100	C7	PZ	0.00000	-0.04156	0.00000	0.04052	0.00000
101	C7	S	-3.42213	0.00000	-0.40277	0.00000	-0.15602
102	C7	PX	2.12006	0.00000	0.49660	0.00000	-0.25673
103	C7	PY	-0.06384	0.00000	1.67289	0.00000	0.76357
104	C7	PZ	0.00000	-0.07668	0.00000	0.09778	0.00000
105	C7	DXX	-0.37362	0.00000	-0.14035	0.00000	0.07530
106	C7	DYY	-0.13943	0.00000	0.16140	0.00000	-0.32310
107	C7	DZZ	0.63637	0.00000	-0.03972	0.00000	0.33386
108	C7	DXY	0.07297	0.00000	-0.43325	0.00000	-0.28744
109	C7	DXZ	0.00000	-0.04702	0.00000	0.11665	0.00000
110	C7	DYZ	0.00000	-0.10114	0.00000	0.18194	0.00000
111	O1	S	0.00396	0.00000	-0.01348	0.00000	0.00579
112	O1	S	0.21801	0.00000	-0.14725	0.00000	0.01844
113	O1	PX	-0.05255	0.00000	0.01676	0.00000	0.00782
114	O1	PY	-0.09748	0.00000	0.03256	0.00000	0.01979
115	O1	PZ	0.00000	-0.06755	0.00000	0.01081	0.00000
116	O1	S	-0.51523	0.00000	0.37501	0.00000	0.05813
117	O1	PX	0.12886	0.00000	0.25967	0.00000	-0.11999
118	O1	PY	0.29666	0.00000	0.25591	0.00000	0.11032
119	O1	PZ	0.00000	0.34653	0.00000	-0.13926	0.00000
120	O1	DXX	0.05416	0.00000	0.04834	0.00000	-0.09045
121	O1	DYY	-0.10359	0.00000	-0.01593	0.00000	-0.03865
122	O1	DZZ	0.11162	0.00000	-0.13310	0.00000	0.14483
123	O1	DXY	-0.06049	0.00000	0.09171	0.00000	0.06246
124	O1	DXZ	0.00000	0.17925	0.00000	-0.03752	0.00000
125	O1	DYZ	0.00000	-0.44969	0.00000	0.08086	0.00000
126	H4	S	-0.06487	0.00000	-0.09955	0.00000	-0.06343
127	H4	S	-0.29381	0.00000	0.11972	0.00000	0.01699
128	H4	PX	0.01704	0.00000	0.00199	0.00000	-0.00181
129	H4	PY	0.01877	0.00000	-0.04552	0.00000	-0.07542

130	H4	PZ	0.00000	0.28218	0.00000	0.20202	0.00000
131	N1	S	0.00589	0.00000	0.01500	0.00000	-0.03705
132	N1	S	0.13653	0.00000	0.42682	0.00000	-0.73216
133	N1	PX	0.04752	0.00000	0.00079	0.00000	-0.04921
134	N1	PY	-0.19050	0.00000	0.19563	0.00000	-0.10502
135	N1	PZ	0.00000	-0.00703	0.00000	0.00311	0.00000
136	N1	S	-1.05454	0.00000	-0.86186	0.00000	2.10120
137	N1	PX	-0.24644	0.00000	-0.39964	0.00000	0.61177
138	N1	PY	-0.41703	0.00000	-0.55387	0.00000	0.31358
139	N1	PZ	0.00000	0.11633	0.00000	0.24790	0.00000
140	N1	DXX	-0.13591	0.00000	-0.16483	0.00000	0.20405
141	N1	DYY	0.01071	0.00000	-0.04649	0.00000	0.18596
142	N1	DZZ	0.07763	0.00000	0.28965	0.00000	-0.47124
143	N1	DXY	-0.10138	0.00000	-0.20238	0.00000	-0.04406
144	N1	DXZ	0.00000	0.25405	0.00000	0.32234	0.00000
145	N1	DYZ	0.00000	-0.00142	0.00000	0.31278	0.00000
146	H6	S	-0.00405	0.00000	0.02674	0.00000	-0.02424
147	H6	S	0.49142	0.00000	-0.09020	0.00000	-0.27315
148	H6	PX	0.04529	0.00000	-0.11073	0.00000	-0.09522
149	H6	PY	0.03635	0.00000	0.25240	0.00000	-0.23252
150	H6	PZ	0.00000	0.23316	0.00000	0.42850	0.00000
151	C8	S	0.00858	0.00000	-0.02703	0.00000	-0.03281
152	C8	S	0.12079	0.00000	-0.15774	0.00000	-0.20266
153	C8	PX	-0.04929	0.00000	-0.01855	0.00000	0.33230
154	C8	PY	0.40261	0.00000	0.33305	0.00000	-0.09032
155	C8	PZ	0.00000	-0.05137	0.00000	-0.02677	0.00000
156	C8	S	0.39122	0.00000	0.25739	0.00000	0.74548
157	C8	PX	0.81962	0.00000	0.56298	0.00000	1.30470
158	C8	PY	0.81077	0.00000	2.45866	0.00000	-0.09003
159	C8	PZ	0.00000	-0.00452	0.00000	-0.09585	0.00000
160	C8	DXX	-0.12315	0.00000	0.12931	0.00000	0.13222
161	C8	DYY	-0.05151	0.00000	-0.07099	0.00000	0.16934
162	C8	DZZ	0.13088	0.00000	-0.15431	0.00000	-0.27216
163	C8	DXY	0.07945	0.00000	0.19001	0.00000	0.17152
164	C8	DXZ	0.00000	0.18136	0.00000	0.22077	0.00000
165	C8	DYZ	0.00000	-0.14356	0.00000	-0.00165	0.00000
166	H8	S	0.14771	0.00000	0.03308	0.00000	0.03559
167	H8	S	-0.71610	0.00000	-0.14237	0.00000	0.15455
168	H8	PX	0.20623	0.00000	-0.01919	0.00000	-0.04950
169	H8	PY	0.03466	0.00000	-0.37573	0.00000	-0.12159
170	H8	PZ	0.00000	0.17238	0.00000	-0.25378	0.00000
171	C10	S	-0.02802	0.00000	-0.04380	0.00000	0.01857
172	C10	S	-0.11720	0.00000	-0.15524	0.00000	0.05194
173	C10	PX	-0.03146	0.00000	-0.08944	0.00000	-0.05822
174	C10	PY	0.11568	0.00000	0.16529	0.00000	-0.15787
175	C10	PZ	0.00000	-0.06960	0.00000	-0.02820	0.00000
176	C10	S	0.80880	0.00000	2.20445	0.00000	-0.75442
177	C10	PX	-0.59340	0.00000	-0.54738	0.00000	-0.50763
178	C10	PY	0.39465	0.00000	1.12096	0.00000	-0.39679
179	C10	PZ	0.00000	-0.09301	0.00000	-0.02490	0.00000
180	C10	DXX	0.00529	0.00000	0.04142	0.00000	0.12211
181	C10	DYY	0.27170	0.00000	0.29455	0.00000	-0.25661
182	C10	DZZ	-0.34811	0.00000	-0.40138	0.00000	0.21332
183	C10	DXY	-0.16105	0.00000	-0.24052	0.00000	-0.14825

184	C10	DXZ	0.00000	0.02258	0.00000	0.07614	0.00000
185	C10	DYZ	0.00000	0.09388	0.00000	0.12312	0.00000
186	H16	S	-0.03304	0.00000	-0.16636	0.00000	0.01308
187	H16	S	0.25606	0.00000	0.33085	0.00000	0.31130
188	H16	PX	-0.09317	0.00000	-0.08921	0.00000	-0.00020
189	H16	PY	-0.01373	0.00000	0.01663	0.00000	0.14474
190	H16	PZ	0.00000	0.19526	0.00000	0.02656	0.00000
191	H18	S	-0.08098	0.00000	-0.05353	0.00000	0.03902
192	H18	S	-0.15393	0.00000	-0.06006	0.00000	-0.25063
193	H18	PX	0.10042	0.00000	0.13297	0.00000	-0.04485
194	H18	PY	-0.08774	0.00000	-0.19724	0.00000	-0.20917
195	H18	PZ	0.00000	0.29512	0.00000	0.25053	0.00000
196	C9	S	-0.01290	0.00000	0.01252	0.00000	0.00826
197	C9	S	-0.10022	0.00000	-0.02069	0.00000	0.10009
198	C9	PX	0.00534	0.00000	0.13067	0.00000	-0.00014
199	C9	PY	-0.01116	0.00000	0.06253	0.00000	-0.06443
200	C9	PZ	0.00000	0.01156	0.00000	0.00540	0.00000
201	C9	S	0.22477	0.00000	-0.46360	0.00000	-0.20327
202	C9	PX	0.02014	0.00000	0.32143	0.00000	0.06986
203	C9	PY	-0.23749	0.00000	-0.04788	0.00000	0.01571
204	C9	PZ	0.00000	-0.31913	0.00000	0.20859	0.00000
205	C9	DXX	-0.06720	0.00000	-0.16421	0.00000	-0.07310
206	C9	DYY	0.06906	0.00000	0.12307	0.00000	0.15025
207	C9	DZZ	-0.00813	0.00000	0.01978	0.00000	-0.06202
208	C9	DXY	0.07929	0.00000	-0.03301	0.00000	0.06600
209	C9	DXZ	0.00000	0.10823	0.00000	-0.13639	0.00000
210	C9	DYZ	0.00000	0.04881	0.00000	-0.03752	0.00000
211	H3	S	-0.01024	0.00000	0.00237	0.00000	-0.03275
212	H3	S	0.10631	0.00000	0.15298	0.00000	0.07882
213	H3	PX	-0.04606	0.00000	-0.19498	0.00000	-0.14386
214	H3	PY	-0.05582	0.00000	-0.06695	0.00000	-0.07490
215	H3	PZ	0.00000	0.20456	0.00000	-0.12716	0.00000
216	H5	S	-0.01327	-0.03353	0.00953	-0.01144	0.04356
217	H5	S	-0.06640	-0.11710	-0.01830	0.11902	-0.03369
218	H5	PX	0.04654	0.09335	-0.04326	-0.12657	0.03215
219	H5	PY	0.01741	-0.00093	0.07069	-0.03100	0.12317
220	H5	PZ	-0.00678	0.09797	-0.04663	-0.05415	-0.05403
221	H7	S	-0.01327	0.03353	0.00953	0.01144	0.04356
222	H7	S	-0.06640	0.11710	-0.01830	-0.11902	-0.03369
223	H7	PX	0.04654	-0.09335	-0.04326	0.12657	0.03215
224	H7	PY	0.01741	0.00093	0.07069	0.03100	0.12317
225	H7	PZ	0.00678	0.09797	0.04663	-0.05415	0.05403

MO:	171	172	173	174	175
Eigenvalues:	2.72457	2.73628	2.76280	2.80715	2.83712
(ev):	74.13948	74.45804	75.17970	76.38635	77.20205

		A	A	A	A	A	
1	H1	S	0.00000	-0.03202	0.02954	0.00000	-0.06280
2	H1	S	0.00000	0.00156	-0.50945	0.00000	0.20956
3	H1	PX	0.00000	0.04783	0.18170	0.00000	0.10954
4	H1	PY	0.00000	-0.15424	0.08144	0.00000	-0.48909
5	H1	PZ	0.24424	0.00000	0.00000	-0.18170	0.00000
6	C1	S	0.00000	-0.02350	-0.00929	0.00000	-0.01151

7	C1	S	0.00000	0.05420	0.18563	0.00000	-0.00423
8	C1	PX	0.00000	-0.14773	-0.00240	0.00000	-0.19002
9	C1	PY	0.00000	0.13470	0.08873	0.00000	0.30004
10	C1	PZ	0.00212	0.00000	0.00000	0.03895	0.00000
11	C1	S	0.00000	0.64513	0.55446	0.00000	0.85161
12	C1	PX	0.00000	-0.34011	0.71822	0.00000	-1.32114
13	C1	PY	0.00000	0.53171	0.28769	0.00000	2.79786
14	C1	PZ	-0.02864	0.00000	0.00000	0.05610	0.00000
15	C1	DXX	0.00000	0.10425	-0.14461	0.00000	0.33545
16	C1	DYY	0.00000	0.09540	0.25361	0.00000	-0.15321
17	C1	DZZ	0.00000	-0.24859	-0.05703	0.00000	-0.16911
18	C1	DXY	0.00000	-0.25706	-0.26850	0.00000	-0.39002
19	C1	DXZ	-0.21870	0.00000	0.00000	0.10843	0.00000
20	C1	DYZ	0.10417	0.00000	0.00000	0.00306	0.00000
21	C2	S	0.00000	0.02475	0.04131	0.00000	-0.01124
22	C2	S	0.00000	0.10944	0.07456	0.00000	-0.04604
23	C2	PX	0.00000	-0.10023	-0.07243	0.00000	0.07203
24	C2	PY	0.00000	-0.17426	-0.08908	0.00000	0.26546
25	C2	PZ	0.03235	0.00000	0.00000	-0.03412	0.00000
26	C2	S	0.00000	-1.20562	-1.54977	0.00000	0.70880
27	C2	PX	0.00000	0.23264	0.34094	0.00000	0.14700
28	C2	PY	0.00000	-0.91993	-0.41933	0.00000	1.11788
29	C2	PZ	0.06577	0.00000	0.00000	-0.04511	0.00000
30	C2	DXX	0.00000	-0.07528	-0.03956	0.00000	0.07450
31	C2	DYY	0.00000	-0.05156	-0.24349	0.00000	0.09753
32	C2	DZZ	0.00000	0.25390	0.36729	0.00000	-0.15119
33	C2	DXY	0.00000	-0.29742	-0.11310	0.00000	0.13241
34	C2	DXZ	-0.33076	0.00000	0.00000	0.06561	0.00000
35	C2	DYZ	-0.07171	0.00000	0.00000	-0.30907	0.00000
36	C3	S	0.00000	-0.02727	-0.01412	0.00000	-0.02697
37	C3	S	0.00000	-0.13934	-0.11295	0.00000	-0.21103
38	C3	PX	0.00000	-0.04052	-0.14851	0.00000	-0.06715
39	C3	PY	0.00000	-0.10936	0.05140	0.00000	0.16808
40	C3	PZ	-0.01167	0.00000	0.00000	0.05351	0.00000
41	C3	S	0.00000	-0.08358	1.90074	0.00000	1.85916
42	C3	PX	0.00000	-0.74275	-0.88551	0.00000	0.62386
43	C3	PY	0.00000	1.32344	-1.38554	0.00000	1.75498
44	C3	PZ	0.05074	0.00000	0.00000	-0.05292	0.00000
45	C3	DXX	0.00000	0.15657	0.09400	0.00000	-0.13141
46	C3	DYY	0.00000	0.00171	-0.04847	0.00000	0.23210
47	C3	DZZ	0.00000	-0.20623	-0.03054	0.00000	-0.14773
48	C3	DXY	0.00000	-0.11912	0.18635	0.00000	0.15537
49	C3	DXZ	-0.20842	0.00000	0.00000	-0.05943	0.00000
50	C3	DYZ	0.07498	0.00000	0.00000	-0.13482	0.00000
51	C4	S	0.00000	0.03290	-0.06013	0.00000	0.03631
52	C4	S	0.00000	0.33217	-0.60384	0.00000	0.08527
53	C4	PX	0.00000	-0.08737	-0.22642	0.00000	-0.21497
54	C4	PY	0.00000	0.38036	-0.03241	0.00000	0.23324
55	C4	PZ	-0.03100	0.00000	0.00000	0.01577	0.00000
56	C4	S	0.00000	-0.65901	2.92770	0.00000	-2.49233
57	C4	PX	0.00000	-0.50097	-2.04873	0.00000	-2.09860
58	C4	PY	0.00000	1.45941	-1.31032	0.00000	0.92642
59	C4	PZ	-0.01860	0.00000	0.00000	-0.01428	0.00000
60	C4	DXX	0.00000	-0.20028	0.02468	0.00000	-0.19133

61	C4	DYY	0.00000	-0.06990	0.21427	0.00000	-0.12260
62	C4	DZZ	0.00000	0.24094	-0.31603	0.00000	0.24312
63	C4	DXY	0.00000	0.03252	0.30431	0.00000	0.30642
64	C4	DXZ	-0.25491	0.00000	0.00000	-0.11961	0.00000
65	C4	DYZ	-0.03726	0.00000	0.00000	-0.07193	0.00000
66	C5	S	0.00000	-0.04030	0.04521	0.00000	0.03638
67	C5	S	0.00000	-0.21084	0.44754	0.00000	0.05789
68	C5	PX	0.00000	0.18071	-0.12854	0.00000	0.01961
69	C5	PY	0.00000	-0.17213	-0.21789	0.00000	0.14492
70	C5	PZ	0.04837	0.00000	0.00000	0.01247	0.00000
71	C5	S	0.00000	1.66548	-2.15379	0.00000	-2.10645
72	C5	PX	0.00000	-0.19692	-2.37672	0.00000	0.03375
73	C5	PY	0.00000	-1.35065	-0.87733	0.00000	0.28860
74	C5	PZ	0.04675	0.00000	0.00000	0.01067	0.00000
75	C5	DXX	0.00000	0.20904	-0.33938	0.00000	0.12127
76	C5	DYY	0.00000	0.10368	0.16261	0.00000	-0.34335
77	C5	DZZ	0.00000	-0.39440	0.25975	0.00000	0.26792
78	C5	DXY	0.00000	-0.20324	0.01946	0.00000	-0.08202
79	C5	DXZ	-0.34307	0.00000	0.00000	-0.08070	0.00000
80	C5	DYZ	0.12565	0.00000	0.00000	-0.34428	0.00000
81	C6	S	0.00000	0.02008	-0.00420	0.00000	0.00389
82	C6	S	0.00000	0.15749	-0.07795	0.00000	0.20742
83	C6	PX	0.00000	0.01939	-0.09810	0.00000	0.05354
84	C6	PY	0.00000	0.02363	0.05134	0.00000	-0.16354
85	C6	PZ	0.03512	0.00000	0.00000	0.00964	0.00000
86	C6	S	0.00000	-0.57155	-1.58051	0.00000	1.21707
87	C6	PX	0.00000	0.05705	-1.13788	0.00000	-0.51592
88	C6	PY	0.00000	-1.08016	0.55522	0.00000	-0.58361
89	C6	PZ	-0.07549	0.00000	0.00000	0.07183	0.00000
90	C6	DXX	0.00000	-0.18783	-0.31250	0.00000	0.14708
91	C6	DYY	0.00000	-0.00439	0.25373	0.00000	-0.06903
92	C6	DZZ	0.00000	0.12517	-0.07025	0.00000	-0.04002
93	C6	DXY	0.00000	-0.07515	-0.08929	0.00000	-0.12556
94	C6	DXZ	-0.23129	0.00000	0.00000	0.01485	0.00000
95	C6	DYZ	-0.02476	0.00000	0.00000	-0.33984	0.00000
96	C7	S	0.00000	-0.03493	0.02605	0.00000	-0.00262
97	C7	S	0.00000	-0.32525	0.27435	0.00000	0.06847
98	C7	PX	0.00000	0.02287	0.02441	0.00000	-0.04470
99	C7	PY	0.00000	-0.10532	0.06999	0.00000	0.04618
100	C7	PZ	0.01379	0.00000	0.00000	0.03920	0.00000
101	C7	S	0.00000	2.42661	-2.23153	0.00000	-0.48934
102	C7	PX	0.00000	-0.98616	1.40206	0.00000	0.13872
103	C7	PY	0.00000	0.12036	0.56375	0.00000	0.48171
104	C7	PZ	0.00697	0.00000	0.00000	0.08760	0.00000
105	C7	DXX	0.00000	0.07689	-0.11770	0.00000	-0.00924
106	C7	DYY	0.00000	0.06790	0.03921	0.00000	0.01752
107	C7	DZZ	0.00000	-0.21937	0.13702	0.00000	-0.05130
108	C7	DXY	0.00000	0.02817	-0.14487	0.00000	-0.24400
109	C7	DXZ	0.05669	0.00000	0.00000	0.34468	0.00000
110	C7	DYZ	0.24457	0.00000	0.00000	-0.07137	0.00000
111	O1	S	0.00000	0.02194	0.01727	0.00000	0.02824
112	O1	S	0.00000	0.53565	-0.17446	0.00000	0.30646
113	O1	PX	0.00000	-0.00918	0.06776	0.00000	-0.04668
114	O1	PY	0.00000	-0.10849	0.20512	0.00000	-0.02736

115	O1	PZ	-0.01000	0.00000	0.00000	-0.00850	0.00000
116	O1	S	0.00000	-1.64641	0.03466	0.00000	-0.98345
117	O1	PX	0.00000	-0.13464	-0.31818	0.00000	0.00884
118	O1	PY	0.00000	0.65495	-0.61625	0.00000	-0.11573
119	O1	PZ	0.01555	0.00000	0.00000	0.03009	0.00000
120	O1	DXX	0.00000	0.01535	-0.08720	0.00000	-0.09386
121	O1	DYY	0.00000	-0.17977	0.15051	0.00000	0.06142
122	O1	DZZ	0.00000	0.29923	-0.03710	0.00000	0.23449
123	O1	DXY	0.00000	-0.01022	-0.20107	0.00000	-0.23117
124	O1	DXZ	0.03725	0.00000	0.00000	0.01318	0.00000
125	O1	DYZ	-0.09501	0.00000	0.00000	-0.06104	0.00000
126	H4	S	0.00000	-0.15612	0.07252	0.00000	0.12674
127	H4	S	0.00000	0.32338	-0.30393	0.00000	0.01548
128	H4	PX	0.00000	0.43042	0.31976	0.00000	-0.01369
129	H4	PY	0.00000	0.05129	0.39808	0.00000	0.00158
130	H4	PZ	-0.50457	0.00000	0.00000	0.19821	0.00000
131	N1	S	0.00000	0.01698	-0.00843	0.00000	0.00922
132	N1	S	0.00000	0.27490	-0.31756	0.00000	0.22652
133	N1	PX	0.00000	-0.01719	-0.08036	0.00000	-0.00578
134	N1	PY	0.00000	-0.00268	-0.10145	0.00000	0.05430
135	N1	PZ	-0.00959	0.00000	0.00000	-0.02926	0.00000
136	N1	S	0.00000	-1.24880	1.03299	0.00000	-1.09906
137	N1	PX	0.00000	-0.27271	0.25991	0.00000	-0.00936
138	N1	PY	0.00000	-0.00376	0.27651	0.00000	-0.78233
139	N1	PZ	0.09513	0.00000	0.00000	-0.04251	0.00000
140	N1	DXX	0.00000	-0.18542	-0.19045	0.00000	0.13931
141	N1	DYY	0.00000	0.06451	0.19745	0.00000	-0.22378
142	N1	DZZ	0.00000	0.12701	-0.07207	0.00000	0.07601
143	N1	DXY	0.00000	0.10064	0.08085	0.00000	-0.17101
144	N1	DXZ	0.28997	0.00000	0.00000	0.09874	0.00000
145	N1	DYZ	-0.15797	0.00000	0.00000	-0.30169	0.00000
146	H6	S	0.00000	0.21095	0.21626	0.00000	-0.03527
147	H6	S	0.00000	-0.07820	0.04532	0.00000	0.19728
148	H6	PX	0.00000	-0.19877	-0.02737	0.00000	0.20792
149	H6	PY	0.00000	-0.01722	-0.08329	0.00000	-0.27043
150	H6	PZ	-0.51345	0.00000	0.00000	0.01502	0.00000
151	C8	S	0.00000	0.00245	-0.01772	0.00000	0.00119
152	C8	S	0.00000	0.19185	-0.11092	0.00000	-0.10254
153	C8	PX	0.00000	-0.18030	-0.02694	0.00000	0.09590
154	C8	PY	0.00000	0.02456	0.13345	0.00000	0.14770
155	C8	PZ	-0.02905	0.00000	0.00000	0.10048	0.00000
156	C8	S	0.00000	-0.46244	0.74863	0.00000	-0.34664
157	C8	PX	0.00000	-0.75020	0.73479	0.00000	0.24877
158	C8	PY	0.00000	-0.81819	1.26521	0.00000	1.61516
159	C8	PZ	-0.03917	0.00000	0.00000	-0.06547	0.00000
160	C8	DXX	0.00000	0.01337	0.12576	0.00000	0.07557
161	C8	DYY	0.00000	-0.01155	-0.01824	0.00000	-0.18858
162	C8	DZZ	0.00000	-0.01892	-0.06384	0.00000	0.08841
163	C8	DXY	0.00000	-0.06900	0.06215	0.00000	0.04859
164	C8	DXZ	0.30450	0.00000	0.00000	0.14943	0.00000
165	C8	DYZ	0.04007	0.00000	0.00000	-0.25336	0.00000
166	H8	S	0.00000	-0.07509	-0.01228	0.00000	-0.01123
167	H8	S	0.00000	0.24994	-0.37649	0.00000	0.03851
168	H8	PX	0.00000	-0.04238	0.08156	0.00000	-0.02931

169	H8	PY	0.00000	0.07120	-0.12719	0.00000	-0.02987
170	H8	PZ	-0.06342	0.00000	0.00000	-0.47328	0.00000
171	C10	S	0.00000	0.00036	-0.01271	0.00000	-0.01931
172	C10	S	0.00000	-0.02156	-0.03107	0.00000	0.00048
173	C10	PX	0.00000	0.05292	-0.02012	0.00000	-0.13213
174	C10	PY	0.00000	-0.01909	0.04483	0.00000	0.18096
175	C10	PZ	-0.01094	0.00000	0.00000	0.01985	0.00000
176	C10	S	0.00000	-0.31807	0.73668	0.00000	1.42042
177	C10	PX	0.00000	0.48475	-0.45814	0.00000	-0.39820
178	C10	PY	0.00000	-0.02156	0.35818	0.00000	0.61832
179	C10	PZ	-0.01261	0.00000	0.00000	0.08908	0.00000
180	C10	DXX	0.00000	-0.05351	0.02764	0.00000	0.05042
181	C10	DYY	0.00000	0.04764	0.07859	0.00000	0.10524
182	C10	DZZ	0.00000	0.00040	-0.11467	0.00000	-0.16841
183	C10	DXY	0.00000	0.13499	-0.02990	0.00000	-0.21872
184	C10	DXZ	0.17443	0.00000	0.00000	0.26941	0.00000
185	C10	DYZ	0.09094	0.00000	0.00000	-0.45213	0.00000
186	H16	S	0.00000	-0.00075	-0.00281	0.00000	-0.08574
187	H16	S	0.00000	-0.22007	0.19860	0.00000	0.23790
188	H16	PX	0.00000	0.03880	-0.03448	0.00000	-0.09834
189	H16	PY	0.00000	-0.09341	-0.07611	0.00000	0.09259
190	H16	PZ	-0.13607	0.00000	0.00000	-0.52364	0.00000
191	H18	S	0.00000	0.00658	-0.08708	0.00000	-0.00261
192	H18	S	0.00000	0.21246	-0.03441	0.00000	-0.14344
193	H18	PX	0.00000	-0.01621	0.01370	0.00000	0.09386
194	H18	PY	0.00000	0.12296	-0.02730	0.00000	-0.20708
195	H18	PZ	0.26500	0.00000	0.00000	-0.20233	0.00000
196	C9	S	0.00000	-0.00768	-0.02227	0.00000	-0.00958
197	C9	S	0.00000	0.01786	-0.00116	0.00000	0.06611
198	C9	PX	0.00000	-0.08499	-0.17147	0.00000	-0.18290
199	C9	PY	0.00000	-0.08806	-0.04673	0.00000	-0.11051
200	C9	PZ	-0.00073	0.00000	0.00000	0.00962	0.00000
201	C9	S	0.00000	0.26034	0.66881	0.00000	0.36019
202	C9	PX	0.00000	0.06704	-0.36853	0.00000	-0.38834
203	C9	PY	0.00000	-0.23356	-0.25567	0.00000	0.11448
204	C9	PZ	0.04538	0.00000	0.00000	-0.00709	0.00000
205	C9	DXX	0.00000	-0.08850	0.09436	0.00000	0.09518
206	C9	DYY	0.00000	0.14769	-0.07600	0.00000	-0.03265
207	C9	DZZ	0.00000	-0.04460	-0.02221	0.00000	0.00915
208	C9	DXY	0.00000	0.22744	-0.03312	0.00000	0.08010
209	C9	DXZ	-0.04949	0.00000	0.00000	-0.01121	0.00000
210	C9	DYZ	-0.02296	0.00000	0.00000	-0.00181	0.00000
211	H3	S	0.00000	-0.01827	-0.01078	0.00000	-0.03929
212	H3	S	0.00000	0.11701	-0.00932	0.00000	-0.15812
213	H3	PX	0.00000	-0.22010	0.21450	0.00000	0.15526
214	H3	PY	0.00000	-0.09291	0.06590	0.00000	0.06620
215	H3	PZ	-0.00803	0.00000	0.00000	-0.00125	0.00000
216	H5	S	-0.01467	0.00961	-0.05795	-0.00200	0.03291
217	H5	S	0.04232	-0.14947	0.04045	0.00283	-0.00550
218	H5	PX	-0.05009	0.06828	0.06834	-0.01717	0.14691
219	H5	PY	-0.02396	0.12915	0.01359	-0.00771	0.06521
220	H5	PZ	-0.00787	-0.03281	0.04439	0.00440	0.07029
221	H7	S	0.01467	0.00961	-0.05795	0.00200	0.03291
222	H7	S	-0.04232	-0.14947	0.04045	-0.00283	-0.00550

223	H7	PX	0.05009	0.06828	0.06834	0.01717	0.14691
224	H7	PY	0.02396	0.12915	0.01359	0.00771	0.06521
225	H7	PZ	-0.00787	0.03281	-0.04439	0.00440	-0.07029

MO:		176	177	178	179	180
Eigenvalues:		2.85185	2.85480	2.88036	2.90289	2.92225
(ev):		77.60292	77.68298	78.37870	78.99170	79.51862

		A	A	A	A	A	
1	H1	S	0.00000	-0.02579	0.00000	-0.05860	0.00125
2	H1	S	0.00000	0.20113	0.00000	0.06948	-0.01798
3	H1	PX	0.00000	-0.06758	0.00000	0.05083	-0.15170
4	H1	PY	0.00000	-0.12370	0.00000	-0.24263	0.08485
5	H1	PZ	-0.19835	0.00000	-0.47410	0.00000	0.00000
6	C1	S	0.00000	-0.00680	0.00000	0.01547	-0.02752
7	C1	S	0.00000	0.01509	0.00000	0.10653	-0.11683
8	C1	PX	0.00000	-0.11314	0.00000	-0.05382	-0.10914
9	C1	PY	0.00000	-0.06232	0.00000	0.08007	-0.05751
10	C1	PZ	0.02689	0.00000	0.02666	0.00000	0.00000
11	C1	S	0.00000	0.12138	0.00000	-1.19992	1.19608
12	C1	PX	0.00000	-0.85678	0.00000	-0.38895	0.19202
13	C1	PY	0.00000	1.74582	0.00000	2.55666	-1.51334
14	C1	PZ	0.09791	0.00000	0.07670	0.00000	0.00000
15	C1	DXX	0.00000	0.18366	0.00000	0.10111	0.04452
16	C1	DYY	0.00000	-0.12211	0.00000	-0.17908	0.09590
17	C1	DZZ	0.00000	-0.07680	0.00000	0.05458	-0.18541
18	C1	DXY	0.00000	-0.05263	0.00000	-0.07906	-0.02486
19	C1	DXZ	0.07471	0.00000	0.42482	0.00000	0.00000
20	C1	DYZ	0.14738	0.00000	-0.02643	0.00000	0.00000
21	C2	S	0.00000	-0.00472	0.00000	0.02982	-0.00031
22	C2	S	0.00000	-0.15250	0.00000	0.08110	-0.08028
23	C2	PX	0.00000	-0.03039	0.00000	-0.24491	0.03306
24	C2	PY	0.00000	-0.31259	0.00000	0.03415	0.17049
25	C2	PZ	-0.01230	0.00000	0.01059	0.00000	0.00000
26	C2	S	0.00000	-0.24168	0.00000	-0.34662	0.69318
27	C2	PX	0.00000	0.76218	0.00000	-0.95677	0.02939
28	C2	PY	0.00000	-3.16160	0.00000	0.13005	1.71444
29	C2	PZ	-0.05736	0.00000	0.01326	0.00000	0.00000
30	C2	DXX	0.00000	0.08494	0.00000	-0.25674	-0.04756
31	C2	DYY	0.00000	-0.19275	0.00000	0.06477	0.10443
32	C2	DZZ	0.00000	0.02553	0.00000	0.22614	-0.02895
33	C2	DXY	0.00000	-0.18388	0.00000	0.06696	0.25564
34	C2	DXZ	-0.00886	0.00000	-0.18071	0.00000	0.00000
35	C2	DYZ	-0.15624	0.00000	0.17096	0.00000	0.00000
36	C3	S	0.00000	0.03151	0.00000	-0.00332	0.03834
37	C3	S	0.00000	0.16185	0.00000	0.10813	0.14918
38	C3	PX	0.00000	0.08206	0.00000	0.02564	0.01485
39	C3	PY	0.00000	-0.06881	0.00000	-0.06122	-0.04287
40	C3	PZ	0.05072	0.00000	0.01453	0.00000	0.00000
41	C3	S	0.00000	-1.81454	0.00000	0.26316	-1.60599
42	C3	PX	0.00000	1.39810	0.00000	1.79603	-2.49757
43	C3	PY	0.00000	2.50947	0.00000	2.54958	-0.57723
44	C3	PZ	-0.04661	0.00000	-0.01754	0.00000	0.00000
45	C3	DXX	0.00000	-0.00636	0.00000	-0.14836	0.08086

46	C3	DYY	0.00000	-0.10407	0.00000	0.24121	-0.29761
47	C3	DZZ	0.00000	0.17753	0.00000	-0.04973	0.28449
48	C3	DXY	0.00000	-0.10077	0.00000	0.02757	0.29818
49	C3	DXZ	0.28833	0.00000	-0.20606	0.00000	0.00000
50	C3	DYZ	-0.09280	0.00000	-0.00504	0.00000	0.00000
51	C4	S	0.00000	0.00774	0.00000	0.05329	0.00386
52	C4	S	0.00000	0.08323	0.00000	-0.14079	0.25524
53	C4	PX	0.00000	-0.12082	0.00000	-0.08141	-0.04034
54	C4	PY	0.00000	0.01951	0.00000	-0.24859	0.21070
55	C4	PZ	0.00180	0.00000	0.08020	0.00000	0.00000
56	C4	S	0.00000	-0.80589	0.00000	-3.04476	0.19176
57	C4	PX	0.00000	-1.58567	0.00000	-0.63164	0.87690
58	C4	PY	0.00000	0.82713	0.00000	-0.47023	0.66033
59	C4	PZ	-0.12398	0.00000	-0.10878	0.00000	0.00000
60	C4	DXX	0.00000	0.22015	0.00000	-0.02251	-0.02138
61	C4	DYY	0.00000	-0.25727	0.00000	-0.27077	0.01359
62	C4	DZZ	0.00000	0.06337	0.00000	0.45339	-0.04567
63	C4	DXY	0.00000	0.08759	0.00000	-0.11411	0.07607
64	C4	DXZ	-0.28439	0.00000	0.14881	0.00000	0.00000
65	C4	DYZ	-0.26463	0.00000	-0.10240	0.00000	0.00000
66	C5	S	0.00000	-0.02906	0.00000	-0.02243	0.01889
67	C5	S	0.00000	-0.14838	0.00000	-0.08370	-0.00208
68	C5	PX	0.00000	-0.10594	0.00000	0.10687	0.00075
69	C5	PY	0.00000	-0.24912	0.00000	-0.07433	0.11854
70	C5	PZ	0.02823	0.00000	-0.02361	0.00000	0.00000
71	C5	S	0.00000	2.09808	0.00000	0.54125	-1.04411
72	C5	PX	0.00000	-1.26176	0.00000	0.78153	0.77038
73	C5	PY	0.00000	-2.09985	0.00000	0.09142	1.13619
74	C5	PZ	0.10768	0.00000	0.02439	0.00000	0.00000
75	C5	DXX	0.00000	-0.23223	0.00000	-0.09613	0.05486
76	C5	DYY	0.00000	0.44134	0.00000	0.13033	-0.18988
77	C5	DZZ	0.00000	-0.25170	0.00000	-0.15249	0.13105
78	C5	DXY	0.00000	0.02540	0.00000	-0.09769	-0.00667
79	C5	DXZ	-0.42214	0.00000	0.13305	0.00000	0.00000
80	C5	DYZ	0.02937	0.00000	0.09933	0.00000	0.00000
81	C6	S	0.00000	0.01189	0.00000	-0.06770	0.00919
82	C6	S	0.00000	0.00791	0.00000	-0.23606	0.12819
83	C6	PX	0.00000	0.02382	0.00000	-0.05915	-0.06712
84	C6	PY	0.00000	0.05413	0.00000	0.23845	0.10244
85	C6	PZ	-0.09556	0.00000	-0.01332	0.00000	0.00000
86	C6	S	0.00000	-0.20785	0.00000	2.85803	-0.59950
87	C6	PX	0.00000	3.20606	0.00000	1.22411	-1.76411
88	C6	PY	0.00000	-0.93276	0.00000	0.19443	-0.30772
89	C6	PZ	-0.03202	0.00000	-0.02224	0.00000	0.00000
90	C6	DXX	0.00000	0.12322	0.00000	0.07860	0.04800
91	C6	DYY	0.00000	-0.18870	0.00000	0.13715	-0.13982
92	C6	DZZ	0.00000	0.11491	0.00000	-0.40052	0.01064
93	C6	DXY	0.00000	0.15783	0.00000	-0.31926	-0.16323
94	C6	DXZ	0.23132	0.00000	-0.21717	0.00000	0.00000
95	C6	DYZ	0.43108	0.00000	0.13161	0.00000	0.00000
96	C7	S	0.00000	0.01913	0.00000	0.02368	0.00038
97	C7	S	0.00000	-0.00004	0.00000	0.01128	-0.00585
98	C7	PX	0.00000	-0.06660	0.00000	0.05158	-0.00226
99	C7	PY	0.00000	0.06327	0.00000	0.03130	0.30030

100	C7	PZ	-0.00919	0.00000	0.02365	0.00000	0.00000
101	C7	S	0.00000	0.86443	0.00000	0.32220	0.45703
102	C7	PX	0.00000	-0.80378	0.00000	-0.42867	0.55457
103	C7	PY	0.00000	0.33971	0.00000	-0.24302	1.77010
104	C7	PZ	0.03857	0.00000	0.01786	0.00000	0.00000
105	C7	DXX	0.00000	0.12226	0.00000	0.01614	0.01442
106	C7	DYY	0.00000	-0.24694	0.00000	-0.15747	0.11877
107	C7	DZZ	0.00000	0.15212	0.00000	0.18602	-0.04140
108	C7	DXY	0.00000	-0.09453	0.00000	0.01232	0.03234
109	C7	DXZ	0.20226	0.00000	0.04633	0.00000	0.00000
110	C7	DYZ	-0.22922	0.00000	0.08859	0.00000	0.00000
111	O1	S	0.00000	0.01548	0.00000	-0.04827	0.02877
112	O1	S	0.00000	0.26894	0.00000	-0.71403	0.53133
113	O1	PX	0.00000	0.00860	0.00000	-0.09597	-0.00538
114	O1	PY	0.00000	-0.06634	0.00000	-0.05995	-0.03172
115	O1	PZ	-0.03179	0.00000	-0.04117	0.00000	0.00000
116	O1	S	0.00000	-0.86704	0.00000	2.63501	-1.68810
117	O1	PX	0.00000	-0.14093	0.00000	0.75024	-0.27792
118	O1	PY	0.00000	-0.22522	0.00000	-0.64965	0.36923
119	O1	PZ	0.19369	0.00000	0.31405	0.00000	0.00000
120	O1	DXX	0.00000	0.10080	0.00000	0.11190	-0.03159
121	O1	DYY	0.00000	-0.01447	0.00000	0.13596	-0.09270
122	O1	DZZ	0.00000	0.09355	0.00000	-0.43195	0.28637
123	O1	DXY	0.00000	-0.33207	0.00000	-0.05288	-0.10348
124	O1	DXZ	0.14239	0.00000	0.33118	0.00000	0.00000
125	O1	DYZ	-0.17908	0.00000	0.19515	0.00000	0.00000
126	H4	S	0.00000	-0.08765	0.00000	-0.02581	0.04896
127	H4	S	0.00000	0.14752	0.00000	0.24942	-0.09222
128	H4	PX	0.00000	0.10868	0.00000	-0.07627	-0.15890
129	H4	PY	0.00000	-0.00322	0.00000	-0.32601	-0.11797
130	H4	PZ	-0.41136	0.00000	0.01925	0.00000	0.00000
131	N1	S	0.00000	-0.01167	0.00000	0.00255	0.02173
132	N1	S	0.00000	-0.08332	0.00000	0.13816	0.28309
133	N1	PX	0.00000	-0.03709	0.00000	0.00601	-0.01347
134	N1	PY	0.00000	0.08219	0.00000	-0.09597	0.12345
135	N1	PZ	0.03790	0.00000	0.00368	0.00000	0.00000
136	N1	S	0.00000	0.43242	0.00000	-0.97303	-1.10556
137	N1	PX	0.00000	-0.00468	0.00000	-0.73782	-0.28494
138	N1	PY	0.00000	-0.08063	0.00000	0.35219	-0.09713
139	N1	PZ	0.13188	0.00000	0.03398	0.00000	0.00000
140	N1	DXX	0.00000	0.09306	0.00000	-0.31642	-0.27747
141	N1	DYY	0.00000	0.02000	0.00000	0.20984	0.15442
142	N1	DZZ	0.00000	-0.09881	0.00000	0.02560	0.19200
143	N1	DXY	0.00000	-0.11645	0.00000	0.04102	0.22865
144	N1	DXZ	-0.02947	0.00000	0.05004	0.00000	0.00000
145	N1	DYZ	0.44553	0.00000	0.08683	0.00000	0.00000
146	H6	S	0.00000	-0.03500	0.00000	-0.01376	0.02275
147	H6	S	0.00000	-0.06557	0.00000	-0.42093	0.20389
148	H6	PX	0.00000	-0.17666	0.00000	-0.16988	0.12695
149	H6	PY	0.00000	0.54267	0.00000	-0.12683	-0.05779
150	H6	PZ	-0.01816	0.00000	-0.13574	0.00000	0.00000
151	C8	S	0.00000	-0.01593	0.00000	-0.00331	-0.06101
152	C8	S	0.00000	-0.02317	0.00000	0.16367	-0.17235
153	C8	PX	0.00000	0.13841	0.00000	-0.20059	-0.23946

154	C8	PY	0.00000	-0.11064	0.00000	0.22780	-0.09399
155	C8	PZ	0.03273	0.00000	-0.01532	0.00000	0.00000
156	C8	S	0.00000	0.34599	0.00000	-0.22664	2.53045
157	C8	PX	0.00000	0.65437	0.00000	-0.65600	0.40921
158	C8	PY	0.00000	-0.84105	0.00000	0.55991	0.60363
159	C8	PZ	-0.04393	0.00000	0.00015	0.00000	0.00000
160	C8	DXX	0.00000	0.00726	0.00000	0.17188	0.12753
161	C8	DYY	0.00000	0.15957	0.00000	-0.15573	0.31115
162	C8	DZZ	0.00000	-0.18499	0.00000	-0.01046	-0.45550
163	C8	DXY	0.00000	-0.00021	0.00000	0.20108	0.13517
164	C8	DXZ	-0.05983	0.00000	-0.01884	0.00000	0.00000
165	C8	DYZ	-0.06489	0.00000	0.07087	0.00000	0.00000
166	H8	S	0.00000	0.01615	0.00000	0.02424	-0.08909
167	H8	S	0.00000	0.30616	0.00000	0.13578	-0.20063
168	H8	PX	0.00000	-0.09163	0.00000	0.01386	-0.00566
169	H8	PY	0.00000	-0.05040	0.00000	-0.11165	-0.60407
170	H8	PZ	-0.24322	0.00000	-0.06633	0.00000	0.00000
171	C10	S	0.00000	0.01719	0.00000	-0.01296	0.00832
172	C10	S	0.00000	0.00250	0.00000	-0.00825	-0.07556
173	C10	PX	0.00000	-0.02770	0.00000	0.06885	0.18009
174	C10	PY	0.00000	-0.17444	0.00000	0.16980	-0.23307
175	C10	PZ	0.00253	0.00000	0.00365	0.00000	0.00000
176	C10	S	0.00000	-0.98273	0.00000	0.70710	-0.40717
177	C10	PX	0.00000	-0.14467	0.00000	0.08062	0.18263
178	C10	PY	0.00000	-0.52170	0.00000	0.50451	-0.08822
179	C10	PZ	0.02411	0.00000	-0.01079	0.00000	0.00000
180	C10	DXX	0.00000	0.05819	0.00000	-0.00836	-0.00548
181	C10	DYY	0.00000	-0.18231	0.00000	0.16861	-0.04494
182	C10	DZZ	0.00000	0.16546	0.00000	-0.13394	0.07352
183	C10	DXY	0.00000	-0.05554	0.00000	0.11776	0.23428
184	C10	DXZ	-0.28846	0.00000	0.17649	0.00000	0.00000
185	C10	DYZ	-0.15242	0.00000	0.12978	0.00000	0.00000
186	H16	S	0.00000	0.03040	0.00000	-0.01714	-0.00880
187	H16	S	0.00000	0.10064	0.00000	-0.04934	-0.09540
188	H16	PX	0.00000	0.01553	0.00000	-0.00038	0.16219
189	H16	PY	0.00000	0.12005	0.00000	-0.22690	-0.17551
190	H16	PZ	0.20861	0.00000	-0.11466	0.00000	0.00000
191	H18	S	0.00000	0.03873	0.00000	-0.06947	-0.03686
192	H18	S	0.00000	-0.17559	0.00000	0.21521	0.22852
193	H18	PX	0.00000	-0.06679	0.00000	0.09349	-0.09500
194	H18	PY	0.00000	-0.08355	0.00000	0.05695	0.22646
195	H18	PZ	-0.34460	0.00000	0.22244	0.00000	0.00000
196	C9	S	0.00000	-0.00856	0.00000	0.03176	-0.01661
197	C9	S	0.00000	0.10304	0.00000	0.00529	0.01416
198	C9	PX	0.00000	-0.21416	0.00000	0.24970	-0.18086
199	C9	PY	0.00000	-0.05340	0.00000	0.15194	-0.07672
200	C9	PZ	-0.01763	0.00000	-0.12769	0.00000	0.00000
201	C9	S	0.00000	0.31421	0.00000	-0.99123	0.45246
202	C9	PX	0.00000	-0.48354	0.00000	0.09080	-0.18902
203	C9	PY	0.00000	0.33737	0.00000	0.80396	-0.26390
204	C9	PZ	-0.17863	0.00000	-0.61639	0.00000	0.00000
205	C9	DXX	0.00000	0.14559	0.00000	0.13381	-0.02907
206	C9	DYY	0.00000	-0.25297	0.00000	-0.14398	-0.00911
207	C9	DZZ	0.00000	0.10042	0.00000	0.05981	0.03014

208	C9	DXY	0.00000	-0.08153	0.00000	-0.23536	0.08737
209	C9	DXZ	0.08762	0.00000	0.43439	0.00000	0.00000
210	C9	DYZ	-0.01716	0.00000	0.04108	0.00000	0.00000
211	H3	S	0.00000	-0.01234	0.00000	-0.00332	0.00218
212	H3	S	0.00000	-0.32981	0.00000	-0.30375	0.04931
213	H3	PX	0.00000	0.34019	0.00000	0.08002	0.07913
214	H3	PY	0.00000	0.13009	0.00000	0.11529	-0.01017
215	H3	PZ	0.12983	0.00000	0.38622	0.00000	0.00000
216	H5	S	0.00108	0.01314	0.03572	0.09777	-0.04116
217	H5	S	-0.08791	0.11899	-0.39100	0.19745	-0.03571
218	H5	PX	0.04817	0.13321	0.34104	-0.11942	0.13245
219	H5	PY	-0.03449	-0.10875	-0.01789	-0.18716	0.06037
220	H5	PZ	0.03520	0.18423	0.07121	0.01686	0.06999
221	H7	S	-0.00108	0.01314	-0.03572	0.09777	-0.04116
222	H7	S	0.08791	0.11899	0.39100	0.19745	-0.03571
223	H7	PX	-0.04817	0.13321	-0.34104	-0.11942	0.13245
224	H7	PY	0.03449	-0.10875	0.01789	-0.18716	0.06037
225	H7	PZ	0.03520	-0.18423	0.07121	-0.01686	-0.06999

MO:	181	182	183	184	185
Eigenvalues:	2.94553	2.94938	2.97878	3.01727	3.01793
(ev):	80.15209	80.25685	81.05685	82.10424	82.12217

		A	A	A	A	A	
1	H1	S	0.00000	-0.10624	0.00000	-0.09706	0.00000
2	H1	S	0.00000	0.05306	0.00000	-0.16669	0.00000
3	H1	PX	0.00000	-0.04889	0.00000	-0.15534	0.00000
4	H1	PY	0.00000	-0.14138	0.00000	0.37878	0.00000
5	H1	PZ	-0.30449	0.00000	-0.06437	0.00000	0.12034
6	C1	S	0.00000	-0.02180	0.00000	-0.04293	0.00000
7	C1	S	0.00000	-0.06441	0.00000	-0.01568	0.00000
8	C1	PX	0.00000	-0.13272	0.00000	-0.11929	0.00000
9	C1	PY	0.00000	-0.07582	0.00000	0.15184	0.00000
10	C1	PZ	0.00010	0.00000	-0.01609	0.00000	0.04020
11	C1	S	0.00000	1.09094	0.00000	0.97688	0.00000
12	C1	PX	0.00000	-0.46340	0.00000	0.98631	0.00000
13	C1	PY	0.00000	1.49613	0.00000	-1.88169	0.00000
14	C1	PZ	0.04819	0.00000	0.03091	0.00000	0.03282
15	C1	DXX	0.00000	0.12368	0.00000	0.10072	0.00000
16	C1	DYY	0.00000	0.03088	0.00000	0.07453	0.00000
17	C1	DZZ	0.00000	-0.17930	0.00000	-0.32900	0.00000
18	C1	DXY	0.00000	-0.05096	0.00000	-0.34579	0.00000
19	C1	DXZ	0.25809	0.00000	0.06739	0.00000	-0.27956
20	C1	DYZ	0.19486	0.00000	0.02565	0.00000	0.24097
21	C2	S	0.00000	0.00451	0.00000	-0.00986	0.00000
22	C2	S	0.00000	0.01171	0.00000	-0.06691	0.00000
23	C2	PX	0.00000	0.05798	0.00000	0.13268	0.00000
24	C2	PY	0.00000	0.06098	0.00000	-0.17526	0.00000
25	C2	PZ	-0.02602	0.00000	0.00966	0.00000	-0.00254
26	C2	S	0.00000	-0.34159	0.00000	0.74961	0.00000
27	C2	PX	0.00000	0.37661	0.00000	0.43237	0.00000
28	C2	PY	0.00000	-0.29825	0.00000	2.05918	0.00000
29	C2	PZ	0.04543	0.00000	-0.01976	0.00000	-0.08845
30	C2	DXX	0.00000	0.13370	0.00000	0.13494	0.00000

31	C2	DYY	0.00000	-0.09548	0.00000	-0.04420	0.00000
32	C2	DZZ	0.00000	0.00634	0.00000	-0.03559	0.00000
33	C2	DXY	0.00000	-0.11161	0.00000	-0.06360	0.00000
34	C2	DXZ	-0.28885	0.00000	0.08565	0.00000	0.38337
35	C2	DYZ	-0.41836	0.00000	-0.08317	0.00000	-0.17567
36	C3	S	0.00000	0.01521	0.00000	-0.05194	0.00000
37	C3	S	0.00000	-0.01264	0.00000	-0.38858	0.00000
38	C3	PX	0.00000	-0.00982	0.00000	-0.16624	0.00000
39	C3	PY	0.00000	-0.02702	0.00000	0.14373	0.00000
40	C3	PZ	0.00744	0.00000	0.02435	0.00000	0.01254
41	C3	S	0.00000	0.20949	0.00000	3.16397	0.00000
42	C3	PX	0.00000	-0.14282	0.00000	-3.93545	0.00000
43	C3	PY	0.00000	0.87176	0.00000	-2.62850	0.00000
44	C3	PZ	-0.05597	0.00000	-0.03368	0.00000	-0.05289
45	C3	DXX	0.00000	0.07350	0.00000	0.32230	0.00000
46	C3	DYY	0.00000	-0.15395	0.00000	-0.14792	0.00000
47	C3	DZZ	0.00000	0.14051	0.00000	-0.21449	0.00000
48	C3	DXY	0.00000	0.13006	0.00000	0.30821	0.00000
49	C3	DXZ	-0.03047	0.00000	0.21142	0.00000	0.06732
50	C3	DYZ	0.23334	0.00000	-0.02828	0.00000	0.15617
51	C4	S	0.00000	-0.00546	0.00000	0.06604	0.00000
52	C4	S	0.00000	0.00829	0.00000	-0.37607	0.00000
53	C4	PX	0.00000	-0.07542	0.00000	-0.09390	0.00000
54	C4	PY	0.00000	0.21648	0.00000	-0.06018	0.00000
55	C4	PZ	-0.01098	0.00000	-0.01363	0.00000	0.01775
56	C4	S	0.00000	0.01155	0.00000	-1.26053	0.00000
57	C4	PX	0.00000	-1.91096	0.00000	1.92200	0.00000
58	C4	PY	0.00000	0.53877	0.00000	-0.71607	0.00000
59	C4	PZ	-0.00781	0.00000	-0.03016	0.00000	-0.04189
60	C4	DXX	0.00000	0.06459	0.00000	-0.34138	0.00000
61	C4	DYY	0.00000	0.02657	0.00000	-0.13310	0.00000
62	C4	DZZ	0.00000	-0.04280	0.00000	0.55948	0.00000
63	C4	DXY	0.00000	0.17933	0.00000	-0.22992	0.00000
64	C4	DXZ	-0.08518	0.00000	-0.03129	0.00000	-0.34299
65	C4	DYZ	-0.15302	0.00000	-0.18367	0.00000	0.28841
66	C5	S	0.00000	0.02613	0.00000	-0.04418	0.00000
67	C5	S	0.00000	0.14533	0.00000	-0.01070	0.00000
68	C5	PX	0.00000	-0.04711	0.00000	0.15678	0.00000
69	C5	PY	0.00000	-0.05078	0.00000	0.09530	0.00000
70	C5	PZ	0.03885	0.00000	0.01496	0.00000	-0.00745
71	C5	S	0.00000	-1.19461	0.00000	0.09875	0.00000
72	C5	PX	0.00000	-1.03628	0.00000	1.43417	0.00000
73	C5	PY	0.00000	-0.66594	0.00000	1.46117	0.00000
74	C5	PZ	-0.04287	0.00000	0.02749	0.00000	0.06639
75	C5	DXX	0.00000	0.01063	0.00000	0.36470	0.00000
76	C5	DYY	0.00000	-0.11086	0.00000	-0.09003	0.00000
77	C5	DZZ	0.00000	0.15563	0.00000	-0.30433	0.00000
78	C5	DXY	0.00000	-0.09357	0.00000	0.21223	0.00000
79	C5	DXZ	0.05174	0.00000	-0.13095	0.00000	-0.26832
80	C5	DYZ	-0.47691	0.00000	0.03148	0.00000	-0.06755
81	C6	S	0.00000	0.01507	0.00000	0.09406	0.00000
82	C6	S	0.00000	0.02100	0.00000	0.53378	0.00000
83	C6	PX	0.00000	0.03549	0.00000	-0.04604	0.00000
84	C6	PY	0.00000	-0.11026	0.00000	-0.04343	0.00000

85	C6	PZ	0.03510	0.00000	-0.02517	0.00000	0.04503
86	C6	S	0.00000	-0.07221	0.00000	-3.87472	0.00000
87	C6	PX	0.00000	-0.04491	0.00000	-4.06144	0.00000
88	C6	PY	0.00000	-0.27124	0.00000	-1.30567	0.00000
89	C6	PZ	0.01778	0.00000	0.03615	0.00000	0.15046
90	C6	DXX	0.00000	0.03998	0.00000	-0.42004	0.00000
91	C6	DYY	0.00000	-0.08354	0.00000	-0.08734	0.00000
92	C6	DZZ	0.00000	0.07095	0.00000	0.50689	0.00000
93	C6	DXY	0.00000	0.01459	0.00000	0.05397	0.00000
94	C6	DXZ	0.14014	0.00000	0.22960	0.00000	0.19998
95	C6	DYZ	-0.09177	0.00000	0.07953	0.00000	-0.48265
96	C7	S	0.00000	0.00770	0.00000	-0.02306	0.00000
97	C7	S	0.00000	0.09074	0.00000	0.12381	0.00000
98	C7	PX	0.00000	-0.07908	0.00000	-0.02505	0.00000
99	C7	PY	0.00000	0.09637	0.00000	0.08347	0.00000
100	C7	PZ	0.01581	0.00000	0.00946	0.00000	0.00631
101	C7	S	0.00000	-0.34322	0.00000	-0.93374	0.00000
102	C7	PX	0.00000	0.15941	0.00000	1.47968	0.00000
103	C7	PY	0.00000	0.81974	0.00000	0.91055	0.00000
104	C7	PZ	0.00715	0.00000	-0.00084	0.00000	-0.00805
105	C7	DXX	0.00000	0.06292	0.00000	-0.07925	0.00000
106	C7	DYY	0.00000	-0.04187	0.00000	0.22083	0.00000
107	C7	DZZ	0.00000	0.01274	0.00000	-0.19546	0.00000
108	C7	DXY	0.00000	-0.03035	0.00000	-0.20135	0.00000
109	C7	DXZ	0.08545	0.00000	0.02060	0.00000	0.08527
110	C7	DYZ	0.21302	0.00000	-0.23470	0.00000	0.09122
111	O1	S	0.00000	-0.01636	0.00000	-0.01922	0.00000
112	O1	S	0.00000	-0.26086	0.00000	-0.47104	0.00000
113	O1	PX	0.00000	-0.12488	0.00000	-0.05475	0.00000
114	O1	PY	0.00000	-0.05306	0.00000	0.03378	0.00000
115	O1	PZ	-0.00183	0.00000	0.00443	0.00000	-0.02918
116	O1	S	0.00000	0.77164	0.00000	1.49566	0.00000
117	O1	PX	0.00000	0.78434	0.00000	0.09720	0.00000
118	O1	PY	0.00000	0.44875	0.00000	-0.76020	0.00000
119	O1	PZ	-0.00286	0.00000	-0.00590	0.00000	0.08473
120	O1	DXX	0.00000	0.29414	0.00000	-0.01142	0.00000
121	O1	DYY	0.00000	-0.37513	0.00000	0.24418	0.00000
122	O1	DZZ	0.00000	-0.10961	0.00000	-0.27604	0.00000
123	O1	DXY	0.00000	0.05906	0.00000	-0.19973	0.00000
124	O1	DXZ	-0.08683	0.00000	-0.08852	0.00000	0.23157
125	O1	DYZ	-0.18102	0.00000	-0.19829	0.00000	0.29123
126	H4	S	0.00000	0.02681	0.00000	-0.02515	0.00000
127	H4	S	0.00000	-0.00689	0.00000	-0.01673	0.00000
128	H4	PX	0.00000	0.23279	0.00000	-0.11097	0.00000
129	H4	PY	0.00000	0.24320	0.00000	-0.04395	0.00000
130	H4	PZ	0.35248	0.00000	-0.12281	0.00000	-0.14693
131	N1	S	0.00000	-0.00133	0.00000	0.01148	0.00000
132	N1	S	0.00000	-0.05055	0.00000	0.15339	0.00000
133	N1	PX	0.00000	-0.02529	0.00000	-0.07559	0.00000
134	N1	PY	0.00000	0.06200	0.00000	0.12618	0.00000
135	N1	PZ	0.00200	0.00000	-0.00503	0.00000	-0.03656
136	N1	S	0.00000	0.16185	0.00000	-0.72554	0.00000
137	N1	PX	0.00000	0.25376	0.00000	0.55895	0.00000
138	N1	PY	0.00000	-0.40143	0.00000	-0.51888	0.00000

139	N1	PZ	-0.08700	0.00000	-0.10471	0.00000	-0.21285
140	N1	DXX	0.00000	0.10064	0.00000	-0.03995	0.00000
141	N1	DYY	0.00000	-0.04845	0.00000	0.01406	0.00000
142	N1	DZZ	0.00000	-0.02268	0.00000	0.01759	0.00000
143	N1	DXY	0.00000	-0.10262	0.00000	0.19492	0.00000
144	N1	DXZ	-0.16035	0.00000	-0.37171	0.00000	-0.22486
145	N1	DYZ	-0.10318	0.00000	0.20450	0.00000	-0.37625
146	H6	S	0.00000	0.04632	0.00000	0.08616	0.00000
147	H6	S	0.00000	0.14018	0.00000	0.35422	0.00000
148	H6	PX	0.00000	0.10782	0.00000	0.06740	0.00000
149	H6	PY	0.00000	-0.12798	0.00000	-0.07620	0.00000
150	H6	PZ	-0.38872	0.00000	0.05253	0.00000	0.30712
151	C8	S	0.00000	-0.02164	0.00000	-0.02474	0.00000
152	C8	S	0.00000	-0.21555	0.00000	-0.11740	0.00000
153	C8	PX	0.00000	0.07314	0.00000	0.02169	0.00000
154	C8	PY	0.00000	-0.12389	0.00000	-0.01814	0.00000
155	C8	PZ	-0.04610	0.00000	-0.00050	0.00000	-0.01931
156	C8	S	0.00000	0.90457	0.00000	1.09164	0.00000
157	C8	PX	0.00000	0.87397	0.00000	0.41679	0.00000
158	C8	PY	0.00000	0.45515	0.00000	0.92350	0.00000
159	C8	PZ	0.04816	0.00000	0.05782	0.00000	0.04928
160	C8	DXX	0.00000	-0.02914	0.00000	0.07594	0.00000
161	C8	DYY	0.00000	0.15935	0.00000	0.04647	0.00000
162	C8	DZZ	0.00000	-0.14042	0.00000	-0.11470	0.00000
163	C8	DXY	0.00000	-0.03134	0.00000	-0.15164	0.00000
164	C8	DXZ	-0.02039	0.00000	-0.51511	0.00000	-0.07251
165	C8	DYZ	0.41800	0.00000	0.11580	0.00000	0.31202
166	H8	S	0.00000	-0.01623	0.00000	-0.12815	0.00000
167	H8	S	0.00000	0.02811	0.00000	-0.46917	0.00000
168	H8	PX	0.00000	-0.04862	0.00000	0.04954	0.00000
169	H8	PY	0.00000	-0.22640	0.00000	0.04697	0.00000
170	H8	PZ	-0.07447	0.00000	-0.04301	0.00000	-0.06336
171	C10	S	0.00000	0.00519	0.00000	-0.00074	0.00000
172	C10	S	0.00000	-0.01553	0.00000	0.01076	0.00000
173	C10	PX	0.00000	-0.02835	0.00000	-0.07265	0.00000
174	C10	PY	0.00000	-0.13020	0.00000	-0.08254	0.00000
175	C10	PZ	0.03590	0.00000	0.01700	0.00000	0.03257
176	C10	S	0.00000	-0.12554	0.00000	0.28854	0.00000
177	C10	PX	0.00000	-0.28942	0.00000	-0.11912	0.00000
178	C10	PY	0.00000	-0.17827	0.00000	0.04894	0.00000
179	C10	PZ	-0.02839	0.00000	-0.02068	0.00000	-0.01013
180	C10	DXX	0.00000	0.02319	0.00000	0.01361	0.00000
181	C10	DYY	0.00000	-0.09123	0.00000	-0.04103	0.00000
182	C10	DZZ	0.00000	0.05988	0.00000	0.01021	0.00000
183	C10	DXY	0.00000	-0.04223	0.00000	-0.07777	0.00000
184	C10	DXZ	-0.25251	0.00000	0.57136	0.00000	-0.07934
185	C10	DYZ	0.36318	0.00000	0.31106	0.00000	0.26569
186	H16	S	0.00000	0.01623	0.00000	-0.02735	0.00000
187	H16	S	0.00000	0.12995	0.00000	0.08198	0.00000
188	H16	PX	0.00000	0.01338	0.00000	0.00248	0.00000
189	H16	PY	0.00000	0.08642	0.00000	0.10939	0.00000
190	H16	PZ	0.32310	0.00000	-0.38499	0.00000	0.12365
191	H18	S	0.00000	-0.00825	0.00000	0.00264	0.00000
192	H18	S	0.00000	-0.15139	0.00000	-0.07729	0.00000

193	H18	PX	0.00000	-0.07553	0.00000	-0.07565	0.00000
194	H18	PY	0.00000	-0.02156	0.00000	-0.05673	0.00000
195	H18	PZ	0.05405	0.00000	0.56250	0.00000	0.09414
196	C9	S	0.00000	0.00945	0.00000	0.01074	0.00000
197	C9	S	0.00000	0.01743	0.00000	-0.02689	0.00000
198	C9	PX	0.00000	0.28896	0.00000	0.02222	0.00000
199	C9	PY	0.00000	0.06940	0.00000	0.10882	0.00000
200	C9	PZ	0.06743	0.00000	0.06276	0.00000	-0.14409
201	C9	S	0.00000	-0.64212	0.00000	-0.23756	0.00000
202	C9	PX	0.00000	0.48525	0.00000	-0.07699	0.00000
203	C9	PY	0.00000	0.75740	0.00000	0.25224	0.00000
204	C9	PZ	0.12664	0.00000	0.14650	0.00000	-0.33854
205	C9	DXX	0.00000	0.13297	0.00000	0.21363	0.00000
206	C9	DYY	0.00000	-0.17627	0.00000	-0.07714	0.00000
207	C9	DZZ	0.00000	-0.02910	0.00000	-0.06668	0.00000
208	C9	DXY	0.00000	0.19488	0.00000	-0.19524	0.00000
209	C9	DXZ	-0.10720	0.00000	-0.10646	0.00000	0.17919
210	C9	DYZ	0.00579	0.00000	-0.00121	0.00000	-0.09657
211	H3	S	0.00000	0.04195	0.00000	-0.02805	0.00000
212	H3	S	0.00000	-0.31088	0.00000	-0.11035	0.00000
213	H3	PX	0.00000	-0.37549	0.00000	0.11509	0.00000
214	H3	PY	0.00000	-0.06509	0.00000	0.10662	0.00000
215	H3	PZ	-0.10582	0.00000	-0.10356	0.00000	0.30184
216	H5	S	-0.00499	0.10071	-0.00252	0.02830	-0.00733
217	H5	S	0.09514	-0.00706	0.10458	0.11632	-0.22112
218	H5	PX	-0.10242	-0.27172	-0.10129	-0.07685	0.17630
219	H5	PY	0.01457	-0.46724	0.01417	-0.05640	-0.10423
220	H5	PZ	0.00390	-0.06996	0.00290	-0.00132	-0.00312
221	H7	S	0.00499	0.10071	0.00252	0.02830	0.00733
222	H7	S	-0.09514	-0.00706	-0.10458	0.11632	0.22112
223	H7	PX	0.10242	-0.27172	0.10129	-0.07685	-0.17630
224	H7	PY	-0.01457	-0.46724	-0.01417	-0.05640	0.10423
225	H7	PZ	0.00390	0.06996	0.00290	0.00132	-0.00312

MO:	186	187	188	189	190
Eigenvalues:	3.04983	3.05511	3.06524	3.07307	3.11348
(ev):	82.99007	83.13370	83.40947	83.62244	84.72227

		A	A	A	A	A	
1	H1	S	0.02461	-0.05763	0.02825	0.00000	0.00000
2	H1	S	-0.06801	-0.16967	0.04274	0.00000	0.00000
3	H1	PX	-0.16996	-0.04958	-0.01648	0.00000	0.00000
4	H1	PY	0.37088	-0.22089	-0.00725	0.00000	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.06853	-0.37760
6	C1	S	0.02807	0.02481	-0.02903	0.00000	0.00000
7	C1	S	0.01190	0.05975	-0.15517	0.00000	0.00000
8	C1	PX	0.08451	-0.00285	0.04147	0.00000	0.00000
9	C1	PY	-0.11395	-0.03502	-0.12089	0.00000	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	-0.00103	-0.06246
11	C1	S	-1.66109	-0.99646	1.37446	0.00000	0.00000
12	C1	PX	1.13983	0.67624	-0.60776	0.00000	0.00000
13	C1	PY	-1.64554	0.47776	0.25580	0.00000	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.01674	0.09695
15	C1	DXX	0.00777	-0.05501	-0.12569	0.00000	0.00000

16	C1	DYY	-0.24396	-0.15170	0.19792	0.00000	0.00000
17	C1	DZZ	0.19377	0.15923	-0.15077	0.00000	0.00000
18	C1	DXY	0.02343	0.21949	0.06493	0.00000	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.02759	0.46115
20	C1	DYZ	0.00000	0.00000	0.00000	-0.37364	0.11814
21	C2	S	0.03214	0.04401	-0.00581	0.00000	0.00000
22	C2	S	0.20701	0.10292	0.06712	0.00000	0.00000
23	C2	PX	-0.05991	0.01529	-0.03664	0.00000	0.00000
24	C2	PY	0.01354	-0.16179	0.16649	0.00000	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.02534	0.04513
26	C2	S	-1.74125	-1.98168	0.66335	0.00000	0.00000
27	C2	PX	-1.39518	-0.66688	0.16521	0.00000	0.00000
28	C2	PY	0.82608	-0.52744	0.33885	0.00000	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	-0.02425	-0.08025
30	C2	DXX	0.02081	0.21234	0.06205	0.00000	0.00000
31	C2	DYY	-0.18808	-0.50465	0.13564	0.00000	0.00000
32	C2	DZZ	0.17191	0.28298	-0.07834	0.00000	0.00000
33	C2	DXY	-0.01117	-0.14704	-0.18412	0.00000	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.09946	0.35805
35	C2	DYZ	0.00000	0.00000	0.00000	0.25939	0.16783
36	C3	S	-0.00248	-0.00351	0.03346	0.00000	0.00000
37	C3	S	0.04305	0.00525	0.07911	0.00000	0.00000
38	C3	PX	-0.02884	0.07070	0.02066	0.00000	0.00000
39	C3	PY	0.14112	-0.10573	-0.04357	0.00000	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.06528	-0.00518
41	C3	S	-1.15054	-0.06232	-1.13603	0.00000	0.00000
42	C3	PX	-1.60069	-1.22803	1.10340	0.00000	0.00000
43	C3	PY	0.28963	1.43577	-0.30214	0.00000	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	-0.02165	-0.10886
45	C3	DXX	0.08556	0.05003	-0.14114	0.00000	0.00000
46	C3	DYY	-0.08105	0.05493	-0.06650	0.00000	0.00000
47	C3	DZZ	-0.01357	-0.03626	0.19326	0.00000	0.00000
48	C3	DXY	0.13323	0.15912	-0.18308	0.00000	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	-0.08793	-0.21080
50	C3	DYZ	0.00000	0.00000	0.00000	-0.48933	0.33871
51	C4	S	-0.02370	0.03154	0.00012	0.00000	0.00000
52	C4	S	0.30033	-0.03043	-0.10749	0.00000	0.00000
53	C4	PX	0.09470	0.20865	-0.00775	0.00000	0.00000
54	C4	PY	0.22918	-0.31733	-0.06606	0.00000	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.01245	0.02027
56	C4	S	1.34063	-0.43817	-0.33023	0.00000	0.00000
57	C4	PX	2.47524	-0.11155	-1.15733	0.00000	0.00000
58	C4	PY	0.56022	-0.25486	-0.25557	0.00000	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	-0.00104	-0.13115
60	C4	DXX	-0.00802	0.21527	0.07480	0.00000	0.00000
61	C4	DYY	0.20927	-0.33006	-0.04783	0.00000	0.00000
62	C4	DZZ	-0.26419	0.23290	0.05161	0.00000	0.00000
63	C4	DXY	-0.32086	-0.17033	-0.17252	0.00000	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.23896	0.06414
65	C4	DYZ	0.00000	0.00000	0.00000	-0.11369	-0.47366
66	C5	S	-0.01414	-0.01792	0.02990	0.00000	0.00000
67	C5	S	-0.14468	0.01344	0.14441	0.00000	0.00000
68	C5	PX	0.02340	-0.09066	0.10475	0.00000	0.00000
69	C5	PY	-0.13987	-0.26888	0.01418	0.00000	0.00000

70	C5	PZ	0.00000	0.00000	0.00000	-0.01844	-0.02997
71	C5	S	1.61399	1.28942	-1.63740	0.00000	0.00000
72	C5	PX	1.47683	0.06075	-0.41987	0.00000	0.00000
73	C5	PY	0.25788	-0.92087	0.23124	0.00000	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.01581	0.08693
75	C5	DXX	0.16883	0.10172	0.04185	0.00000	0.00000
76	C5	DYY	-0.00445	0.18131	-0.23411	0.00000	0.00000
77	C5	DZZ	-0.07381	-0.16138	0.20290	0.00000	0.00000
78	C5	DXY	-0.01662	0.11678	-0.26150	0.00000	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.06570	-0.19574
80	C5	DYZ	0.00000	0.00000	0.00000	0.27606	0.33410
81	C6	S	0.00206	0.02740	-0.03400	0.00000	0.00000
82	C6	S	-0.21595	-0.17599	0.09616	0.00000	0.00000
83	C6	PX	-0.05536	-0.02014	0.16063	0.00000	0.00000
84	C6	PY	0.05830	0.17198	-0.35123	0.00000	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00722	0.01910
86	C6	S	0.23245	-0.41966	2.24589	0.00000	0.00000
87	C6	PX	-1.72500	-0.77896	0.75456	0.00000	0.00000
88	C6	PY	1.09928	0.09430	-0.39517	0.00000	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.05113	0.12980
90	C6	DXX	0.03295	0.15193	0.06915	0.00000	0.00000
91	C6	DYY	-0.00623	-0.27397	0.18647	0.00000	0.00000
92	C6	DZZ	0.05372	0.24359	-0.29637	0.00000	0.00000
93	C6	DXY	-0.22948	-0.20080	0.14168	0.00000	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	-0.20846	-0.02731
95	C6	DYZ	0.00000	0.00000	0.00000	-0.10152	-0.36184
96	C7	S	-0.04790	-0.00728	0.00321	0.00000	0.00000
97	C7	S	-0.22038	-0.04888	0.00320	0.00000	0.00000
98	C7	PX	-0.13216	0.03676	0.04192	0.00000	0.00000
99	C7	PY	0.05248	-0.02441	-0.00730	0.00000	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	-0.04450	0.04515
101	C7	S	2.47411	1.21218	-0.31117	0.00000	0.00000
102	C7	PX	-1.09525	-0.61773	-0.03725	0.00000	0.00000
103	C7	PY	0.39425	1.17450	-0.36658	0.00000	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.01284	0.03302
105	C7	DXX	0.02377	0.03127	-0.01691	0.00000	0.00000
106	C7	DYY	0.17668	0.10485	0.01641	0.00000	0.00000
107	C7	DZZ	-0.24629	-0.02930	-0.00290	0.00000	0.00000
108	C7	DXY	0.02474	0.26707	-0.04477	0.00000	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.63885	-0.24954
110	C7	DYZ	0.00000	0.00000	0.00000	-0.06660	0.25577
111	O1	S	0.01172	-0.03303	-0.03840	0.00000	0.00000
112	O1	S	0.33916	-0.23000	-0.43793	0.00000	0.00000
113	O1	PX	0.01398	0.04074	-0.00709	0.00000	0.00000
114	O1	PY	0.02300	-0.09240	0.01231	0.00000	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.01683	0.00340
116	O1	S	-1.08795	0.99106	1.48115	0.00000	0.00000
117	O1	PX	0.05752	0.04177	0.89276	0.00000	0.00000
118	O1	PY	0.72743	-0.30972	0.07079	0.00000	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	-0.03607	0.09853
120	O1	DXX	0.35148	-0.06230	0.39229	0.00000	0.00000
121	O1	DYY	-0.40844	0.23941	-0.04378	0.00000	0.00000
122	O1	DZZ	0.09456	-0.25540	-0.44027	0.00000	0.00000
123	O1	DXY	-0.02159	0.14689	0.22658	0.00000	0.00000

124	O1	DXZ	0.00000	0.00000	0.00000	-0.07896	-0.07438
125	O1	DYZ	0.00000	0.00000	0.00000	-0.09081	-0.35774
126	H4	S	0.00217	0.01961	-0.01157	0.00000	0.00000
127	H4	S	0.24148	0.17228	0.06761	0.00000	0.00000
128	H4	PX	0.05666	0.16967	0.18728	0.00000	0.00000
129	H4	PY	-0.03329	0.17368	0.03567	0.00000	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	-0.12174	-0.31742
131	N1	S	-0.02287	-0.04662	0.04143	0.00000	0.00000
132	N1	S	-0.31827	-0.33974	0.39955	0.00000	0.00000
133	N1	PX	0.03899	0.07379	-0.00515	0.00000	0.00000
134	N1	PY	0.02596	0.17500	-0.13874	0.00000	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	-0.01430	-0.02621
136	N1	S	1.68648	2.23953	-2.24460	0.00000	0.00000
137	N1	PX	0.82885	1.19929	-0.74519	0.00000	0.00000
138	N1	PY	0.08233	-0.38114	-0.47734	0.00000	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	-0.06192	-0.10480
140	N1	DXX	0.23408	0.28413	-0.06230	0.00000	0.00000
141	N1	DYY	0.03386	0.17584	-0.32902	0.00000	0.00000
142	N1	DZZ	-0.19472	-0.37005	0.34430	0.00000	0.00000
143	N1	DXY	-0.08055	-0.33816	-0.07540	0.00000	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	-0.04851	0.03269
145	N1	DYZ	0.00000	0.00000	0.00000	-0.14489	-0.29961
146	H6	S	-0.05917	-0.02137	0.01090	0.00000	0.00000
147	H6	S	-0.25836	-0.08523	-0.02263	0.00000	0.00000
148	H6	PX	0.03664	0.13473	-0.02563	0.00000	0.00000
149	H6	PY	-0.25357	-0.15982	-0.29716	0.00000	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.14144	0.31971
151	C8	S	0.06846	0.03396	-0.05097	0.00000	0.00000
152	C8	S	-0.05560	-0.36532	0.09592	0.00000	0.00000
153	C8	PX	0.08569	0.14607	-0.07326	0.00000	0.00000
154	C8	PY	0.00204	-0.17143	-0.00001	0.00000	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	-0.01565	-0.00518
156	C8	S	-2.91273	-0.94441	1.98405	0.00000	0.00000
157	C8	PX	-0.01211	1.62555	-0.45817	0.00000	0.00000
158	C8	PY	0.11526	-0.21848	-0.81615	0.00000	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	-0.01442	0.01630
160	C8	DXX	-0.05445	-0.40432	-0.07811	0.00000	0.00000
161	C8	DYY	-0.29640	0.18325	0.24622	0.00000	0.00000
162	C8	DZZ	0.48744	0.29165	-0.37200	0.00000	0.00000
163	C8	DXY	0.11011	0.04530	-0.19987	0.00000	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.03313	0.11228
165	C8	DYZ	0.00000	0.00000	0.00000	0.45204	-0.04023
166	H8	S	0.03727	0.02876	0.00501	0.00000	0.00000
167	H8	S	0.24040	0.11051	0.03140	0.00000	0.00000
168	H8	PX	-0.10473	0.09970	0.03579	0.00000	0.00000
169	H8	PY	-0.00670	-0.37004	0.08641	0.00000	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	-0.50780	0.17888
171	C10	S	-0.02080	-0.01092	0.01616	0.00000	0.00000
172	C10	S	-0.04683	-0.01498	0.07040	0.00000	0.00000
173	C10	PX	-0.06770	-0.00780	0.03950	0.00000	0.00000
174	C10	PY	0.30477	-0.02708	-0.27800	0.00000	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.05310	-0.00780
176	C10	S	1.14471	-0.03790	-1.26441	0.00000	0.00000
177	C10	PX	-0.01293	-0.34999	0.36164	0.00000	0.00000

178	C10	PY	0.74790	-0.12700	-0.79892	0.00000	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.01121	-0.00570
180	C10	DXX	0.00735	-0.10477	-0.08644	0.00000	0.00000
181	C10	DYY	0.14041	0.05286	-0.06911	0.00000	0.00000
182	C10	DZZ	-0.16306	-0.06008	0.13172	0.00000	0.00000
183	C10	DXY	-0.00634	-0.01294	-0.04917	0.00000	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	-0.18740	-0.06045
185	C10	DYZ	0.00000	0.00000	0.00000	0.32647	-0.06093
186	H16	S	-0.04883	0.04509	0.01668	0.00000	0.00000
187	H16	S	0.03600	0.08121	-0.18026	0.00000	0.00000
188	H16	PX	-0.14986	-0.00179	0.16521	0.00000	0.00000
189	H16	PY	-0.16523	0.03198	0.25704	0.00000	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.20033	0.03315
191	H18	S	-0.02203	-0.02373	0.09250	0.00000	0.00000
192	H18	S	0.17531	-0.10743	-0.13803	0.00000	0.00000
193	H18	PX	0.19158	-0.07516	-0.21730	0.00000	0.00000
194	H18	PY	-0.03771	0.14229	0.06485	0.00000	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.03943	-0.06020
196	C9	S	0.01651	0.01599	0.03379	0.00000	0.00000
197	C9	S	0.01946	-0.09438	-0.36275	0.00000	0.00000
198	C9	PX	-0.02835	0.08498	0.34259	0.00000	0.00000
199	C9	PY	0.03935	0.06692	0.21129	0.00000	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.05065	0.10837
201	C9	S	-0.44751	-0.23999	-0.87462	0.00000	0.00000
202	C9	PX	-0.06127	0.06635	0.10983	0.00000	0.00000
203	C9	PY	0.44322	-0.21460	0.05813	0.00000	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.14492	0.13979
205	C9	DXX	-0.26155	-0.01188	-0.41210	0.00000	0.00000
206	C9	DYY	-0.16181	0.13726	0.07421	0.00000	0.00000
207	C9	DZZ	0.33374	-0.05633	0.37831	0.00000	0.00000
208	C9	DXY	0.01530	-0.26328	-0.35548	0.00000	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	-0.04265	-0.05065
210	C9	DYZ	0.00000	0.00000	0.00000	0.08725	0.07175
211	H3	S	0.03040	-0.01525	0.01902	0.00000	0.00000
212	H3	S	-0.22456	0.18883	0.11626	0.00000	0.00000
213	H3	PX	0.04827	0.14965	0.19920	0.00000	0.00000
214	H3	PY	-0.02709	0.04293	-0.00967	0.00000	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	-0.15009	-0.15462
216	H5	S	0.04124	-0.01249	0.00129	0.00484	0.01741
217	H5	S	0.15965	0.00315	0.17074	0.09152	0.11078
218	H5	PX	0.20780	-0.05310	0.16102	-0.04907	-0.10140
219	H5	PY	-0.18707	0.23856	0.06481	0.06950	0.06901
220	H5	PZ	0.31495	-0.08472	0.17628	-0.00137	0.03463
221	H7	S	0.04124	-0.01249	0.00129	-0.00484	-0.01741
222	H7	S	0.15965	0.00315	0.17074	-0.09152	-0.11078
223	H7	PX	0.20780	-0.05310	0.16102	0.04907	0.10140
224	H7	PY	-0.18707	0.23856	0.06481	-0.06950	-0.06901
225	H7	PZ	-0.31495	0.08472	-0.17628	-0.00137	0.03463

MO:	191	192	193	194	195
Eigenvalues:	3.13185	3.15634	3.19293	3.20217	3.25015
(ev):	85.22204	85.88837	86.88420	87.13548	88.44107

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1	H1	S	-0.00388	0.03913	0.04692	0.00000	0.03307
2	H1	S	0.00207	0.00954	0.25529	0.00000	0.06769
3	H1	PX	-0.14110	-0.18187	-0.03400	0.00000	0.01418
4	H1	PY	0.15532	0.19337	0.17907	0.00000	-0.34834
5	H1	PZ	0.00000	0.00000	0.00000	-0.05135	0.00000
6	C1	S	-0.03690	0.03761	-0.08698	0.00000	-0.00627
7	C1	S	-0.03078	0.10998	-0.34813	0.00000	-0.13811
8	C1	PX	-0.10937	0.01718	-0.06223	0.00000	-0.06394
9	C1	PY	-0.15204	-0.06112	-0.01923	0.00000	0.06334
10	C1	PZ	0.00000	0.00000	0.00000	-0.03358	0.00000
11	C1	S	1.51080	-2.73604	3.31032	0.00000	-0.00980
12	C1	PX	-0.10765	1.01229	-1.54630	0.00000	-0.31360
13	C1	PY	-0.75837	-0.84329	-0.58870	0.00000	0.54341
14	C1	PZ	0.00000	0.00000	0.00000	0.01530	0.00000
15	C1	DXX	0.02943	0.05594	-0.01489	0.00000	-0.20744
16	C1	DYY	0.11487	-0.32986	0.44296	0.00000	0.23484
17	C1	DZZ	-0.19326	0.23169	-0.47632	0.00000	-0.04132
18	C1	DXY	-0.03671	0.03988	-0.24940	0.00000	0.23042
19	C1	DXZ	0.00000	0.00000	0.00000	0.10725	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.08920	0.00000
21	C2	S	0.00039	0.09448	-0.03057	0.00000	0.02582
22	C2	S	-0.08404	0.22033	-0.02988	0.00000	0.23508
23	C2	PX	0.05929	-0.13713	-0.10814	0.00000	-0.01324
24	C2	PY	0.15395	-0.09499	0.01294	0.00000	-0.26541
25	C2	PZ	0.00000	0.00000	0.00000	0.00840	0.00000
26	C2	S	0.43055	-3.39969	1.24342	0.00000	-1.61824
27	C2	PX	0.76053	-1.97480	0.18487	0.00000	-0.77992
28	C2	PY	0.33434	0.49419	-1.51763	0.00000	-0.89103
29	C2	PZ	0.00000	0.00000	0.00000	0.01577	0.00000
30	C2	DXX	0.05898	0.02255	0.03626	0.00000	0.08559
31	C2	DYY	0.03955	-0.55076	0.13760	0.00000	-0.20730
32	C2	DZZ	-0.00915	0.55711	-0.19932	0.00000	0.14242
33	C2	DXY	0.00790	0.15546	-0.15383	0.00000	-0.02237
34	C2	DXZ	0.00000	0.00000	0.00000	-0.00083	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.06571	0.00000
36	C3	S	0.02291	0.01438	0.13139	0.00000	0.05019
37	C3	S	0.04951	0.08924	0.57733	0.00000	0.13397
38	C3	PX	0.09938	0.00940	-0.11402	0.00000	-0.05314
39	C3	PY	-0.08171	0.20705	0.05184	0.00000	-0.11192
40	C3	PZ	0.00000	0.00000	0.00000	0.00640	0.00000
41	C3	S	-0.11655	-1.29324	-8.82005	0.00000	-3.21012
42	C3	PX	-0.60884	-0.07866	1.31677	0.00000	0.05385
43	C3	PY	-1.37014	1.12372	1.68518	0.00000	2.57296
44	C3	PZ	0.00000	0.00000	0.00000	-0.02917	0.00000
45	C3	DXX	0.32958	-0.09774	-0.34130	0.00000	-0.21488
46	C3	DYY	-0.33329	0.01131	-0.35561	0.00000	-0.05214
47	C3	DZZ	0.11216	0.08977	0.67138	0.00000	0.26043
48	C3	DXY	-0.24497	0.13861	-0.11819	0.00000	0.39007
49	C3	DXZ	0.00000	0.00000	0.00000	-0.04004	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.03523	0.00000
51	C4	S	-0.00432	-0.01886	0.00668	0.00000	0.05101
52	C4	S	-0.19448	-0.06421	0.01032	0.00000	0.05557
53	C4	PX	-0.05319	0.09037	-0.27980	0.00000	0.14857
54	C4	PY	-0.04126	0.01487	0.00573	0.00000	-0.15596

55	C4	PZ	0.00000	0.00000	0.00000	-0.00523	0.00000
56	C4	S	0.61891	0.72569	-1.42566	0.00000	-1.83065
57	C4	PX	-0.78105	2.18853	-1.11977	0.00000	0.07674
58	C4	PY	-0.45863	-0.59287	0.85108	0.00000	0.64301
59	C4	PZ	0.00000	0.00000	0.00000	0.04221	0.00000
60	C4	DXX	0.27679	0.20268	-0.05528	0.00000	-0.24118
61	C4	DYY	-0.31740	-0.07163	-0.15893	0.00000	0.16551
62	C4	DZZ	0.04690	-0.16499	0.08201	0.00000	0.27032
63	C4	DXY	0.10265	-0.13637	0.06686	0.00000	-0.07143
64	C4	DXZ	0.00000	0.00000	0.00000	0.15623	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.08699	0.00000
66	C5	S	0.02907	-0.03246	0.02410	0.00000	-0.05224
67	C5	S	0.04984	-0.17407	0.09967	0.00000	-0.00223
68	C5	PX	-0.03317	-0.15093	0.10367	0.00000	0.00614
69	C5	PY	0.01704	-0.36263	-0.03067	0.00000	-0.02788
70	C5	PZ	0.00000	0.00000	0.00000	0.01009	0.00000
71	C5	S	-1.48760	2.51261	0.05863	0.00000	2.38702
72	C5	PX	-0.77748	1.34061	-0.63073	0.00000	0.49051
73	C5	PY	0.13589	-0.36389	-0.46177	0.00000	-0.99937
74	C5	PZ	0.00000	0.00000	0.00000	-0.03072	0.00000
75	C5	DXX	0.01863	-0.02972	-0.17731	0.00000	0.07783
76	C5	DYY	-0.18583	0.31373	0.02350	0.00000	0.19577
77	C5	DZZ	0.16150	-0.21156	0.16846	0.00000	-0.28651
78	C5	DXY	-0.12683	0.19478	-0.12767	0.00000	0.20624
79	C5	DXZ	0.00000	0.00000	0.00000	0.05420	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.07234	0.00000
81	C6	S	0.01117	-0.07728	-0.04558	0.00000	-0.02570
82	C6	S	0.23309	0.29062	-0.43326	0.00000	0.12204
83	C6	PX	-0.03910	-0.11605	0.16041	0.00000	-0.05751
84	C6	PY	-0.18803	-0.40532	0.01757	0.00000	-0.27679
85	C6	PZ	0.00000	0.00000	0.00000	0.00040	0.00000
86	C6	S	-0.42369	4.74689	2.08432	0.00000	2.48750
87	C6	PX	-0.66173	-1.02418	3.65630	0.00000	0.74553
88	C6	PY	-0.73060	-0.02007	0.17558	0.00000	-0.68726
89	C6	PZ	0.00000	0.00000	0.00000	0.00378	0.00000
90	C6	DXX	0.03247	0.10177	0.21641	0.00000	-0.15013
91	C6	DYY	-0.00304	0.37714	0.11261	0.00000	0.39838
92	C6	DZZ	-0.04767	-0.60063	-0.19257	0.00000	-0.21683
93	C6	DXY	0.04089	-0.27754	0.16924	0.00000	0.39661
94	C6	DXZ	0.00000	0.00000	0.00000	-0.03782	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.00046	0.00000
96	C7	S	0.01344	-0.03386	-0.07912	0.00000	-0.05479
97	C7	S	-0.07392	-0.09889	-0.57189	0.00000	-0.21680
98	C7	PX	-0.21171	-0.09583	-0.17138	0.00000	-0.10761
99	C7	PY	-0.02236	0.13480	0.09364	0.00000	0.10887
100	C7	PZ	0.00000	0.00000	0.00000	-0.00189	0.00000
101	C7	S	-1.03979	2.12009	5.92529	0.00000	4.00236
102	C7	PX	0.66763	-1.14026	-3.37981	0.00000	-1.97237
103	C7	PY	0.10793	-0.24080	0.47090	0.00000	0.49776
104	C7	PZ	0.00000	0.00000	0.00000	0.01420	0.00000
105	C7	DXX	0.06324	0.00636	-0.00870	0.00000	0.07493
106	C7	DYY	-0.31107	0.15053	0.47244	0.00000	0.35446
107	C7	DZZ	0.10165	-0.17200	-0.41696	0.00000	-0.30193
108	C7	DXY	0.04772	-0.08302	-0.02145	0.00000	0.19249

109	C7	DXZ	0.00000	0.00000	0.00000	0.02202	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.01265	0.00000
111	O1	S	-0.02014	0.02504	0.01349	0.00000	-0.01607
112	O1	S	-0.19444	0.20171	0.07105	0.00000	-0.14971
113	O1	PX	-0.00072	0.04992	-0.03710	0.00000	0.02115
114	O1	PY	-0.07576	-0.02794	-0.00015	0.00000	0.05375
115	O1	PZ	0.00000	0.00000	0.00000	-0.01339	0.00000
116	O1	S	0.69308	-0.59793	-0.50529	0.00000	0.45838
117	O1	PX	0.22000	-0.75861	-0.10516	0.00000	0.02097
118	O1	PY	-0.12767	-0.21932	-0.36132	0.00000	-0.13902
119	O1	PZ	0.00000	0.00000	0.00000	-0.08233	0.00000
120	O1	DXX	0.07799	-0.18502	-0.16952	0.00000	-0.05687
121	O1	DYY	0.09928	0.03027	0.19700	0.00000	0.08571
122	O1	DZZ	-0.18761	0.29772	0.04886	0.00000	-0.15509
123	O1	DXY	0.15011	-0.17585	-0.31991	0.00000	0.09372
124	O1	DXZ	0.00000	0.00000	0.00000	-0.36682	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.09993	0.00000
126	H4	S	0.00003	0.06310	-0.00101	0.00000	-0.01962
127	H4	S	-0.08620	0.23816	-0.01676	0.00000	0.12695
128	H4	PX	0.19380	0.04529	-0.02061	0.00000	-0.10347
129	H4	PY	0.10958	-0.04540	-0.13727	0.00000	0.10915
130	H4	PZ	0.00000	0.00000	0.00000	-0.00075	0.00000
131	N1	S	0.02647	0.05978	-0.02313	0.00000	0.02624
132	N1	S	0.21536	0.65613	-0.35731	0.00000	0.12988
133	N1	PX	-0.06485	-0.08086	0.16027	0.00000	-0.05073
134	N1	PY	0.01290	-0.16659	-0.19146	0.00000	-0.24117
135	N1	PZ	0.00000	0.00000	0.00000	-0.00038	0.00000
136	N1	S	-1.21382	-3.41394	1.61447	0.00000	-1.46792
137	N1	PX	-0.04434	-0.47269	0.14307	0.00000	0.01162
138	N1	PY	-0.51652	-1.12161	0.38847	0.00000	-0.60494
139	N1	PZ	0.00000	0.00000	0.00000	0.00095	0.00000
140	N1	DXX	0.10840	-0.00002	0.33792	0.00000	0.15432
141	N1	DYY	-0.28201	-0.62860	-0.09450	0.00000	-0.47617
142	N1	DZZ	0.18736	0.50604	-0.15834	0.00000	0.19281
143	N1	DXY	0.18928	-0.01198	-0.30195	0.00000	0.21248
144	N1	DXZ	0.00000	0.00000	0.00000	0.01398	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.00843	0.00000
146	H6	S	0.09882	-0.02019	-0.17662	0.00000	-0.09417
147	H6	S	0.30894	-0.36644	-0.23144	0.00000	-0.28122
148	H6	PX	0.10378	0.06821	-0.17022	0.00000	-0.16864
149	H6	PY	-0.00769	-0.13464	-0.05876	0.00000	0.06477
150	H6	PZ	0.00000	0.00000	0.00000	0.00457	0.00000
151	C8	S	0.01112	-0.02310	0.07735	0.00000	0.01954
152	C8	S	0.09353	0.19628	0.14078	0.00000	0.21059
153	C8	PX	0.00807	-0.13640	0.04943	0.00000	-0.10708
154	C8	PY	-0.10461	0.11813	0.00398	0.00000	-0.26582
155	C8	PZ	0.00000	0.00000	0.00000	-0.00082	0.00000
156	C8	S	-0.32107	0.28527	-3.17514	0.00000	-1.51075
157	C8	PX	-0.04975	-1.14106	-0.20840	0.00000	-0.64014
158	C8	PY	1.04011	-0.63971	-3.22424	0.00000	-0.95155
159	C8	PZ	0.00000	0.00000	0.00000	-0.00328	0.00000
160	C8	DXX	0.34673	0.06214	-0.37615	0.00000	0.03160
161	C8	DYY	-0.21324	-0.09579	-0.05376	0.00000	-0.04831
162	C8	DZZ	-0.00232	-0.15514	0.41551	0.00000	0.01611

163	C8	DXY	0.14793	-0.21015	0.09009	0.00000	-0.31103
164	C8	DXZ	0.00000	0.00000	0.00000	0.01337	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.01166	0.00000
166	H8	S	0.02317	0.04480	0.12877	0.00000	0.01333
167	H8	S	-0.00488	0.28066	0.80107	0.00000	0.40070
168	H8	PX	-0.40454	-0.03691	-0.09520	0.00000	0.06158
169	H8	PY	-0.03334	0.10753	-0.03937	0.00000	-0.23238
170	H8	PZ	0.00000	0.00000	0.00000	-0.02035	0.00000
171	C10	S	0.01860	0.00537	-0.01077	0.00000	0.02502
172	C10	S	-0.15630	0.11758	-0.07112	0.00000	-0.27346
173	C10	PX	-0.02506	-0.05028	0.07016	0.00000	-0.10632
174	C10	PY	0.15404	-0.04757	0.08356	0.00000	-0.03439
175	C10	PZ	0.00000	0.00000	0.00000	0.00174	0.00000
176	C10	S	0.72460	-0.45702	-1.17341	0.00000	-0.33979
177	C10	PX	-0.16899	0.65601	0.61569	0.00000	0.37600
178	C10	PY	0.60939	-0.29012	-0.23568	0.00000	0.24106
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.29446	-0.08228	-0.13380	0.00000	0.21412
181	C10	DYY	-0.20485	0.06348	0.15532	0.00000	-0.29450
182	C10	DZZ	0.10283	0.02909	-0.08242	0.00000	0.17155
183	C10	DXY	0.12593	-0.09586	-0.02024	0.00000	0.06424
184	C10	DXZ	0.00000	0.00000	0.00000	-0.01012	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00471	0.00000
186	H16	S	-0.02791	-0.06094	-0.03952	0.00000	-0.03339
187	H16	S	0.17602	-0.26715	-0.22025	0.00000	0.08126
188	H16	PX	-0.20784	0.09827	0.01306	0.00000	-0.28214
189	H16	PY	-0.32952	0.19265	-0.01276	0.00000	-0.10340
190	H16	PZ	0.00000	0.00000	0.00000	0.00747	0.00000
191	H18	S	-0.03835	0.12136	0.12650	0.00000	0.08769
192	H18	S	0.15722	0.00653	0.22834	0.00000	0.21988
193	H18	PX	0.33126	-0.12211	0.07962	0.00000	0.28985
194	H18	PY	-0.21829	-0.01891	0.16399	0.00000	-0.18881
195	H18	PZ	0.00000	0.00000	0.00000	-0.00352	0.00000
196	C9	S	0.00367	-0.01685	-0.02792	0.00000	0.01080
197	C9	S	-0.21206	0.25981	0.03818	0.00000	-0.00810
198	C9	PX	0.15378	-0.23977	-0.14782	0.00000	0.02904
199	C9	PY	0.06568	-0.10711	-0.02266	0.00000	0.04226
200	C9	PZ	0.00000	0.00000	0.00000	0.03652	0.00000
201	C9	S	-0.03907	0.51227	0.59341	0.00000	-0.20527
202	C9	PX	0.12141	-0.13933	-0.12283	0.00000	0.00868
203	C9	PY	-0.39551	-0.03387	-0.25037	0.00000	0.13856
204	C9	PZ	0.00000	0.00000	0.00000	-0.10230	0.00000
205	C9	DXX	0.04112	0.31198	0.27027	0.00000	-0.17441
206	C9	DYY	0.09637	-0.07767	-0.03450	0.00000	0.05604
207	C9	DZZ	-0.09674	-0.27815	-0.21334	0.00000	0.14414
208	C9	DXY	-0.29270	0.03157	0.01970	0.00000	0.10429
209	C9	DXZ	0.00000	0.00000	0.00000	-0.31192	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.85972	0.00000
211	H3	S	0.00911	-0.02821	-0.03098	0.00000	-0.00946
212	H3	S	0.26715	-0.06933	0.03629	0.00000	-0.05052
213	H3	PX	0.17211	0.02645	0.03489	0.00000	-0.11202
214	H3	PY	-0.01206	0.04859	0.06990	0.00000	0.01002
215	H3	PZ	0.00000	0.00000	0.00000	0.59188	0.00000
216	H5	S	-0.04433	-0.00687	-0.03944	0.02484	0.01649

217	H5	S	-0.04201	-0.06439	-0.08057	-0.06015	0.04392
218	H5	PX	-0.10663	-0.11940	-0.07851	-0.19444	0.08970
219	H5	PY	0.18667	0.02605	0.01488	-0.46070	-0.04081
220	H5	PZ	-0.14138	-0.11652	-0.11325	0.05273	0.09787
221	H7	S	-0.04433	-0.00687	-0.03944	-0.02484	0.01649
222	H7	S	-0.04201	-0.06439	-0.08057	0.06015	0.04392
223	H7	PX	-0.10663	-0.11940	-0.07851	0.19444	0.08970
224	H7	PY	0.18667	0.02605	0.01488	0.46070	-0.04081
225	H7	PZ	0.14138	0.11652	0.11325	0.05273	-0.09787

MO:	196	197	198	199	200
Eigenvalues:	3.30396	3.34005	3.35844	3.43095	3.45749
(ev):	89.90539	90.88745	91.38780	93.36103	94.08322

			A	A	A	A	A
1	H1	S	-0.14225	0.01944	-0.01062	-0.10608	0.18676
2	H1	S	-0.50753	0.06258	0.03420	-0.18966	0.31540
3	H1	PX	0.38430	-0.11079	-0.06560	0.13371	-0.40927
4	H1	PY	0.07788	-0.07082	0.11540	0.18505	-0.06589
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02773	-0.00881	0.02010	-0.00407	0.02745
7	C1	S	0.20121	-0.11992	-0.05674	0.05459	-0.37374
8	C1	PX	0.28877	-0.14105	0.09197	0.10689	-0.01752
9	C1	PY	-0.10761	-0.05109	-0.02154	0.21541	-0.19185
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.12890	1.34093	-0.28940	0.40862	-0.34332
12	C1	PX	1.02338	-0.00813	0.28880	0.27916	-0.18930
13	C1	PY	-0.90841	-1.15185	-0.49948	-0.12334	0.00489
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.18470	-0.04583	0.08182	0.18464	-0.11945
16	C1	DYY	0.29562	0.13361	-0.22364	-0.20375	-0.15669
17	C1	DZZ	-0.17172	-0.01385	0.13106	-0.03684	0.22409
18	C1	DXY	0.13677	0.13499	-0.03839	-0.27078	0.03780
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00170	-0.03718	-0.03117	-0.02120	-0.02427
22	C2	S	-0.23685	-0.05394	0.06836	0.15211	0.30111
23	C2	PX	-0.04356	-0.18634	-0.10003	-0.00618	0.02783
24	C2	PY	-0.10570	-0.05462	0.03790	0.04770	0.13781
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.75069	1.07542	0.76943	0.18703	0.20713
27	C2	PX	0.37277	0.25950	-0.03966	0.55460	0.08805
28	C2	PY	1.86914	0.72854	1.04182	0.07907	-0.30036
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.10726	-0.10728	-0.01841	-0.08759	0.03912
31	C2	DYY	-0.18845	0.21793	0.14567	0.20653	0.18447
32	C2	DZZ	0.05041	-0.21365	-0.20098	-0.13041	-0.19307
33	C2	DXY	-0.19490	-0.03231	-0.12217	0.24147	0.02063
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03998	-0.00779	-0.03910	-0.06488	-0.01843
37	C3	S	-0.18788	0.04899	0.04783	0.14006	0.08412
38	C3	PX	0.13665	-0.08421	0.03495	0.17867	0.10363
39	C3	PY	-0.34531	-0.11065	0.00862	-0.13058	0.00395

40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	3.84317	-0.19678	2.17177	2.31791	0.75772
42	C3	PX	-2.09938	-1.56112	-0.50079	-1.40423	0.60200
43	C3	PY	-2.37624	-1.30951	-1.48753	-0.88078	-0.76650
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.40259	0.39535	-0.09072	-0.23542	-0.18650
46	C3	DYY	-0.07540	-0.27453	0.23118	0.48306	0.24019
47	C3	DZZ	-0.19458	-0.04863	-0.17685	-0.33436	-0.12472
48	C3	DXY	-0.49737	0.24052	-0.02058	-0.17331	0.03000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00076	-0.01380	-0.05249	-0.01283	-0.03765
52	C4	S	-0.19111	0.35641	0.20510	0.09964	-0.36328
53	C4	PX	-0.00458	-0.05070	-0.05801	-0.01243	0.05982
54	C4	PY	-0.26900	0.08817	0.09456	0.30209	-0.45878
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.14686	0.32343	1.10964	0.58890	0.39663
57	C4	PX	1.07922	0.12446	0.35017	-0.09675	-0.20206
58	C4	PY	-1.10239	0.47571	-0.21797	0.33418	-0.85339
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.08772	0.04977	0.14780	-0.23092	0.44433
61	C4	DYY	0.06112	-0.01409	-0.08835	0.17056	-0.49713
62	C4	DZZ	0.06992	-0.11451	-0.32104	-0.09202	-0.14197
63	C4	DXY	-0.22263	0.19950	-0.12087	0.01268	-0.40521
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.01102	0.02132	0.04749	-0.01827	0.06359
67	C5	S	0.09847	-0.06215	-0.11729	-0.13099	-0.26710
68	C5	PX	0.04204	0.05648	0.07656	0.06925	0.09649
69	C5	PY	-0.12501	0.00035	-0.09609	0.19325	0.01433
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.05358	-1.00513	-1.51959	0.00323	-0.75147
72	C5	PX	0.80413	0.23339	0.29055	-0.10974	-0.43686
73	C5	PY	1.17786	0.45802	0.69141	-0.18168	-0.15754
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.13818	-0.30561	-0.13026	0.20736	0.24954
76	C5	DYY	0.22899	0.11599	-0.03890	-0.24648	-0.35128
77	C5	DZZ	-0.09387	0.14395	0.28086	-0.06575	0.37886
78	C5	DXY	0.05375	-0.08961	-0.15754	0.01798	-0.15030
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.02665	0.02650	0.02485	0.01157	0.01666
82	C6	S	0.56473	-0.00678	0.09544	0.65635	-0.09658
83	C6	PX	0.04813	-0.09744	0.15041	-0.04508	0.01665
84	C6	PY	-0.31262	-0.03882	-0.07241	-0.37335	0.04125
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-1.00395	-1.67050	-0.95616	-0.81205	-0.54640
87	C6	PX	-3.02262	-1.06017	-1.26323	-1.34403	0.24054
88	C6	PY	-1.59435	-0.23783	0.33223	-1.67518	0.33891
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.18825	-0.46403	-0.15809	-0.37133	0.00600
91	C6	DYY	0.08908	0.30564	0.04678	0.51037	0.00619
92	C6	DZZ	-0.00456	0.12975	0.14065	-0.09865	0.10945
93	C6	DXY	-0.26598	-0.22087	-0.08222	0.19708	0.35888

94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.05182	-0.01986	0.00281	0.02755	0.00994
97	C7	S	0.12463	-0.00281	0.31039	0.08279	0.03832
98	C7	PX	0.04330	-0.29204	0.35662	0.33553	0.05447
99	C7	PY	-0.26300	-0.07779	-0.16427	-0.19040	-0.07745
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-3.74140	0.22525	-2.01191	-1.81835	-1.02117
102	C7	PX	2.16096	0.15012	1.47045	1.24057	0.42871
103	C7	PY	0.62249	0.45881	-0.15446	0.76519	-0.47846
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00557	0.05286	0.10108	0.08966	0.02133
106	C7	DYY	-0.41204	0.04847	-0.02134	-0.24872	-0.07117
107	C7	DZZ	0.28602	-0.09853	-0.03721	0.13024	0.04906
108	C7	DXY	0.36409	0.34899	0.16735	0.45275	0.23066
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00467	-0.01136	0.02154	0.01988	0.01281
112	O1	S	-0.06431	0.17978	0.22771	0.05013	-0.09109
113	O1	PX	0.02891	-0.03610	-0.02140	-0.03189	0.08591
114	O1	PY	0.06739	-0.04745	-0.03898	0.01618	0.00107
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.33518	-0.45389	-0.74357	-0.47011	0.26255
117	O1	PX	-0.43854	0.15477	-0.08514	0.21665	-0.51868
118	O1	PY	-0.65054	0.45029	0.16038	0.42949	-1.02059
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.37439	0.09341	0.02369	0.29053	-0.43735
121	O1	DYY	0.36160	-0.23211	-0.11547	-0.29832	0.71567
122	O1	DZZ	0.04205	-0.00299	0.21253	0.09377	0.00432
123	O1	DXY	-0.22500	0.12455	-0.21309	-0.03371	-0.26249
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.03829	0.08122	0.11529	-0.00592	0.09736
127	H4	S	0.02520	0.08082	0.14739	0.02129	0.14045
128	H4	PX	-0.15363	-0.06094	0.10583	0.09296	0.36068
129	H4	PY	-0.23953	-0.28938	-0.27538	0.10281	-0.00029
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.01412	0.01067	-0.00343	0.00386	0.00579
132	N1	S	0.21860	-0.27698	0.09305	-0.06108	-0.09196
133	N1	PX	-0.06909	-0.14820	-0.01722	-0.02370	-0.01201
134	N1	PY	0.02361	-0.05620	0.00796	-0.19440	0.01243
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-1.23713	0.49140	-0.10836	-0.43587	0.23862
137	N1	PX	0.63897	0.16554	-0.16017	0.96664	-0.07708
138	N1	PY	-1.53342	0.13652	-0.04786	-1.53177	0.32685
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.23447	-0.11770	-0.22724	0.58220	0.00065
141	N1	DYY	-0.38450	0.09802	0.10468	-0.75496	0.02637
142	N1	DZZ	0.09331	0.00673	0.02549	0.06188	0.00781
143	N1	DXY	-0.28568	-0.03255	-0.23615	-0.10810	0.31465
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.09856	-0.03690	-0.03229	-0.02236	-0.08378
147	H6	S	0.29640	-0.05682	-0.07999	0.14768	-0.10163

148	H6	PX	0.14122	-0.21527	-0.11777	-0.22407	-0.19369
149	H6	PY	-0.22825	-0.06671	-0.20585	0.20690	-0.01339
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.01405	0.03382	-0.03601	0.03132	0.01564
152	C8	S	-0.32214	-0.28164	0.15152	-0.46027	-0.13565
153	C8	PX	0.09876	-0.15801	0.05044	0.10698	-0.09819
154	C8	PY	-0.14035	0.15572	-0.39700	-0.03459	0.08911
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	1.71287	-0.13974	1.30611	0.35530	0.00696
157	C8	PX	1.66252	0.31957	0.17777	1.71494	-0.24931
158	C8	PY	1.47201	-0.21700	1.04683	0.57322	0.19427
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.03972	0.34668	-0.27227	-0.00067	0.27022
161	C8	DYY	0.14215	-0.46003	0.49473	-0.04611	-0.26923
162	C8	DZZ	-0.05071	0.23190	-0.25018	0.22160	0.09791
163	C8	DXY	0.04430	-0.38832	-0.42191	0.31492	0.02732
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00496	0.03702	-0.24166	-0.14641	-0.00489
167	H8	S	-0.40924	0.02926	-0.62598	-0.38421	-0.11544
168	H8	PX	-0.20407	-0.24100	0.51682	0.21453	0.01470
169	H8	PY	-0.20877	-0.21891	-0.08099	-0.37454	-0.09836
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.01320	-0.02624	0.04174	-0.00580	-0.01662
172	C10	S	0.01090	0.19869	-0.39494	0.17076	0.17558
173	C10	PX	-0.03756	-0.41575	-0.11225	0.12495	-0.04118
174	C10	PY	-0.06801	0.04571	-0.24172	0.07250	0.06869
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.17891	0.11352	-0.08847	0.10802	0.33219
177	C10	PX	-0.64817	-0.34974	-0.36179	-0.40534	-0.04308
178	C10	PY	-0.18907	-0.12738	0.11358	-0.20966	0.03565
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.04980	-0.15264	0.19982	0.00035	-0.01112
181	C10	DYY	-0.09340	0.33590	-0.58190	0.13538	0.18362
182	C10	DZZ	0.08443	-0.20954	0.34097	-0.07820	-0.14181
183	C10	DXY	0.02330	-0.13884	0.19604	-0.09258	-0.04132
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.08350	0.10957	0.16308	-0.06085	-0.03735
187	H16	S	0.19825	0.19488	0.37533	0.00103	-0.05032
188	H16	PX	-0.02666	-0.12658	-0.45191	0.24326	0.11521
189	H16	PY	-0.00481	0.33087	-0.05649	-0.05803	0.02789
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.06296	-0.17090	0.00395	-0.00774	-0.08627
192	H18	S	-0.28037	-0.35519	0.00809	-0.20626	-0.08941
193	H18	PX	-0.04828	-0.36107	0.28043	-0.06969	-0.14749
194	H18	PY	-0.03474	-0.26136	-0.13139	0.08430	-0.07711
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.02681	0.00281	-0.01217	0.01844	-0.04368
197	C9	S	0.22951	-0.16023	0.06812	-0.16036	0.37647
198	C9	PX	-0.18115	0.06271	-0.10934	0.01594	-0.17839
199	C9	PY	-0.00685	0.01309	-0.03163	0.00467	0.03265
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.50918	-0.07527	0.23325	-0.29584	0.92058

202	C9	PX	-0.21703	0.14154	-0.04753	0.07719	-0.30348
203	C9	PY	-0.00386	-0.29267	-0.05751	-0.00126	0.13734
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.05128	0.01938	0.21356	0.14736	-0.09106
206	C9	DYY	0.00531	0.01308	-0.06867	-0.06072	0.11426
207	C9	DZZ	0.04471	-0.01819	-0.16402	-0.08021	-0.02192
208	C9	DXY	0.27644	-0.09911	-0.07007	-0.14351	0.19287
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.06556	0.05540	-0.01385	0.05993	-0.22580
212	H3	S	-0.13643	0.19656	-0.01174	0.07286	-0.29099
213	H3	PX	-0.19091	0.08719	0.09661	0.13654	-0.20600
214	H3	PY	0.13289	-0.06882	0.03588	-0.09709	0.32954
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.05527	-0.02720	-0.00106	0.05259	-0.06167
217	H5	S	0.02908	-0.04699	-0.04288	0.03421	-0.08369
218	H5	PX	0.13535	-0.04767	-0.07912	-0.11949	0.15549
219	H5	PY	-0.13516	0.09337	0.03126	0.05955	-0.12571
220	H5	PZ	0.04483	-0.04346	-0.06851	0.02485	-0.05603
221	H7	S	-0.05527	-0.02720	-0.00106	0.05259	-0.06167
222	H7	S	0.02908	-0.04699	-0.04288	0.03421	-0.08369
223	H7	PX	0.13535	-0.04767	-0.07912	-0.11949	0.15549
224	H7	PY	-0.13516	0.09337	0.03126	0.05955	-0.12571
225	H7	PZ	-0.04483	0.04346	0.06851	-0.02485	0.05603

M0:	201	202	203	204	205
Eigenvalues:	3.52337	3.56160	3.57691	3.66981	3.72630
(ev):	95.87591	96.91612	97.33263	99.86077	101.39790

		A	A	A	A	A	
1	H1	S	-0.04330	0.22972	-0.12081	0.07766	0.01208
2	H1	S	-0.04892	0.17382	0.06527	0.04686	-0.02133
3	H1	PX	0.03345	-0.48068	0.17057	-0.11620	0.02010
4	H1	PY	0.28089	-0.03319	0.05683	-0.01976	-0.18129
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02783	0.01993	-0.00250	-0.00094	0.00516
7	C1	S	0.12237	-0.01099	0.07455	-0.02621	-0.10345
8	C1	PX	-0.06844	-0.43907	0.08044	-0.04071	0.10548
9	C1	PY	0.10772	-0.02461	0.07589	-0.06373	-0.12162
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.21798	-0.28041	-0.00538	-0.05516	0.18004
12	C1	PX	-0.19315	0.34797	-0.12836	-0.00760	-0.03680
13	C1	PY	0.10923	-0.64942	0.07576	-0.01609	0.34903
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.21334	-0.01351	0.12247	-0.07204	-0.20603
16	C1	DYY	-0.09252	-0.01939	-0.04721	0.00402	0.12190
17	C1	DZZ	-0.16691	0.11194	-0.04326	0.01162	0.05378
18	C1	DXY	-0.34679	-0.25386	0.01800	-0.05104	0.24815
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.03757	-0.01840	0.00687	-0.02469	-0.00260
22	C2	S	0.00708	0.05198	-0.02142	0.31002	0.02111
23	C2	PX	0.09138	-0.19026	-0.00157	-0.53312	0.02921
24	C2	PY	0.31312	-0.05451	0.00696	-0.02880	0.18859

25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.82855	0.00948	-0.29814	0.46780	0.19785
27	C2	PX	-0.22269	0.09300	-0.05542	-0.18562	0.32766
28	C2	PY	-1.33167	0.55636	-0.26845	0.12978	-0.05588
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.37435	-0.09137	-0.02114	0.48035	-0.17527
31	C2	DYY	0.22956	0.04339	0.02069	-0.18586	0.24494
32	C2	DZZ	0.18962	-0.11140	0.03559	-0.19847	-0.02977
33	C2	DXY	0.46416	0.14964	0.06521	0.36348	0.24760
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.04138	-0.03755	0.00318	-0.02117	-0.02119
37	C3	S	0.49682	-0.17578	0.04073	-0.03274	-0.15879
38	C3	PX	0.07199	-0.21220	0.01623	0.01842	-0.13103
39	C3	PY	-0.05722	0.14774	-0.02031	-0.03902	-0.04589
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-3.93029	2.12391	-0.78744	0.93063	1.15737
42	C3	PX	1.01872	-1.71149	-0.06786	-0.17098	-0.22691
43	C3	PY	1.60404	-1.24683	0.80794	-0.35110	-0.24459
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.18164	0.34661	-0.03317	0.06061	0.15575
46	C3	DYY	0.07402	-0.25248	0.01874	-0.02194	-0.10610
47	C3	DZZ	0.14634	-0.12148	0.00992	-0.10152	-0.08814
48	C3	DXY	-0.31001	0.29485	0.00411	-0.12906	0.17675
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.04210	0.02001	0.00824	-0.01580	-0.02340
52	C4	S	-0.47560	-0.39648	0.21990	0.06096	0.21246
53	C4	PX	-0.08959	-0.15226	0.01045	-0.05688	0.19821
54	C4	PY	-0.10540	-0.16898	0.23514	-0.02474	0.01191
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.76218	0.07911	0.12966	0.29282	0.35252
57	C4	PX	-0.05911	0.55566	0.10248	-0.08438	-0.53524
58	C4	PY	0.00715	-0.56913	1.02540	-0.13796	0.15796
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.08397	0.27424	-0.17810	0.07595	-0.15672
61	C4	DYY	-0.22739	-0.26249	0.24361	-0.11232	0.13295
62	C4	DZZ	0.30375	0.16929	-0.01684	-0.05713	-0.15891
63	C4	DXY	0.22416	0.46639	0.02809	-0.05668	-0.36013
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02493	0.00871	-0.02843	-0.02934	0.00694
67	C5	S	-0.12959	-0.17323	0.07780	0.38183	-0.09475
68	C5	PX	-0.00287	-0.06244	-0.00917	-0.46541	0.16997
69	C5	PY	0.23847	0.00958	0.09251	0.42146	0.12011
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	1.64690	-0.11980	0.71506	-0.01255	-0.52998
72	C5	PX	-0.36408	0.19356	0.11338	-0.34813	-0.27857
73	C5	PY	-0.74542	0.16376	-0.34142	0.44268	-0.13798
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.22826	-0.25146	0.05380	0.19384	0.26588
76	C5	DYY	-0.32672	0.15302	-0.03769	0.08071	-0.35964
77	C5	DZZ	-0.08849	0.07307	-0.14448	-0.23430	0.06613
78	C5	DXY	0.05602	0.04203	-0.02114	-0.63341	0.06324

79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.06717	0.03664	-0.00936	0.00213	0.00724
82	C6	S	-0.06331	0.45840	-0.01763	0.10348	0.11921
83	C6	PX	-0.04213	-0.13794	-0.01701	-0.04036	-0.12819
84	C6	PY	0.28394	-0.34399	0.03413	0.07136	-0.03186
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	1.67318	-1.16995	0.25425	-0.26772	-0.61482
87	C6	PX	2.32562	-1.99389	0.35934	-0.33953	-0.20961
88	C6	PY	0.36907	-0.93803	-0.04974	-0.02825	-0.32726
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.18889	-0.49842	0.02654	0.08225	-0.21428
91	C6	DYY	-0.09350	0.48283	-0.01191	-0.14066	0.18624
92	C6	DZZ	-0.25724	0.06403	-0.03760	0.02771	0.00424
93	C6	DXY	-0.46909	-0.33222	-0.04701	-0.18543	-0.17918
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.03317	0.01105	-0.01032	0.01652	0.05935
97	C7	S	-0.26032	0.23308	-0.07486	0.01827	-0.12055
98	C7	PX	0.02184	0.06698	-0.00593	-0.03744	-0.25661
99	C7	PY	-0.17920	0.17567	0.00385	-0.04819	0.11060
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	2.99782	-1.54857	1.09591	-0.92887	-1.42964
102	C7	PX	-1.68849	1.11861	-0.53213	0.48753	0.35177
103	C7	PY	-0.05911	0.69608	0.13648	-0.00696	0.33282
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.09461	0.02385	0.01901	-0.06640	-0.21728
106	C7	DYY	0.06197	-0.00965	0.03464	-0.04205	0.17075
107	C7	DZZ	-0.10835	-0.00472	-0.03611	0.09314	0.29821
108	C7	DXY	0.35948	-0.40767	0.03382	0.03402	-0.10839
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.02087	-0.03397	-0.00930	0.01001	0.03029
112	O1	S	-0.22877	-0.18839	0.25334	0.06897	0.05540
113	O1	PX	0.03799	0.05226	0.09661	-0.00299	-0.00773
114	O1	PY	0.01042	-0.00155	0.03900	-0.03608	0.01767
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.75921	0.91385	-0.65507	-0.22716	-0.50142
117	O1	PX	-0.15213	-0.20550	0.32177	-0.05606	0.12727
118	O1	PY	-0.45387	-0.37647	0.74708	-0.02298	0.12663
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.16382	-0.18159	0.38862	-0.04282	0.11972
121	O1	DYY	0.34434	0.29402	-0.40886	0.05924	-0.06391
122	O1	DZZ	-0.22499	-0.23688	-0.03124	0.06777	0.15228
123	O1	DXY	0.23075	0.40851	0.11948	-0.10724	-0.22264
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.05327	0.07282	-0.06516	-0.66170	0.09229
127	H4	S	-0.10378	0.04702	0.00659	-0.52909	0.05767
128	H4	PX	0.12152	0.00427	-0.07847	-0.67502	0.21443
129	H4	PY	0.22825	-0.13826	0.11849	0.77471	0.00415
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00554	-0.01430	-0.00009	-0.00733	0.01633
132	N1	S	0.05886	-0.02327	-0.01197	0.15799	-0.13916

133	N1	PX	-0.04687	-0.00887	-0.00354	-0.01653	-0.04352
134	N1	PY	0.03635	-0.16052	-0.00094	0.09070	-0.04052
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.20124	-0.01286	0.03132	-0.20249	0.00393
137	N1	PX	-0.52594	0.80459	-0.02538	-0.08928	0.13212
138	N1	PY	0.48560	-1.15778	0.06273	-0.07989	-0.15471
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.29822	0.35953	-0.01556	-0.12279	0.12554
141	N1	DYY	0.22896	-0.49884	0.02583	0.04630	-0.02287
142	N1	DZZ	0.01283	-0.02196	-0.00099	-0.01281	0.05035
143	N1	DXY	-0.26914	-0.42790	-0.01697	-0.04627	-0.11714
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.09616	-0.05448	-0.00051	-0.54816	0.04483
147	H6	S	-0.05241	-0.02089	-0.00256	-0.36532	0.09953
148	H6	PX	0.15231	-0.22623	0.00157	-0.83240	-0.02283
149	H6	PY	0.40813	0.04393	0.05207	-0.30872	0.17700
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.01591	-0.00818	0.00426	-0.01745	-0.05743
152	C8	S	0.18458	-0.11796	0.02822	0.00926	-0.13032
153	C8	PX	-0.17195	0.29686	-0.02368	-0.02587	0.02702
154	C8	PY	-0.01400	-0.05992	0.00031	-0.00079	0.16730
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.71764	0.43475	-0.32034	0.60693	1.61330
157	C8	PX	-0.50617	1.31217	-0.10968	0.12368	0.69720
158	C8	PY	-1.73495	0.76284	-0.35358	0.40581	-0.21013
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.06496	-0.30181	-0.00941	-0.01876	-0.07688
161	C8	DYY	-0.05225	0.31352	-0.01803	0.03678	-0.03658
162	C8	DZZ	0.04092	0.00037	0.01458	-0.08174	-0.25933
163	C8	DXY	-0.40112	0.27148	-0.04179	-0.03044	0.11192
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.01393	-0.11391	0.00234	0.05100	0.28861
167	H8	S	0.35156	-0.33190	0.11356	-0.08210	0.12656
168	H8	PX	0.06404	0.15573	0.01094	-0.10225	-0.40664
169	H8	PY	-0.13781	0.10698	-0.02612	0.00982	0.05165
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.01404	0.01150	0.00117	0.00795	0.09051
172	C10	S	-0.13216	-0.05780	-0.02370	-0.04316	-0.50768
173	C10	PX	-0.32827	0.25320	-0.03935	-0.05511	0.02391
174	C10	PY	-0.06217	0.02034	0.00092	-0.00381	0.43752
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-1.08140	0.09360	-0.15098	0.01850	-1.52800
177	C10	PX	0.15496	-0.21926	0.07397	-0.12325	-0.09125
178	C10	PY	-0.30492	-0.03788	-0.01248	-0.01434	-0.28136
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.15078	0.03255	-0.02480	-0.04691	-0.58250
181	C10	DYY	0.02528	-0.15359	0.01632	-0.00159	0.27791
182	C10	DZZ	0.09754	0.09839	0.00853	0.05495	0.55602
183	C10	DXY	0.11620	-0.11116	0.01072	0.04084	-0.31767
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.22888	-0.07290	0.01925	0.07883	0.41186

187	H16	S	0.14295	0.00278	0.00464	0.07424	0.30491
188	H16	PX	-0.39604	0.14283	-0.04816	-0.09689	-0.49024
189	H16	PY	0.20695	-0.10658	0.02377	0.03975	0.35215
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.03187	0.15554	0.00569	-0.01224	0.50952
192	H18	S	-0.02822	0.00979	0.02620	-0.03704	0.27717
193	H18	PX	-0.07806	0.19885	-0.00318	-0.00928	0.45334
194	H18	PY	-0.12108	0.22346	-0.00765	0.00743	0.66980
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.01042	-0.00752	-0.09889	-0.00163	-0.00135
197	C9	S	-0.02925	0.06745	0.76442	-0.00249	0.00138
198	C9	PX	0.03747	0.18516	0.55603	-0.09595	-0.13456
199	C9	PY	-0.02325	-0.03751	0.16306	0.00664	0.16491
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.05268	0.14581	0.55897	0.10142	0.03702
202	C9	PX	-0.04814	0.04195	0.40811	-0.06858	-0.07105
203	C9	PY	0.07221	-0.02163	0.21225	-0.01767	0.11522
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.19540	-0.31544	-0.42529	0.05183	0.06903
206	C9	DYY	0.07056	0.05824	-0.12481	0.03014	0.16963
207	C9	DZZ	0.12344	0.24658	0.33190	-0.08737	-0.21190
208	C9	DXY	0.15352	0.08758	-0.58926	0.04786	-0.06405
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.01256	-0.00159	-0.26969	-0.02369	-0.16659
212	H3	S	-0.01871	-0.00113	-0.30931	-0.01801	-0.11839
213	H3	PX	-0.12717	-0.14497	0.01125	0.00095	0.01594
214	H3	PY	-0.06379	-0.01722	0.57637	0.02743	0.23671
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.01601	-0.08832	-0.37629	0.03258	0.08354
217	H5	S	0.04728	-0.06395	-0.37822	0.01138	0.04182
218	H5	PX	0.07257	0.17062	0.38718	-0.03792	-0.09289
219	H5	PY	-0.04884	-0.06392	-0.16235	0.01463	0.03369
220	H5	PZ	0.09180	-0.06026	-0.64438	0.04193	0.06972
221	H7	S	0.01601	-0.08832	-0.37629	0.03258	0.08354
222	H7	S	0.04728	-0.06395	-0.37822	0.01138	0.04182
223	H7	PX	0.07257	0.17062	0.38718	-0.03792	-0.09289
224	H7	PY	-0.04884	-0.06392	-0.16235	0.01463	0.03369
225	H7	PZ	-0.09180	0.06026	0.64438	-0.04193	-0.06972

MO:	206	207	208	209	210
Eigenvalues:	3.78192	3.79244	3.84127	3.87761	3.98970
(ev):	102.91138	103.19748	104.52633	105.51517	108.56519

		A	A	A	A	A	
1	H1	S	0.04729	0.00000	-0.02568	0.75223	0.03842
2	H1	S	-0.04375	0.00000	-0.09396	0.56436	-0.07560
3	H1	PX	-0.11510	0.00000	0.09291	-0.93001	-0.09735
4	H1	PY	0.17433	0.00000	-0.12664	-0.36155	0.09844
5	H1	PZ	0.00000	-0.02276	0.00000	0.00000	0.00000
6	C1	S	0.01696	0.00000	0.00546	0.07856	0.03767
7	C1	S	0.02584	0.00000	-0.11078	-0.43974	-0.06232
8	C1	PX	-0.13033	0.00000	0.16523	-0.52787	-0.08681
9	C1	PY	0.17030	0.00000	-0.10709	-0.18431	0.19475

10	C1	PZ	0.00000	0.00379	0.00000	0.00000	0.00000
11	C1	S	-0.33049	0.00000	0.02727	-1.12745	-0.84565
12	C1	PX	0.36053	0.00000	0.05360	-0.40697	0.45924
13	C1	PY	-0.66705	0.00000	-0.09691	0.09465	-0.01387
14	C1	PZ	0.00000	-0.04473	0.00000	0.00000	0.00000
15	C1	DXX	0.20063	0.00000	-0.13141	-0.69217	0.16165
16	C1	DYY	-0.16759	0.00000	0.10680	0.54936	-0.11371
17	C1	DZZ	0.06140	0.00000	0.04931	0.46015	0.14254
18	C1	DXY	-0.34421	0.00000	0.27869	-0.48140	-0.29480
19	C1	DXZ	0.00000	0.04292	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.01082	0.00000	0.00000	0.00000
21	C2	S	-0.00684	0.00000	-0.00633	0.05563	-0.02176
22	C2	S	-0.04420	0.00000	0.12274	-0.28990	0.07525
23	C2	PX	0.03191	0.00000	-0.07862	0.32636	-0.06188
24	C2	PY	-0.26505	0.00000	0.13592	0.14317	-0.10915
25	C2	PZ	0.00000	0.00026	0.00000	0.00000	0.00000
26	C2	S	0.14879	0.00000	-0.00216	-0.56304	0.20857
27	C2	PX	-0.00750	0.00000	-0.05279	0.10474	-0.04568
28	C2	PY	0.61787	0.00000	-0.24098	0.09170	0.39210
29	C2	PZ	0.00000	0.01353	0.00000	0.00000	0.00000
30	C2	DXX	0.23746	0.00000	-0.03464	-0.36873	0.09393
31	C2	DYY	-0.27822	0.00000	0.09376	0.33859	-0.15664
32	C2	DZZ	-0.00211	0.00000	-0.06809	0.32257	-0.09577
33	C2	DXY	-0.37756	0.00000	0.30035	-0.31467	0.02762
34	C2	DXZ	0.00000	0.00306	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00694	0.00000	0.00000	0.00000
36	C3	S	-0.03406	0.00000	0.00829	-0.03121	-0.08786
37	C3	S	0.09045	0.00000	-0.05516	0.03048	0.17810
38	C3	PX	0.21555	0.00000	-0.10083	-0.00635	0.02063
39	C3	PY	0.04336	0.00000	-0.03453	-0.18246	-0.00068
40	C3	PZ	0.00000	-0.00444	0.00000	0.00000	0.00000
41	C3	S	1.16356	0.00000	-0.37156	0.64553	2.49330
42	C3	PX	-0.63667	0.00000	0.01213	0.24956	-0.29754
43	C3	PY	-1.04549	0.00000	0.16556	0.27177	-0.71765
44	C3	PZ	0.00000	0.03084	0.00000	0.00000	0.00000
45	C3	DXX	-0.31491	0.00000	0.13479	-0.09564	-0.51703
46	C3	DYY	0.32801	0.00000	-0.14464	0.04557	0.37045
47	C3	DZZ	-0.16996	0.00000	0.03772	-0.16649	-0.39417
48	C3	DXY	-0.16663	0.00000	0.10350	-0.28506	0.02189
49	C3	DXZ	0.00000	-0.00544	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00605	0.00000	0.00000	0.00000
51	C4	S	0.01782	0.00000	0.01042	-0.03835	-0.00276
52	C4	S	-0.29156	0.00000	-0.06824	0.25686	-0.13951
53	C4	PX	-0.22311	0.00000	0.16722	-0.11911	-0.08903
54	C4	PY	-0.01447	0.00000	-0.15586	0.08441	0.09410
55	C4	PZ	0.00000	-0.02358	0.00000	0.00000	0.00000
56	C4	S	0.13151	0.00000	0.09312	0.23315	0.56294
57	C4	PX	0.78630	0.00000	-0.11947	0.23658	0.38576
58	C4	PY	-0.47668	0.00000	0.01132	0.34802	-0.34398
59	C4	PZ	0.00000	0.01585	0.00000	0.00000	0.00000
60	C4	DXX	0.16049	0.00000	0.00462	-0.38714	-0.05322
61	C4	DYY	-0.10402	0.00000	0.08647	0.21303	0.04442
62	C4	DZZ	0.13309	0.00000	0.02062	-0.21133	0.00865
63	C4	DXY	0.33953	0.00000	-0.42773	-0.11679	0.20640

64	C4	DXZ	0.00000	0.03387	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	-0.09218	0.00000	0.00000	0.00000
66	C5	S	0.00353	0.00000	0.01350	-0.05711	0.01481
67	C5	S	0.06969	0.00000	-0.13683	0.26443	-0.05527
68	C5	PX	-0.14079	0.00000	0.13612	-0.05548	0.02111
69	C5	PY	-0.18424	0.00000	0.07632	0.21217	-0.12053
70	C5	PZ	0.00000	0.00408	0.00000	0.00000	0.00000
71	C5	S	-0.08536	0.00000	-0.00694	0.57427	-0.38136
72	C5	PX	0.36684	0.00000	-0.06941	0.04931	0.16441
73	C5	PY	0.47101	0.00000	-0.21495	0.09315	0.28421
74	C5	PZ	0.00000	-0.01602	0.00000	0.00000	0.00000
75	C5	DXX	-0.29463	0.00000	0.29226	-0.03921	-0.08136
76	C5	DYY	0.40371	0.00000	-0.29712	0.00568	0.08390
77	C5	DZZ	-0.02178	0.00000	0.09410	-0.30115	0.07367
78	C5	DXY	-0.01983	0.00000	0.08344	-0.31659	0.19302
79	C5	DXZ	0.00000	0.00036	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.01242	0.00000	0.00000	0.00000
81	C6	S	0.01174	0.00000	0.00114	-0.01667	0.00679
82	C6	S	-0.03211	0.00000	0.03766	0.06404	0.11738
83	C6	PX	0.14618	0.00000	-0.09801	0.08441	0.07618
84	C6	PY	0.03218	0.00000	0.00842	-0.04223	0.07304
85	C6	PZ	0.00000	0.00129	0.00000	0.00000	0.00000
86	C6	S	-0.57866	0.00000	-0.03019	0.37994	-0.90544
87	C6	PX	-0.95566	0.00000	0.22587	-0.04892	-0.83661
88	C6	PY	-0.13015	0.00000	0.02429	-0.09758	0.15435
89	C6	PZ	0.00000	-0.01617	0.00000	0.00000	0.00000
90	C6	DXX	0.16254	0.00000	-0.06380	-0.08622	0.01576
91	C6	DYY	-0.20778	0.00000	0.08405	0.04323	-0.09684
92	C6	DZZ	0.05468	0.00000	0.00455	-0.08785	0.03439
93	C6	DXY	0.42157	0.00000	-0.21106	-0.02602	0.06040
94	C6	DXZ	0.00000	-0.00416	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	-0.00143	0.00000	0.00000	0.00000
96	C7	S	0.01627	0.00000	0.01213	0.01764	0.12393
97	C7	S	-0.05967	0.00000	-0.05777	-0.18601	-0.52593
98	C7	PX	0.10101	0.00000	-0.14480	0.04996	-0.50752
99	C7	PY	-0.09597	0.00000	0.05669	-0.12849	-0.09881
100	C7	PZ	0.00000	0.00098	0.00000	0.00000	0.00000
101	C7	S	-1.01012	0.00000	0.10279	-0.23357	-2.54037
102	C7	PX	0.64453	0.00000	-0.19334	-0.01940	0.65015
103	C7	PY	0.08204	0.00000	0.03575	-0.09894	-0.08237
104	C7	PZ	0.00000	-0.00900	0.00000	0.00000	0.00000
105	C7	DXX	-0.00673	0.00000	-0.11605	-0.00446	-0.73029
106	C7	DYY	-0.08285	0.00000	0.14599	0.00188	0.76712
107	C7	DZZ	0.08711	0.00000	0.06831	0.10202	0.65335
108	C7	DXY	0.24648	0.00000	-0.08236	0.14791	0.40053
109	C7	DXZ	0.00000	-0.00042	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00065	0.00000	0.00000	0.00000
111	O1	S	-0.02174	0.00000	0.03003	0.05677	-0.00424
112	O1	S	-0.06448	0.00000	0.01854	0.04798	-0.03224
113	O1	PX	0.00361	0.00000	-0.00308	-0.00381	0.00440
114	O1	PY	-0.00608	0.00000	0.02153	0.05499	0.01552
115	O1	PZ	0.00000	-0.01481	0.00000	0.00000	0.00000
116	O1	S	0.46037	0.00000	-0.41479	-0.81581	0.16300
117	O1	PX	-0.19866	0.00000	-0.15781	0.06650	-0.01149

118	O1	PY	-0.17270	0.00000	-0.18847	0.23186	0.06597
119	O1	PZ	0.00000	0.06877	0.00000	0.00000	0.00000
120	O1	DXX	-0.11208	0.00000	-0.01397	0.25300	0.03996
121	O1	DYY	0.09899	0.00000	0.18524	-0.03604	-0.05822
122	O1	DZZ	-0.13145	0.00000	0.05067	0.21649	-0.01375
123	O1	DXY	0.17386	0.00000	-0.32174	-0.17195	0.13234
124	O1	DXZ	0.00000	-0.05729	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	-0.14977	0.00000	0.00000	0.00000
126	H4	S	-0.03565	0.00000	0.09228	-0.28875	0.13253
127	H4	S	-0.02751	0.00000	0.08881	-0.17269	0.04526
128	H4	PX	-0.17361	0.00000	0.20173	-0.31169	0.08410
129	H4	PY	-0.09448	0.00000	0.01729	0.21885	-0.15207
130	H4	PZ	0.00000	-0.00199	0.00000	0.00000	0.00000
131	N1	S	0.03613	0.00000	-0.01552	0.00697	0.00294
132	N1	S	-0.02891	0.00000	0.02441	-0.06368	0.00404
133	N1	PX	-0.00442	0.00000	-0.00504	0.00495	-0.02371
134	N1	PY	0.09936	0.00000	-0.02682	-0.04401	0.05013
135	N1	PZ	0.00000	-0.00040	0.00000	0.00000	0.00000
136	N1	S	-0.45477	0.00000	0.21232	-0.03638	0.06202
137	N1	PX	0.06841	0.00000	-0.00279	0.07758	0.00096
138	N1	PY	0.05631	0.00000	-0.04246	-0.12230	-0.05502
139	N1	PZ	0.00000	0.00420	0.00000	0.00000	0.00000
140	N1	DXX	0.07134	0.00000	-0.04745	0.08152	-0.16173
141	N1	DYY	0.11243	0.00000	-0.03556	-0.01497	0.18733
142	N1	DZZ	0.11176	0.00000	-0.04451	0.01490	0.01002
143	N1	DXY	0.38257	0.00000	-0.16928	-0.09427	-0.08285
144	N1	DXZ	0.00000	0.00090	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00052	0.00000	0.00000	0.00000
146	H6	S	0.00939	0.00000	-0.10995	0.43963	-0.08729
147	H6	S	0.05698	0.00000	-0.08930	0.27649	-0.04669
148	H6	PX	0.06245	0.00000	-0.17682	0.57221	-0.11630
149	H6	PY	-0.21893	0.00000	0.08216	0.15956	-0.06658
150	H6	PZ	0.00000	-0.00093	0.00000	0.00000	0.00000
151	C8	S	-0.02899	0.00000	0.00185	0.00975	-0.02446
152	C8	S	-0.20518	0.00000	0.08719	-0.03861	0.05164
153	C8	PX	-0.12877	0.00000	0.04285	0.00961	-0.03294
154	C8	PY	0.17401	0.00000	-0.06634	-0.06549	-0.21778
155	C8	PZ	0.00000	0.00006	0.00000	0.00000	0.00000
156	C8	S	1.26456	0.00000	-0.25488	-0.13479	0.81944
157	C8	PX	0.11475	0.00000	0.05854	0.15057	0.22129
158	C8	PY	-0.04178	0.00000	-0.01010	0.02830	0.80860
159	C8	PZ	0.00000	0.00053	0.00000	0.00000	0.00000
160	C8	DXX	0.24312	0.00000	-0.13852	-0.07676	-0.27063
161	C8	DYY	-0.28171	0.00000	0.13652	0.09150	0.28297
162	C8	DZZ	-0.12210	0.00000	0.00125	0.03945	-0.13307
163	C8	DXY	0.08833	0.00000	-0.05437	0.00635	-0.42037
164	C8	DXZ	0.00000	0.00168	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	-0.00035	0.00000	0.00000	0.00000
166	H8	S	0.00072	0.00000	0.12414	0.05181	0.73192
167	H8	S	-0.17716	0.00000	0.12712	0.02112	0.24212
168	H8	PX	-0.02342	0.00000	-0.16475	-0.05007	-0.95600
169	H8	PY	-0.13100	0.00000	0.06528	-0.03212	-0.00717
170	H8	PZ	0.00000	0.00216	0.00000	0.00000	0.00000
171	C10	S	0.06815	0.00000	-0.01885	-0.00686	-0.02857

172	C10	S	-0.31628	0.00000	0.06674	0.02482	0.02399
173	C10	PX	-0.08883	0.00000	0.03634	-0.08219	0.32525
174	C10	PY	0.40527	0.00000	-0.14451	-0.08390	-0.25392
175	C10	PZ	0.00000	-0.00032	0.00000	0.00000	0.00000
176	C10	S	-1.00652	0.00000	0.22597	0.09216	0.56594
177	C10	PX	-0.02733	0.00000	0.00653	-0.12838	0.02184
178	C10	PY	-0.12520	0.00000	0.00518	-0.03403	0.08364
179	C10	PZ	0.00000	0.00037	0.00000	0.00000	0.00000
180	C10	DXX	-0.47623	0.00000	0.14443	0.01262	0.38577
181	C10	DYY	0.38702	0.00000	-0.15028	-0.01738	-0.47863
182	C10	DZZ	0.37661	0.00000	-0.09496	-0.03491	-0.12158
183	C10	DXY	-0.20115	0.00000	0.06051	0.15413	-0.27076
184	C10	DXZ	0.00000	0.00018	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	-0.00032	0.00000	0.00000	0.00000
186	H16	S	0.34076	0.00000	-0.09643	0.05304	-0.34964
187	H16	S	0.24068	0.00000	-0.07155	0.03543	-0.17729
188	H16	PX	-0.40442	0.00000	0.11145	-0.05872	0.41377
189	H16	PY	0.30485	0.00000	-0.09193	-0.01547	-0.18972
190	H16	PZ	0.00000	-0.00013	0.00000	0.00000	0.00000
191	H18	S	0.31086	0.00000	-0.07886	-0.12254	0.09833
192	H18	S	0.20822	0.00000	-0.05820	-0.09852	0.00097
193	H18	PX	0.23677	0.00000	-0.05342	-0.10821	0.18093
194	H18	PY	0.42954	0.00000	-0.11291	-0.10738	-0.00558
195	H18	PZ	0.00000	-0.00020	0.00000	0.00000	0.00000
196	C9	S	0.00446	0.00000	0.00489	0.00023	0.00156
197	C9	S	-0.05035	0.00000	-0.11121	0.01756	0.02525
198	C9	PX	0.22494	0.00000	0.22789	0.02425	0.02421
199	C9	PY	-0.39396	0.00000	-0.72340	-0.05344	0.06142
200	C9	PZ	0.00000	-0.93616	0.00000	0.00000	0.00000
201	C9	S	0.01718	0.00000	0.20625	0.05685	-0.07997
202	C9	PX	0.11032	0.00000	0.09555	-0.01239	0.01638
203	C9	PY	-0.32189	0.00000	-0.62238	0.07837	0.10418
204	C9	PZ	0.00000	-0.55713	0.00000	0.00000	0.00000
205	C9	DXX	0.06524	0.00000	0.46152	0.10463	-0.09004
206	C9	DYY	-0.48476	0.00000	-1.01742	-0.11797	0.09306
207	C9	DZZ	0.42974	0.00000	0.65516	0.02691	-0.03130
208	C9	DXY	0.08953	0.00000	0.10217	-0.07092	-0.02453
209	C9	DXZ	0.00000	-1.10350	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.49943	0.00000	0.00000	0.00000
211	H3	S	0.40557	0.00000	0.74563	0.02812	-0.06534
212	H3	S	0.29232	0.00000	0.52271	-0.03563	-0.06350
213	H3	PX	0.04819	0.00000	0.19897	0.05916	-0.02394
214	H3	PY	-0.56000	0.00000	-1.00211	-0.04927	0.08310
215	H3	PZ	0.00000	-0.00307	0.00000	0.00000	0.00000
216	H5	S	-0.19784	-0.71098	-0.35269	-0.01789	0.03059
217	H5	S	-0.10270	-0.44057	-0.19370	-0.05420	0.02038
218	H5	PX	0.15861	0.50274	0.20699	0.00201	-0.00728
219	H5	PY	-0.05918	-0.25740	-0.08314	-0.00525	0.00027
220	H5	PZ	-0.18438	-0.81389	-0.35222	-0.06184	0.02568
221	H7	S	-0.19784	0.71098	-0.35269	-0.01789	0.03059
222	H7	S	-0.10270	0.44057	-0.19370	-0.05420	0.02038
223	H7	PX	0.15861	-0.50274	0.20699	0.00201	-0.00728
224	H7	PY	-0.05918	0.25740	-0.08314	-0.00525	0.00027
225	H7	PZ	0.18438	-0.81389	0.35222	0.06184	-0.02568

MO:	211	212	213	214	215
Eigenvalues:	4.01961	4.19924	4.46531	4.49945	4.55630
(ev):	109.37924	114.26708	121.50731	122.43635	123.98333

		A	A	A	A	A	
1	H1	S	0.05238	0.42060	-0.06761	-0.09032	-0.03515
2	H1	S	0.01356	0.32660	-0.14795	0.02661	-0.03198
3	H1	PX	-0.06556	-0.43544	0.01258	0.02020	0.00685
4	H1	PY	-0.01971	-0.19557	0.05414	-0.01975	-0.01138
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01999	0.04512	0.06293	0.16187	0.03114
7	C1	S	-0.04619	-0.27769	-0.29317	-1.19692	-0.17674
8	C1	PX	-0.05582	-0.30012	-0.00676	0.11692	-0.00723
9	C1	PY	0.06887	-0.08434	0.10595	-0.10577	-0.06703
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.37984	-0.05877	-0.51838	0.08766	0.06404
12	C1	PX	0.08708	-0.50947	0.61954	-0.06755	-0.00018
13	C1	PY	0.18770	0.13066	-0.38015	0.65409	0.33653
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.01559	-0.40195	0.26057	0.52667	0.07609
16	C1	DYY	0.02539	0.60482	0.08740	0.72219	0.14779
17	C1	DZZ	0.07429	0.21936	0.22961	0.65584	0.13701
18	C1	DXY	-0.10868	-0.36305	-0.07794	0.04189	0.05479
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.03254	-0.07363	0.11051	0.07582	-0.22201
22	C2	S	0.13303	0.35253	-0.74492	-0.52691	1.41148
23	C2	PX	-0.11047	-0.32000	-0.05947	-0.03800	0.10979
24	C2	PY	-0.12884	-0.19698	0.05785	-0.06610	-0.00394
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.31091	0.57541	-0.17422	-0.02858	0.81783
27	C2	PX	0.05714	-0.25511	-0.05617	0.07850	0.07984
28	C2	PY	0.13701	-0.19040	0.05197	0.01583	-0.17378
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.18451	0.40217	0.41835	0.28124	-0.92516
31	C2	DYY	-0.25284	-0.70467	0.47280	0.24147	-0.83209
32	C2	DZZ	-0.15799	-0.34741	0.43214	0.30145	-0.83647
33	C2	DXY	0.11911	0.49278	0.07797	-0.02098	-0.13922
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03354	0.03721	0.22553	0.01669	-0.00069
37	C3	S	-0.09321	-0.12448	-1.52284	-0.16268	0.02789
38	C3	PX	-0.05431	0.08836	0.03605	-0.00775	-0.15385
39	C3	PY	0.06655	-0.16434	0.05906	-0.07350	0.10518
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.65074	-0.59460	-0.22710	0.71858	-0.07820
42	C3	PX	-0.11892	0.47811	-0.62781	0.35906	0.86752
43	C3	PY	-0.33187	0.24652	-0.30534	-0.29222	-0.28731
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.16359	0.16446	0.80085	0.09009	0.04776
46	C3	DYY	0.08562	-0.02752	0.93418	0.02692	-0.16576
47	C3	DZZ	-0.12379	0.13589	0.89966	0.06567	0.02166
48	C3	DXY	0.06089	-0.48724	-0.02334	-0.08949	0.09120

49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00436	-0.00375	-0.02745	0.24471	0.02087
52	C4	S	-0.10246	0.03484	0.03021	-1.68713	-0.18352
53	C4	PX	0.00466	0.01836	-0.04067	0.03539	-0.02618
54	C4	PY	0.06286	0.15536	0.03116	0.19308	0.00069
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.21485	-0.01328	0.91840	-1.25031	-0.38393
57	C4	PX	-0.01885	-0.20606	0.37129	-0.82026	-0.41615
58	C4	PY	-0.09793	0.53027	-0.36590	-0.91350	-0.58718
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.09138	-0.56634	-0.07325	0.83555	0.14058
61	C4	DYY	0.12945	0.42866	-0.08616	1.25198	0.13297
62	C4	DZZ	0.01646	-0.04352	-0.09662	0.97941	0.10906
63	C4	DXY	0.09569	0.09651	0.05211	-0.12535	-0.04021
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02315	0.03976	-0.00807	0.22534	-0.06199
67	C5	S	-0.12148	-0.17299	0.05796	-1.38566	0.61563
68	C5	PX	0.07803	0.21768	0.01758	-0.08912	-0.01496
69	C5	PY	-0.15886	-0.30873	0.05657	0.03795	-0.13449
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.41042	-0.37465	-0.05383	-0.99791	-0.34589
72	C5	PX	0.07477	0.20863	-0.05074	-0.40540	-0.34855
73	C5	PY	-0.00342	-0.26822	0.23193	0.17674	0.23719
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00571	0.11468	-0.05639	0.84479	-0.32066
76	C5	DYY	0.05003	0.00874	-0.11059	0.90651	-0.24310
77	C5	DZZ	0.11939	0.20612	-0.02683	0.86193	-0.24736
78	C5	DXY	0.32048	0.83126	-0.00444	-0.12804	0.00947
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01696	-0.00645	0.18480	-0.00099	-0.23363
82	C6	S	0.12234	-0.05298	-1.09991	-0.05776	1.31616
83	C6	PX	-0.03291	-0.03362	-0.05681	0.01765	-0.05894
84	C6	PY	-0.09705	0.19202	-0.23172	-0.03329	0.07959
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.39371	0.13958	-2.24508	0.21419	0.28892
87	C6	PX	-0.49657	0.56608	-0.43436	0.04325	0.78034
88	C6	PY	-0.31092	0.25014	0.97916	0.15625	0.75503
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.04410	0.43170	0.58175	-0.02206	-0.79131
91	C6	DYY	0.03900	-0.39870	0.91161	0.02741	-0.96278
92	C6	DZZ	0.02936	0.01322	0.72441	-0.01041	-0.86131
93	C6	DXY	0.10864	-0.20361	0.03490	0.00351	-0.05320
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.07185	-0.05628	0.16091	-0.00690	0.16726
97	C7	S	-0.29192	0.22557	-1.12748	0.14890	-1.03616
98	C7	PX	-0.06768	0.17838	0.09264	0.01377	0.05661
99	C7	PY	0.15070	-0.19337	-0.11562	-0.04993	0.08142
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.61883	0.57561	-0.22347	-0.83128	-0.49679
102	C7	PX	0.65247	-0.08131	-0.11361	0.43866	0.04054

103	C7	PY	0.01226	-0.16872	0.39227	-0.10957	-0.57377
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.24434	0.17728	0.67985	-0.06044	0.76859
106	C7	DYY	0.30826	-0.44821	0.56582	-0.11399	0.61964
107	C7	DZZ	0.32297	-0.23907	0.64082	-0.03516	0.61664
108	C7	DXY	-0.19324	0.11906	0.07442	0.01787	-0.15719
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00788	0.04304	0.02189	-0.30999	-0.14067
112	O1	S	-0.03432	-0.02952	0.01443	-0.29474	-0.14924
113	O1	PX	0.00129	-0.01209	0.01159	-0.10694	-0.04640
114	O1	PY	0.02632	0.09279	-0.00872	0.16350	0.04107
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00284	-0.56689	-0.21340	3.76790	1.80192
117	O1	PX	0.03887	0.18628	-0.08698	0.53648	0.22410
118	O1	PY	0.07617	0.33040	0.02472	-0.23892	-0.23820
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.08159	0.29480	0.07141	-0.94077	-0.45566
121	O1	DYY	-0.04544	-0.11730	0.07566	-1.21863	-0.44666
122	O1	DZZ	0.02575	0.12811	0.07856	-1.04829	-0.48461
123	O1	DXY	0.06685	0.02756	0.02196	-0.06374	-0.03226
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.22385	0.50903	0.00094	-0.20086	0.02974
127	H4	S	0.13849	0.29796	-0.07197	-0.03274	-0.18423
128	H4	PX	0.18874	0.41591	0.00861	-0.10504	0.03014
129	H4	PY	-0.19603	-0.37822	-0.02558	0.13864	-0.00134
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01223	0.00140	-0.34702	0.02680	-0.06725
132	N1	S	0.10594	0.13094	0.28687	-0.04322	0.09092
133	N1	PX	0.11167	-0.02741	-0.15981	0.01099	-0.06525
134	N1	PY	-0.03901	0.18457	-0.20052	-0.00132	0.12438
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.05925	-0.04821	4.42827	-0.25263	1.06290
137	N1	PX	0.26939	-0.29924	0.86802	-0.10374	-0.14208
138	N1	PY	-0.36115	0.31523	0.54607	-0.04736	0.60450
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.23748	-0.20333	-1.04354	0.08676	-0.36600
141	N1	DYY	-0.24407	0.22959	-1.16156	0.07326	-0.01533
142	N1	DZZ	-0.02881	0.00515	-1.10089	0.09095	-0.21733
143	N1	DXY	0.00259	0.06411	0.02702	-0.02515	0.07938
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.18256	-0.50238	-0.08590	-0.02774	0.18270
147	H6	S	-0.05331	-0.30603	0.03516	0.05986	-0.14565
148	H6	PX	-0.22448	-0.53618	-0.05925	-0.01748	0.15721
149	H6	PY	-0.06795	-0.14587	-0.02667	0.01034	0.03025
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.02125	0.00373	0.05600	-0.01328	0.22719
152	C8	S	0.00917	0.00839	-0.47320	0.03205	-1.40937
153	C8	PX	0.02347	-0.05968	-0.12728	0.01893	-0.05201
154	C8	PY	-0.06597	0.05703	0.01759	-0.00490	0.05432
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.46260	-0.03588	-0.80560	0.42349	-0.77918

157	C8	PX	0.59320	-0.38131	1.01949	0.04977	-0.39607
158	C8	PY	0.63985	-0.05400	-0.40167	0.32567	-0.31359
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.34037	0.20348	0.36855	-0.04595	0.93621
161	C8	DYY	0.31135	-0.17232	0.14782	-0.01243	0.81223
162	C8	DZZ	-0.08884	0.01366	0.26245	-0.04932	0.87388
163	C8	DXY	0.54789	-0.12296	-0.11313	0.01978	-0.07895
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.21110	-0.21033	-0.10048	-0.00764	-0.17952
167	H8	S	-0.04600	-0.11455	0.13187	-0.11605	0.04454
168	H8	PX	-0.27900	0.24804	0.08306	-0.00346	0.16293
169	H8	PY	0.11133	-0.05603	-0.03499	-0.00304	0.06147
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00273	0.00251	0.06266	-0.00949	0.14411
172	C10	S	-0.02826	0.01936	-0.37344	0.07356	-1.03245
173	C10	PX	-0.66643	0.09712	0.00442	0.00573	0.03998
174	C10	PY	-0.20270	0.09686	0.00485	0.00441	-0.13293
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.22659	-0.00831	-0.41056	0.11917	-0.32244
177	C10	PX	-0.63937	0.12325	-0.21821	-0.08952	0.11720
178	C10	PY	-0.08717	0.05896	-0.15835	0.00267	0.07726
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.35242	0.03256	0.23775	-0.04356	0.66984
181	C10	DYY	0.35324	-0.01470	0.22984	-0.04810	0.55412
182	C10	DZZ	0.02019	0.00544	0.25101	-0.03585	0.54174
183	C10	DXY	1.13664	-0.24974	-0.08317	0.00231	0.00663
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.64166	-0.10022	-0.02476	0.01855	-0.12642
187	H16	S	0.33609	-0.03704	0.10428	0.02219	0.04429
188	H16	PX	-0.74491	0.11376	0.04591	-0.00619	0.09459
189	H16	PY	0.08201	0.01810	0.00859	0.00260	-0.01655
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.68099	0.13862	0.00024	-0.00378	-0.09496
192	H18	S	-0.37589	0.08352	-0.04942	-0.03903	0.15639
193	H18	PX	-0.67291	0.13016	-0.00405	0.00329	-0.05655
194	H18	PY	-0.42637	0.08859	0.02605	0.00426	-0.04170
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00292	0.01130	0.00487	-0.07958	-0.02992
197	C9	S	-0.00740	-0.08705	-0.03635	0.45887	0.17939
198	C9	PX	0.02418	0.06893	0.00023	-0.03155	-0.01291
199	C9	PY	0.04680	0.07240	0.00125	0.05252	0.00922
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.05380	-0.10988	0.06452	-0.56474	-0.24850
202	C9	PX	0.00913	0.04618	-0.01730	0.26417	0.09877
203	C9	PY	0.07192	0.09396	-0.03955	0.06331	0.04008
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.04568	-0.00834	0.00288	-0.16729	-0.05081
206	C9	DYY	0.06795	0.09321	0.02603	-0.31244	-0.13468
207	C9	DZZ	-0.01609	0.02582	0.02905	-0.43285	-0.15698
208	C9	DXY	-0.03038	-0.09392	-0.00212	0.04006	0.02405
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

211	H3	S	-0.04774	-0.06284	-0.00650	0.10588	0.05090
212	H3	S	-0.04305	-0.04268	0.00993	0.03247	0.01716
213	H3	PX	-0.00914	0.01227	-0.00402	0.04407	0.01424
214	H3	PY	0.05857	0.07393	0.00370	-0.02470	-0.02433
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.02019	0.01318	-0.01453	0.12670	0.04988
217	H5	S	0.01100	-0.00880	0.00125	0.03032	0.01902
218	H5	PX	-0.00938	-0.01180	0.00432	-0.07579	-0.02415
219	H5	PY	0.00234	0.00417	-0.00085	0.02840	0.00543
220	H5	PZ	0.01291	-0.01067	-0.00189	0.05548	0.02051
221	H7	S	0.02019	0.01318	-0.01453	0.12670	0.04988
222	H7	S	0.01100	-0.00880	0.00125	0.03032	0.01902
223	H7	PX	-0.00938	-0.01180	0.00432	-0.07579	-0.02415
224	H7	PY	0.00234	0.00417	-0.00085	0.02840	0.00543
225	H7	PZ	-0.01291	0.01067	0.00189	-0.05548	-0.02051

MO:	216	217	218	219	220
Eigenvalues:	4.59956	4.67304	4.70236	4.83284	4.88374
(ev):	125.16054	127.15986	127.95773	131.50831	132.89343

		A	A	A	A	A	
1	H1	S	-0.23702	-0.16601	-0.10093	0.07080	-0.21583
2	H1	S	-0.00931	0.29199	0.00026	0.05627	-0.00724
3	H1	PX	0.17444	0.20987	0.07876	-0.04839	0.20319
4	H1	PY	0.09700	0.09270	0.02133	-0.05525	0.06766
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.22343	0.16795	0.12073	-0.05839	0.22856
7	C1	S	-1.42321	-1.13744	-0.70925	0.25662	-1.27556
8	C1	PX	0.04287	0.08541	0.02106	0.02478	-0.00735
9	C1	PY	0.11549	0.13744	-0.00654	-0.03635	-0.07733
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.31807	-0.43618	-0.53642	0.57502	-1.72029
12	C1	PX	0.28932	-0.39508	0.16287	-0.37658	0.51530
13	C1	PY	-0.22476	-0.59465	0.25951	0.22574	0.17688
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	1.08640	0.95993	0.52779	-0.29664	1.05935
16	C1	DYY	0.76041	0.58369	0.46883	-0.14959	1.03708
17	C1	DZZ	0.84655	0.59650	0.46004	-0.20455	0.82433
18	C1	DXY	-0.02205	0.06129	-0.00314	0.03661	0.08725
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.18761	0.07713	-0.01431	0.05594	0.20479
22	C2	S	1.22312	-0.52336	0.19327	-0.31505	-1.15705
23	C2	PX	0.03966	-0.06708	-0.01033	-0.06408	0.02110
24	C2	PY	0.09869	-0.08269	0.15160	0.13203	0.07154
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.32372	-0.48718	-0.35597	0.27026	-1.45564
27	C2	PX	0.16691	-0.07137	-0.13398	0.25138	-0.55155
28	C2	PY	0.25386	0.30870	-0.02369	0.30788	-0.44133
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.84693	0.35837	-0.12992	0.28969	0.99797
31	C2	DYY	-0.67837	0.27481	0.00005	0.26367	0.96904
32	C2	DZZ	-0.72659	0.27167	-0.07066	0.18168	0.72728
33	C2	DXY	-0.03247	0.03215	0.08250	0.19464	0.05129

34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.20885	0.10994	-0.05899	-0.07183	-0.19306
37	C3	S	-1.33722	-0.70541	0.38799	0.39964	1.21808
38	C3	PX	0.00214	0.00140	0.08414	0.01702	-0.05621
39	C3	PY	-0.07103	-0.09750	-0.14352	0.07309	-0.02630
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.03445	-0.68501	0.83563	1.09511	0.45288
42	C3	PX	-0.43950	-0.04198	-0.12515	0.12894	0.02863
43	C3	PY	-0.57256	0.50408	-0.07284	-0.03955	0.48535
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.86781	0.45049	-0.27904	-0.34939	-0.74893
46	C3	DYY	0.83977	0.37835	-0.13241	-0.36148	-1.06712
47	C3	DZZ	0.80893	0.40979	-0.23002	-0.26199	-0.70670
48	C3	DXY	-0.03639	0.00383	-0.09388	-0.04419	0.05390
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00572	0.04456	0.02070	0.06792	-0.02227
52	C4	S	-0.14780	-0.13260	-0.20119	-0.34050	0.03381
53	C4	PX	-0.15404	-0.04261	-0.09216	0.03161	-0.13913
54	C4	PY	0.05650	0.05701	0.02844	-0.01560	0.03527
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.03088	0.59373	-0.37235	-1.08016	0.45110
57	C4	PX	0.12397	0.66453	-0.06212	-0.43289	0.39796
58	C4	PY	-0.25562	1.65213	-0.34641	-0.00526	-0.21974
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.11257	0.08827	0.16020	0.33976	-0.05545
61	C4	DYY	-0.07709	0.00284	0.05980	0.28043	-0.15458
62	C4	DZZ	0.04840	0.11247	0.09640	0.24084	-0.05926
63	C4	DXY	0.10032	0.11719	0.04748	-0.02110	0.10537
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.19065	0.05662	-0.17808	-0.16842	-0.14296
67	C5	S	1.17305	-0.64774	1.09261	0.95383	0.85926
68	C5	PX	-0.03799	-0.06620	0.01437	0.01512	0.08417
69	C5	PY	-0.06423	0.07587	-0.00255	0.04020	0.08751
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.37235	0.53776	0.66316	0.26837	1.27344
72	C5	PX	0.15225	0.71391	0.08389	0.26824	0.07745
73	C5	PY	0.01208	-0.49611	-0.08170	-0.03103	-0.30875
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.76796	0.32649	-0.75137	-0.71027	-0.63589
76	C5	DYY	-0.72151	0.36161	-0.81222	-0.81735	-0.82197
77	C5	DZZ	-0.73849	0.20112	-0.65903	-0.61452	-0.48817
78	C5	DXY	-0.01368	-0.08543	0.02731	0.05786	0.05804
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00981	0.00425	0.13073	0.17498	-0.11369
82	C6	S	0.07306	-0.10131	-0.71158	-1.01782	0.59394
83	C6	PX	-0.09500	0.01025	0.01927	0.04688	0.07034
84	C6	PY	0.02477	0.04576	-0.04893	0.00192	-0.02914
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00910	2.45219	-0.78808	0.92326	-0.28447
87	C6	PX	-0.60903	0.07322	-0.47914	-0.05260	0.21694

88	C6	PY	-0.44221	-1.42148	0.20905	-1.71882	1.01258
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.10104	-0.02436	0.50674	0.76345	-0.36687
91	C6	DYY	0.05670	-0.04021	0.60112	0.74290	-0.55509
92	C6	DZZ	0.01018	-0.00805	0.48072	0.61777	-0.38834
93	C6	DXY	-0.09288	-0.07837	0.00757	-0.02720	0.13663
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00870	0.03577	-0.25576	0.10037	-0.01818
97	C7	S	-0.00776	-0.26321	1.63117	-0.46407	0.09228
98	C7	PX	0.03972	0.04914	-0.07919	0.03125	-0.04857
99	C7	PY	-0.15294	0.05404	-0.00790	0.09633	0.14459
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.77910	0.51992	0.40229	-0.88280	0.78622
102	C7	PX	0.54319	0.40822	0.00630	0.73908	-0.63494
103	C7	PY	0.33380	-0.28523	-0.00463	-0.35477	-0.00600
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.02747	0.11113	-1.27872	0.43726	0.04081
106	C7	DYY	-0.03741	0.12216	-0.99848	0.31940	-0.02053
107	C7	DZZ	0.03235	0.12498	-0.95394	0.35207	-0.08335
108	C7	DXY	0.13214	-0.07160	0.06478	-0.14025	-0.17312
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.02841	0.30629	-0.06192	-0.00959	-0.00992
112	O1	S	-0.03270	0.42378	-0.08973	-0.08976	0.01571
113	O1	PX	-0.00639	0.08651	-0.01317	0.01191	-0.00203
114	O1	PY	0.00046	-0.09221	0.02333	0.04070	-0.01514
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.38070	-4.23414	0.86931	0.22036	0.14587
117	O1	PX	-0.02031	-0.44584	0.07920	0.24429	-0.15917
118	O1	PY	-0.13779	0.66237	-0.16846	-0.01482	-0.09894
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.12156	0.96785	-0.19648	0.13243	-0.12787
121	O1	DYY	-0.03260	0.91864	-0.17521	-0.04367	0.00664
122	O1	DZZ	-0.10487	1.06392	-0.21504	-0.06098	-0.02019
123	O1	DXY	-0.00791	0.02024	-0.00147	0.07985	-0.03983
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.11225	-0.05519	0.14563	0.17913	0.16749
127	H4	S	-0.05679	0.35752	-0.07228	0.04499	-0.04546
128	H4	PX	0.06183	-0.07908	0.10623	0.12439	0.13782
129	H4	PY	-0.04155	0.03928	-0.08104	-0.12226	-0.11381
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.08354	0.32783	-0.05731	0.19385	-0.14160
132	N1	S	-0.09199	-0.05407	0.01567	0.16417	0.03845
133	N1	PX	0.05388	0.05722	-0.02078	-0.01759	-0.05427
134	N1	PY	0.00816	0.09429	-0.08550	-0.03305	0.04110
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-1.11517	-5.37241	0.85244	-4.06551	2.54112
137	N1	PX	0.02295	-1.18051	0.27510	-0.89350	0.40758
138	N1	PY	-0.39299	-0.81665	-0.08781	-0.82270	0.63645
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.36194	0.77167	-0.13777	0.32614	-0.46444
141	N1	DYY	0.20741	0.91617	-0.25795	0.34350	-0.30390

142	N1	DZZ	0.26257	1.05857	-0.16806	0.66209	-0.44761
143	N1	DXY	-0.03213	0.00383	-0.05729	0.02178	0.08504
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.19035	-0.05189	0.01301	-0.08547	-0.23025
147	H6	S	0.00514	0.09539	-0.03824	0.10716	-0.08060
148	H6	PX	0.13605	-0.06020	0.00213	-0.11403	-0.20134
149	H6	PY	0.03208	-0.02882	0.00424	-0.04167	-0.06211
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.15084	0.16390	-0.02370	0.15775	0.11415
152	C8	S	0.91522	-1.03423	-0.00453	-0.96729	-0.62044
153	C8	PX	0.04814	0.02600	0.01005	-0.01009	0.00131
154	C8	PY	-0.10497	0.02947	0.21523	-0.09822	-0.08522
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.93127	0.64352	0.06198	0.43864	-1.37084
157	C8	PX	0.25139	-1.56695	0.33203	-0.98218	0.30543
158	C8	PY	0.54209	0.86153	0.03900	0.89092	-0.73896
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.63862	0.57649	-0.07013	0.67931	0.53040
161	C8	DYY	-0.51877	0.72134	-0.10275	0.79495	0.55356
162	C8	DZZ	-0.58103	0.59326	-0.05543	0.55504	0.40936
163	C8	DXY	0.02656	-0.03422	0.12713	-0.08655	-0.02481
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00180	-0.12087	0.27993	-0.16621	0.00298
167	H8	S	-0.13230	-0.23539	-0.11884	-0.20858	0.17791
168	H8	PX	-0.02840	0.03460	-0.26200	0.10948	0.04597
169	H8	PY	-0.04558	0.03204	0.01786	0.02466	0.02014
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.17145	0.11681	0.28615	-0.10806	-0.14820
172	C10	S	1.15690	-0.88498	-1.78566	0.61256	0.90562
173	C10	PX	-0.02157	0.02057	0.00238	0.01321	0.01245
174	C10	PY	0.09383	-0.16419	-0.02108	-0.11004	-0.04015
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.56679	0.36499	-0.92199	0.98859	0.26158
177	C10	PX	-0.12299	0.50031	-0.14692	0.30103	-0.08463
178	C10	PY	0.01449	0.38533	-0.14687	0.30326	-0.03250
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.78854	0.62460	1.32665	-0.49590	-0.76275
181	C10	DYY	-0.70612	0.44062	1.28688	-0.61176	-0.74012
182	C10	DZZ	-0.64096	0.42342	1.04785	-0.37656	-0.50747
183	C10	DXY	-0.01251	0.08550	0.04390	0.03826	-0.00523
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.14073	-0.18207	-0.19152	0.04038	0.15849
187	H16	S	-0.05472	-0.09818	0.20777	-0.18720	-0.04903
188	H16	PX	-0.11586	0.08662	0.20409	-0.09337	-0.14652
189	H16	PY	0.02565	-0.03635	-0.06475	0.03210	0.05307
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.11504	-0.08872	-0.25285	0.11579	0.13525
192	H18	S	-0.14119	0.27903	0.08047	0.04618	-0.10210
193	H18	PX	0.08603	-0.06932	-0.19088	0.07837	0.11056
194	H18	PY	0.06744	-0.08711	-0.14997	0.05747	0.10958
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

196	C9	S	-0.00942	0.07415	-0.05039	-0.31279	0.13478
197	C9	S	0.02628	-0.47960	0.30243	1.79162	-0.75850
198	C9	PX	-0.01958	0.00203	-0.01503	-0.00527	-0.01631
199	C9	PY	0.00294	-0.01282	0.00145	0.00964	-0.00665
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.03700	0.51542	0.04841	1.19174	-0.53494
202	C9	PX	-0.01943	-0.22675	0.01835	0.05833	-0.06863
203	C9	PY	-0.05574	-0.14440	0.02342	-0.10667	0.06237
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.01334	0.17870	-0.17734	-1.28943	0.56455
206	C9	DYY	-0.02663	0.36710	-0.21508	-1.33828	0.58301
207	C9	DZZ	-0.04728	0.36473	-0.24007	-1.36087	0.56716
208	C9	DXY	0.02284	-0.03469	0.02382	0.04139	-0.00065
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.01234	-0.12238	0.04237	0.20883	-0.09203
212	H3	S	0.02296	-0.01248	-0.02796	-0.16867	0.06123
213	H3	PX	0.00101	-0.02439	0.00955	0.04760	-0.02109
214	H3	PY	-0.00907	0.07541	-0.03427	-0.21223	0.09395
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00165	-0.11447	0.04554	0.17447	-0.07017
217	H5	S	0.00925	-0.03190	-0.00912	-0.24676	0.13651
218	H5	PX	-0.00526	0.04561	-0.02418	-0.11078	0.04381
219	H5	PY	0.00700	-0.00144	0.01160	0.07179	-0.02718
220	H5	PZ	0.01224	-0.04430	0.03577	0.16701	-0.05924
221	H7	S	0.00165	-0.11447	0.04554	0.17447	-0.07017
222	H7	S	0.00925	-0.03190	-0.00912	-0.24676	0.13651
223	H7	PX	-0.00526	0.04561	-0.02418	-0.11078	0.04381
224	H7	PY	0.00700	-0.00144	0.01160	0.07179	-0.02718
225	H7	PZ	-0.01224	0.04430	-0.03577	-0.16701	0.05924

MO:	221	222	223	224	225
Eigenvalues:	4.89251	4.92769	5.06080	5.28515	0.00000
(ev):	133.13204	134.08936	137.71148	143.81642	0.00000

		A	A	A	A	A	
1	H1	S	0.09346	-0.06041	0.06639	-0.21002	0.00000
2	H1	S	0.04702	-0.10299	-0.11770	0.05064	0.00000
3	H1	PX	-0.10617	0.01232	-0.07722	0.21722	0.00000
4	H1	PY	-0.06427	0.00144	-0.03359	0.06089	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.08281	0.03569	-0.04754	0.17578	0.00000
7	C1	S	0.47862	-0.12461	0.36196	-1.08680	0.00000
8	C1	PX	-0.00939	-0.15496	0.06027	-0.08382	0.00000
9	C1	PY	-0.04214	0.15465	-0.12731	-0.03084	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.33368	-0.88738	-0.35963	-0.77295	0.00000
12	C1	PX	-0.18921	0.38004	0.32227	0.26037	0.00000
13	C1	PY	1.04042	0.80883	0.02492	-0.11260	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.42772	0.25985	-0.39589	1.00996	0.00000
16	C1	DYY	-0.32503	0.17235	-0.23743	1.06417	0.00000
17	C1	DZZ	-0.30377	0.11503	-0.16049	0.57514	0.00000
18	C1	DXY	-0.07650	-0.20896	0.09998	0.02774	0.00000

19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02437	0.19802	0.12539	-0.12073	0.00000
22	C2	S	0.42765	-0.96543	-0.80088	0.78448	0.00000
23	C2	PX	-0.04067	0.02161	-0.01137	-0.04662	0.00000
24	C2	PY	0.09087	0.00956	0.09658	-0.04038	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.23847	-1.25845	-0.49613	0.54674	0.00000
27	C2	PX	-0.20649	-0.59415	0.10130	0.13753	0.00000
28	C2	PY	0.11268	0.00428	0.11199	0.49312	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.26847	0.91708	0.72894	-0.70034	0.00000
31	C2	DYY	-0.28255	0.73894	0.68465	-0.75367	0.00000
32	C2	DZZ	-0.09857	0.71030	0.41462	-0.39118	0.00000
33	C2	DXY	0.15299	0.07508	0.08880	0.02072	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00106	0.11886	-0.05102	-0.23896	0.00000
37	C3	S	-0.06705	-0.68532	0.14849	1.31333	0.00000
38	C3	PX	0.02836	-0.06362	-0.05113	-0.04128	0.00000
39	C3	PY	0.05840	0.03274	0.10010	0.11990	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.92839	0.77741	0.98672	3.54694	0.00000
42	C3	PX	0.92653	1.15505	-0.61171	-0.45155	0.00000
43	C3	PY	0.01278	-0.58529	0.44803	-1.49973	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.11252	0.49300	-0.11666	-0.99628	0.00000
46	C3	DYY	0.11879	0.54992	-0.32746	-1.42173	0.00000
47	C3	DZZ	0.00964	0.45045	-0.16608	-0.80478	0.00000
48	C3	DXY	-0.09812	-0.02578	0.06662	0.00518	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.05296	-0.33158	0.15541	-0.16242	0.00000
52	C4	S	0.08884	1.70011	-0.98668	0.96792	0.00000
53	C4	PX	-0.00730	-0.07317	0.02185	-0.07101	0.00000
54	C4	PY	-0.01102	-0.03980	-0.00560	0.03009	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-1.70585	-0.41176	-0.24861	0.79490	0.00000
57	C4	PX	-0.03679	-0.35053	0.32155	0.01884	0.00000
58	C4	PY	-1.32242	-2.80458	0.27834	-0.64663	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.14618	-1.39938	0.82027	-0.89523	0.00000
61	C4	DYY	-0.07287	-1.52755	0.85078	-0.92386	0.00000
62	C4	DZZ	-0.14875	-1.09457	0.52801	-0.51989	0.00000
63	C4	DXY	-0.09316	0.05196	-0.05459	0.08533	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.07279	-0.00762	-0.16721	0.11891	0.00000
67	C5	S	0.24223	-0.04684	1.00836	-0.76651	0.00000
68	C5	PX	-0.00013	0.12863	0.02194	-0.01775	0.00000
69	C5	PY	0.02754	0.11305	0.06007	-0.05061	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.64915	-0.08422	0.89446	-1.09936	0.00000
72	C5	PX	0.31477	-0.20223	0.23080	-0.03810	0.00000

73	C5	PY	-0.13743	0.21329	-0.08945	0.27026	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.18161	0.12279	-0.83276	0.68019	0.00000
76	C5	DYY	-0.22224	-0.13890	-0.91561	0.72201	0.00000
77	C5	DZZ	-0.25735	0.00963	-0.57765	0.38957	0.00000
78	C5	DXY	0.07328	0.19239	0.00689	0.03912	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.21712	-0.10956	-0.02869	0.17258	0.00000
82	C6	S	-1.30622	0.67355	0.33600	-0.94616	0.00000
83	C6	PX	0.01006	0.02866	0.05497	0.03664	0.00000
84	C6	PY	-0.00620	0.05163	0.05234	-0.03197	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	1.61407	2.29136	0.20874	-1.58260	0.00000
87	C6	PX	-0.12085	-0.00564	-0.44926	-1.27490	0.00000
88	C6	PY	-1.38513	-0.04505	-0.87342	-0.11920	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.94364	-0.54792	-0.19026	0.85472	0.00000
91	C6	DYY	1.03417	-0.58832	-0.33861	0.85364	0.00000
92	C6	DZZ	0.76754	-0.38966	-0.10778	0.58259	0.00000
93	C6	DXY	-0.09342	0.03984	0.02196	-0.07114	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.04941	0.03224	0.22165	0.19696	0.00000
97	C7	S	-0.01281	0.00915	-1.37657	-0.88369	0.00000
98	C7	PX	0.04173	0.03952	-0.00831	-0.06528	0.00000
99	C7	PY	0.02768	-0.08473	-0.00666	0.11046	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.74996	-1.71308	-0.94904	-3.34480	0.00000
102	C7	PX	1.04456	0.78614	0.34438	1.50370	0.00000
103	C7	PY	-0.67554	-0.57788	0.26874	-0.07256	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.05693	0.01688	1.31150	1.13803	0.00000
106	C7	DYY	0.02234	-0.00773	0.97939	0.80039	0.00000
107	C7	DZZ	0.16890	0.10434	0.77049	0.62722	0.00000
108	C7	DXY	-0.06143	0.05737	0.03050	-0.14478	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.29479	-0.31360	0.00288	-0.00679	0.00000
112	O1	S	-0.40830	-0.72873	0.12183	-0.13395	0.00000
113	O1	PX	-0.09187	-0.05487	-0.00493	0.00594	0.00000
114	O1	PY	0.07987	0.03579	0.03988	-0.04355	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	4.30221	5.26465	-0.30448	0.43167	0.00000
117	O1	PX	0.10611	0.26452	-0.05632	-0.02207	0.00000
118	O1	PY	-0.86678	-1.44792	0.27550	-0.35403	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-1.16238	-0.99111	-0.05036	0.00698	0.00000
121	O1	DYY	-0.86669	-0.50778	-0.21346	0.22990	0.00000
122	O1	DZZ	-0.96421	-1.17050	0.07947	-0.09158	0.00000
123	O1	DXY	-0.12945	0.08457	-0.06473	0.04718	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.08071	0.07338	0.18114	-0.12123	0.00000

127	H4	S	0.02883	-0.11161	-0.02750	0.05060	0.00000
128	H4	PX	0.04064	0.07618	0.13890	-0.10360	0.00000
129	H4	PY	-0.00147	-0.03597	-0.13509	0.10492	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.21093	0.14726	0.09760	-0.00031	0.00000
132	N1	S	0.17583	-0.02917	-0.13189	-0.00016	0.00000
133	N1	PX	-0.02006	0.07564	0.10082	-0.01716	0.00000
134	N1	PY	-0.06514	0.11983	0.08081	-0.08267	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-4.42498	-2.30867	-1.49012	-0.11350	0.00000
137	N1	PX	-0.94960	-0.44646	0.03209	0.16656	0.00000
138	N1	PY	-1.01870	-0.39475	-0.41104	-0.35322	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.39911	0.46477	0.50419	0.04735	0.00000
141	N1	DYY	0.32443	0.50624	0.38808	-0.16000	0.00000
142	N1	DZZ	0.72498	0.42907	0.23110	0.02707	0.00000
143	N1	DXY	-0.02206	-0.00108	-0.03864	-0.04840	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.03335	-0.20908	-0.15992	0.16014	0.00000
147	H6	S	-0.08007	-0.09102	0.13545	0.00762	0.00000
148	H6	PX	0.01559	-0.19285	-0.17869	0.14517	0.00000
149	H6	PY	0.02045	-0.05205	-0.05673	0.04058	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.11536	-0.03803	-0.22898	-0.12074	0.00000
152	C8	S	-0.80719	0.18561	1.43806	0.61520	0.00000
153	C8	PX	0.00518	0.03596	-0.02563	-0.02623	0.00000
154	C8	PY	-0.05986	0.02921	0.07084	0.01051	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.84140	1.04860	1.47076	1.45934	0.00000
157	C8	PX	-1.02884	-0.44385	0.16645	0.53095	0.00000
158	C8	PY	1.49287	0.72345	0.32873	1.14297	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.51150	-0.22073	-1.07312	-0.45797	0.00000
161	C8	DYY	0.66431	-0.16036	-1.34656	-0.69701	0.00000
162	C8	DZZ	0.40703	-0.13816	-0.80498	-0.39763	0.00000
163	C8	DXY	-0.04165	0.04173	-0.00788	-0.02217	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.05397	-0.00950	-0.30967	-0.30024	0.00000
167	H8	S	-0.27934	-0.18689	0.02933	-0.25497	0.00000
168	H8	PX	0.00846	-0.00669	0.29606	0.28165	0.00000
169	H8	PY	0.04348	0.02889	-0.04631	-0.01240	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.02941	0.06726	0.14305	0.05454	0.00000
172	C10	S	0.13818	-0.40920	-0.82223	-0.26165	0.00000
173	C10	PX	0.01247	0.00586	-0.03342	-0.01735	0.00000
174	C10	PY	-0.09568	0.00428	0.17395	0.12645	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	1.05459	0.06772	-0.61864	0.14606	0.00000
177	C10	PX	0.21109	0.02124	-0.00649	-0.27023	0.00000
178	C10	PY	0.33826	0.05003	-0.07421	0.01936	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.11395	0.35014	0.76414	0.29009	0.00000

181	C10	DYY	-0.25076	0.32313	0.86239	0.34212	0.00000
182	C10	DZZ	-0.09171	0.22821	0.45047	0.16389	0.00000
183	C10	DXY	0.06360	0.03468	-0.09010	-0.08222	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.01345	-0.05988	-0.17128	-0.05348	0.00000
187	H16	S	-0.13817	0.00955	0.09842	0.10513	0.00000
188	H16	PX	-0.02980	0.06282	0.17986	0.08230	0.00000
189	H16	PY	0.00684	-0.02542	-0.05895	-0.02022	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.02688	-0.08358	-0.12739	-0.05548	0.00000
192	H18	S	0.03786	0.03155	0.08875	-0.06606	0.00000
193	H18	PX	0.01532	-0.05952	-0.10154	-0.03501	0.00000
194	H18	PY	0.00276	-0.05858	-0.10774	-0.02983	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.29822	-0.10087	0.07642	-0.03611	0.00000
197	C9	S	-1.62497	0.65390	-0.42883	0.19492	0.00000
198	C9	PX	-0.00664	0.03848	-0.03491	0.02533	0.00000
199	C9	PY	-0.00924	0.00335	-0.00482	0.00743	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-1.91832	-0.24309	-0.35666	0.20795	0.00000
202	C9	PX	0.07457	0.09937	0.00461	-0.04599	0.00000
203	C9	PY	0.39597	0.22999	0.01075	-0.01508	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	1.36754	-0.34854	0.35046	-0.17750	0.00000
206	C9	DYY	1.22742	-0.52374	0.34758	-0.17139	0.00000
207	C9	DZZ	1.22523	-0.45998	0.30688	-0.14085	0.00000
208	C9	DXY	-0.00551	0.02695	0.00728	-0.00537	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.14699	0.13096	-0.05146	0.02488	0.00000
212	H3	S	0.13980	-0.05010	0.03971	-0.01266	0.00000
213	H3	PX	-0.03433	0.00266	-0.00059	-0.00429	0.00000
214	H3	PY	0.18446	-0.12806	0.07016	-0.04185	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.06975	0.12650	-0.03607	0.01048	0.00000
217	H5	S	0.34042	0.02561	0.07178	-0.01627	0.00000
218	H5	PX	0.08325	-0.03232	0.01390	-0.00241	0.00000
219	H5	PY	-0.08522	-0.00953	-0.00871	0.00298	0.00000
220	H5	PZ	-0.14281	0.06738	-0.03657	0.02290	0.00000
221	H7	S	-0.06975	0.12650	-0.03607	0.01048	0.00000
222	H7	S	0.34042	0.02561	0.07178	-0.01627	0.00000
223	H7	PX	0.08325	-0.03232	0.01390	-0.00241	0.00000
224	H7	PY	-0.08522	-0.00953	-0.00871	0.00298	0.00000
225	H7	PZ	0.14281	-0.06738	0.03657	-0.02290	0.00000

Mulliken Population Analysis

AO	atom type	Occupancy
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1	H1 S	0.532517
2	H1 S	0.298367
3	H1 PX	0.009181

4	H1	PY	0.002289
5	H1	PZ	0.003103
6	C1	S	1.996405
7	C1	S	0.655863
8	C1	PX	0.726659
9	C1	PY	0.716440
10	C1	PZ	0.597250
11	C1	S	0.437520
12	C1	PX	0.278377
13	C1	PY	0.218376
14	C1	PZ	0.530178
15	C1	DXX	0.018328
16	C1	DYY	0.019897
17	C1	DZZ	-0.017491
18	C1	DXY	0.014336
19	C1	DXZ	0.005073
20	C1	DYZ	0.005884
21	C2	S	1.996577
22	C2	S	0.674998
23	C2	PX	0.724961
24	C2	PY	0.759276
25	C2	PZ	0.518959
26	C2	S	0.465593
27	C2	PX	0.301499
28	C2	PY	0.165506
29	C2	PZ	0.450104
30	C2	DXX	0.017019
31	C2	DYY	0.020276
32	C2	DZZ	-0.018189
33	C2	DXY	0.016380
34	C2	DXZ	0.002249
35	C2	DYZ	0.008470
36	C3	S	1.996663
37	C3	S	0.673620
38	C3	PX	0.721380
39	C3	PY	0.755201
40	C3	PZ	0.534254
41	C3	S	0.433570
42	C3	PX	0.211720
43	C3	PY	0.230966
44	C3	PZ	0.451643
45	C3	DXX	0.017682
46	C3	DYY	0.031068
47	C3	DZZ	-0.017546
48	C3	DXY	0.014666
49	C3	DXZ	0.004221
50	C3	DYZ	0.011640
51	C4	S	1.996668
52	C4	S	0.679027
53	C4	PX	0.774123
54	C4	PY	0.627839
55	C4	PZ	0.520384
56	C4	S	0.341095
57	C4	PX	0.142984

58	C4	PY	0.030891
59	C4	PZ	0.386812
60	C4	DXX	0.024767
61	C4	DYY	0.031904
62	C4	DZZ	-0.020395
63	C4	DXY	0.022756
64	C4	DXZ	0.008435
65	C4	DYZ	0.019842
66	C5	S	1.996586
67	C5	S	0.674449
68	C5	PX	0.703647
69	C5	PY	0.772905
70	C5	PZ	0.515694
71	C5	S	0.505642
72	C5	PX	0.252806
73	C5	PY	0.246684
74	C5	PZ	0.461436
75	C5	DXX	0.016760
76	C5	DYY	0.021398
77	C5	DZZ	-0.018695
78	C5	DXY	0.015684
79	C5	DXZ	0.003175
80	C5	DYZ	0.007607
81	C6	S	1.996714
82	C6	S	0.692307
83	C6	PX	0.727693
84	C6	PY	0.750531
85	C6	PZ	0.487710
86	C6	S	0.343431
87	C6	PX	0.190641
88	C6	PY	0.130764
89	C6	PZ	0.371023
90	C6	DXX	0.020123
91	C6	DYY	0.030987
92	C6	DZZ	-0.019967
93	C6	DXY	0.030036
94	C6	DXZ	0.005444
95	C6	DYZ	0.016082
96	C7	S	1.996657
97	C7	S	0.670549
98	C7	PX	0.728845
99	C7	PY	0.733341
100	C7	PZ	0.536088
101	C7	S	0.448949
102	C7	PX	0.320615
103	C7	PY	0.186017
104	C7	PZ	0.480038
105	C7	DXX	0.022761
106	C7	DYY	0.014997
107	C7	DZZ	-0.017778
108	C7	DXY	0.016465
109	C7	DXZ	0.003892
110	C7	DYZ	0.007348
111	O1	S	1.995297

112	01	S	0.885512
113	01	PX	0.942983
114	01	PY	0.859023
115	01	PZ	1.115339
116	01	S	0.948862
117	01	PX	0.597882
118	01	PY	0.511108
119	01	PZ	0.738701
120	01	DXX	0.016537
121	01	DYY	0.025687
122	01	DZZ	-0.000113
123	01	DXY	0.006043
124	01	DXZ	0.002863
125	01	DYZ	0.004840
126	H4	S	0.531560
127	H4	S	0.276527
128	H4	PX	0.005579
129	H4	PY	0.006053
130	H4	PZ	0.002260
131	N1	S	1.996242
132	N1	S	0.787125
133	N1	PX	0.865540
134	N1	PY	0.833170
135	N1	PZ	0.661960
136	N1	S	0.962512
137	N1	PX	0.516183
138	N1	PY	0.371284
139	N1	PZ	0.545098
140	N1	DXX	0.008194
141	N1	DYY	0.014474
142	N1	DZZ	-0.011320
143	N1	DXY	0.008872
144	N1	DXZ	0.004584
145	N1	DYZ	0.011447
146	H6	S	0.530699
147	H6	S	0.276199
148	H6	PX	0.009342
149	H6	PY	0.002422
150	H6	PZ	0.002302
151	C8	S	1.996661
152	C8	S	0.680929
153	C8	PX	0.660898
154	C8	PY	0.774976
155	C8	PZ	0.535776
156	C8	S	0.377242
157	C8	PX	0.097228
158	C8	PY	0.120073
159	C8	PZ	0.427158
160	C8	DXX	0.020848
161	C8	DYY	0.029138
162	C8	DZZ	-0.019142
163	C8	DXY	0.025485
164	C8	DXZ	0.010042
165	C8	DYZ	0.010054

166	H8	S	0.531217
167	H8	S	0.294522
168	H8	PX	0.010160
169	H8	PY	0.001670
170	H8	PZ	0.002661
171	C10	S	1.996636
172	C10	S	0.678138
173	C10	PX	0.725035
174	C10	PY	0.768638
175	C10	PZ	0.470293
176	C10	S	0.565066
177	C10	PX	0.360903
178	C10	PY	0.244104
179	C10	PZ	0.451542
180	C10	DXX	0.012351
181	C10	DYY	0.018690
182	C10	DZZ	-0.020290
183	C10	DXY	0.013151
184	C10	DXZ	0.000362
185	C10	DYZ	0.007672
186	H16	S	0.533306
187	H16	S	0.308514
188	H16	PX	0.009115
189	H16	PY	0.002490
190	H16	PZ	0.002273
191	H18	S	0.529207
192	H18	S	0.291436
193	H18	PX	0.006576
194	H18	PY	0.005231
195	H18	PZ	0.002164
196	C9	S	1.996709
197	C9	S	0.648252
198	C9	PX	0.572181
199	C9	PY	0.686169
200	C9	PZ	0.722477
201	C9	S	0.547280
202	C9	PX	0.151609
203	C9	PY	0.318498
204	C9	PZ	0.322838
205	C9	DXX	0.012056
206	C9	DYY	0.010736
207	C9	DZZ	0.004387
208	C9	DXY	0.014913
209	C9	DXZ	0.020755
210	C9	DYZ	0.003392
211	H3	S	0.540886
212	H3	S	0.304305
213	H3	PX	0.001138
214	H3	PY	0.009288
215	H3	PZ	0.002049
216	H5	S	0.540933
217	H5	S	0.327826
218	H5	PX	0.003466
219	H5	PY	0.002066

220	H5	PZ	0.007116
221	H7	S	0.540933
222	H7	S	0.327826
223	H7	PX	0.003466
224	H7	PY	0.002066
225	H7	PZ	0.007116

Atom	Occupancy	Charge
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H1	0.845457	0.154543
C1	6.203094	-0.203094
C2	6.103680	-0.103680
C3	6.070746	-0.070746
C4	5.587132	0.412868
C5	6.175780	-0.175780
C6	5.773520	0.226480
C7	6.148785	-0.148785
O1	8.650564	-0.650564
H4	0.821980	0.178020
N1	7.575365	-0.575365
H6	0.820965	0.179035
C8	5.747366	0.252634
H8	0.840231	0.159769
C10	6.292292	-0.292292
H16	0.855698	0.144302
H18	0.834613	0.165387
C9	6.032253	-0.032253
H3	0.857666	0.142334
H5	0.881406	0.118594
H7	0.881406	0.118594

Total Charge = 0.000000

Natural Atomic Orbital Populations

Nao	Atom	Type	Basis	Occupancy
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1	H1	S	MIN	0.760102
2	H1	S	RYD	0.000860
3	H1	PX	RYD	0.000507
4	H1	PY	RYD	0.000070
5	H1	PZ	RYD	0.000117
6	C1	S	MIN	1.998920
7	C1	S	MIN	0.938227
8	C1	S	RYD	0.000856
9	C1	S	RYD	0.000027
10	C1	PX	MIN	1.201661
11	C1	PX	RYD	0.004427
12	C1	PY	MIN	1.065741
13	C1	PY	RYD	0.005363
14	C1	PZ	MIN	1.134184

15	C1	PZ	RVD	0.002329
16	C1	DXY	RVD	0.001729
17	C1	DXZ	RVD	0.001214
18	C1	DYZ	RVD	0.000560
19	C1	DXX-YY	RVD	0.001401
20	C1	D3ZZ-RR	RVD	0.001197
21	C2	S	MIN	1.998987
22	C2	S	MIN	0.959355
23	C2	S	RVD	0.001088
24	C2	S	RVD	0.000036
25	C2	PX	MIN	1.186574
26	C2	PX	RVD	0.005910
27	C2	PY	MIN	1.075491
28	C2	PY	RVD	0.006953
29	C2	PZ	MIN	0.976752
30	C2	PZ	RVD	0.001688
31	C2	DXY	RVD	0.001824
32	C2	DXZ	RVD	0.000417
33	C2	DYZ	RVD	0.001288
34	C2	DXX-YY	RVD	0.001505
35	C2	D3ZZ-RR	RVD	0.001225
36	C3	S	MIN	1.998989
37	C3	S	MIN	0.878637
38	C3	S	RVD	0.001423
39	C3	S	RVD	0.000050
40	C3	PX	MIN	1.075588
41	C3	PX	RVD	0.008844
42	C3	PY	MIN	1.106043
43	C3	PY	RVD	0.004179
44	C3	PZ	MIN	1.013808
45	C3	PZ	RVD	0.001066
46	C3	DXY	RVD	0.001368
47	C3	DXZ	RVD	0.000397
48	C3	DYZ	RVD	0.001620
49	C3	DXX-YY	RVD	0.001625
50	C3	D3ZZ-RR	RVD	0.001064
51	C4	S	MIN	1.998783
52	C4	S	MIN	0.822480
53	C4	S	RVD	0.001487
54	C4	S	RVD	0.000114
55	C4	PX	MIN	1.071846
56	C4	PX	RVD	0.005692
57	C4	PY	MIN	0.753903
58	C4	PY	RVD	0.009798
59	C4	PZ	MIN	0.926714
60	C4	PZ	RVD	0.001710
61	C4	DXY	RVD	0.002106
62	C4	DXZ	RVD	0.001076
63	C4	DYZ	RVD	0.002641
64	C4	DXX-YY	RVD	0.002773
65	C4	D3ZZ-RR	RVD	0.001038
66	C5	S	MIN	1.999024
67	C5	S	MIN	0.966354
68	C5	S	RVD	0.000852

69	C5	S	RYD	0.000031
70	C5	PX	MIN	1.102095
71	C5	PX	RYD	0.005945
72	C5	PY	MIN	1.154844
73	C5	PY	RYD	0.006763
74	C5	PZ	MIN	0.983121
75	C5	PZ	RYD	0.001731
76	C5	DXY	RYD	0.001684
77	C5	DXZ	RYD	0.000281
78	C5	DYZ	RYD	0.001397
79	C5	DXX-YY	RYD	0.001711
80	C5	D3ZZ-RR	RYD	0.001302
81	C6	S	MIN	1.999151
82	C6	S	MIN	0.837925
83	C6	S	RYD	0.003711
84	C6	S	RYD	0.000112
85	C6	PX	MIN	1.033983
86	C6	PX	RYD	0.008355
87	C6	PY	MIN	0.948168
88	C6	PY	RYD	0.009704
89	C6	PZ	MIN	0.875846
90	C6	PZ	RYD	0.001174
91	C6	DXY	RYD	0.002901
92	C6	DXZ	RYD	0.000530
93	C6	DYZ	RYD	0.002381
94	C6	DXX-YY	RYD	0.001822
95	C6	D3ZZ-RR	RYD	0.001023
96	C7	S	MIN	1.998873
97	C7	S	MIN	0.953736
98	C7	S	RYD	0.000711
99	C7	S	RYD	0.000041
100	C7	PX	MIN	1.200778
101	C7	PX	RYD	0.004175
102	C7	PY	MIN	1.040786
103	C7	PY	RYD	0.005468
104	C7	PZ	MIN	1.008539
105	C7	PZ	RYD	0.001671
106	C7	DXY	RYD	0.001779
107	C7	DXZ	RYD	0.000860
108	C7	DYZ	RYD	0.000911
109	C7	DXX-YY	RYD	0.001433
110	C7	D3ZZ-RR	RYD	0.001216
111	O1	S	MIN	1.999715
112	O1	S	MIN	1.570738
113	O1	S	RYD	0.000895
114	O1	S	RYD	0.000026
115	O1	PX	MIN	1.642862
116	O1	PX	RYD	0.002596
117	O1	PY	MIN	1.499321
118	O1	PY	RYD	0.001512
119	O1	PZ	MIN	1.874311
120	O1	PZ	RYD	0.003659
121	O1	DXY	RYD	0.001613
122	O1	DXZ	RYD	0.001127

123	O1	DYZ	RVD	0.001173
124	O1	DXX-YY	RVD	0.003951
125	O1	D3ZZ-RR	RVD	0.002029
126	H4	S	MIN	0.749192
127	H4	S	RVD	0.000751
128	H4	PX	RVD	0.000309
129	H4	PY	RVD	0.000321
130	H4	PZ	RVD	0.000066
131	N1	S	MIN	1.999380
132	N1	S	MIN	1.379731
133	N1	S	RVD	0.000496
134	N1	S	RVD	0.000017
135	N1	PX	MIN	1.511466
136	N1	PX	RVD	0.004266
137	N1	PY	MIN	1.371089
138	N1	PY	RVD	0.003967
139	N1	PZ	MIN	1.227123
140	N1	PZ	RVD	0.001209
141	N1	DXY	RVD	0.002218
142	N1	DXZ	RVD	0.001760
143	N1	DYZ	RVD	0.002970
144	N1	DXX-YY	RVD	0.004686
145	N1	D3ZZ-RR	RVD	0.002870
146	H6	S	MIN	0.748692
147	H6	S	RVD	0.000747
148	H6	PX	RVD	0.000524
149	H6	PY	RVD	0.000079
150	H6	PZ	RVD	0.000072
151	C8	S	MIN	1.999037
152	C8	S	MIN	0.866006
153	C8	S	RVD	0.002899
154	C8	S	RVD	0.000106
155	C8	PX	MIN	0.907783
156	C8	PX	RVD	0.009129
157	C8	PY	MIN	1.089210
158	C8	PY	RVD	0.008116
159	C8	PZ	MIN	1.005298
160	C8	PZ	RVD	0.001574
161	C8	DXY	RVD	0.002297
162	C8	DXZ	RVD	0.001228
163	C8	DYZ	RVD	0.001517
164	C8	DXX-YY	RVD	0.002114
165	C8	D3ZZ-RR	RVD	0.001111
166	H8	S	MIN	0.762543
167	H8	S	RVD	0.000423
168	H8	PX	RVD	0.000592
169	H8	PY	RVD	0.000018
170	H8	PZ	RVD	0.000096
171	C10	S	MIN	1.998991
172	C10	S	MIN	1.045350
173	C10	S	RVD	0.001147
174	C10	S	RVD	0.000015
175	C10	PX	MIN	1.213224
176	C10	PX	RVD	0.004486

177	C10	PY	MIN	1.134888
178	C10	PY	RYD	0.003455
179	C10	PZ	MIN	0.904125
180	C10	PZ	RYD	0.002294
181	C10	DXY	RYD	0.001829
182	C10	DXZ	RYD	0.000071
183	C10	DYZ	RYD	0.001483
184	C10	DXX-YY	RYD	0.002032
185	C10	D3ZZ-RR	RYD	0.001512
186	H16	S	MIN	0.782926
187	H16	S	RYD	0.000407
188	H16	PX	RYD	0.000547
189	H16	PY	RYD	0.000073
190	H16	PZ	RYD	0.000088
191	H18	S	MIN	0.766048
192	H18	S	RYD	0.000814
193	H18	PX	RYD	0.000383
194	H18	PY	RYD	0.000240
195	H18	PZ	RYD	0.000075
196	C9	S	MIN	1.999446
197	C9	S	MIN	1.081286
198	C9	S	RYD	0.001539
199	C9	S	RYD	0.000031
200	C9	PX	MIN	0.814459
201	C9	PX	RYD	0.003582
202	C9	PY	MIN	1.119362
203	C9	PY	RYD	0.003414
204	C9	PZ	MIN	1.206820
205	C9	PZ	RYD	0.000454
206	C9	DXY	RYD	0.002107
207	C9	DXZ	RYD	0.002936
208	C9	DYZ	RYD	0.000667
209	C9	DXX-YY	RYD	0.002293
210	C9	D3ZZ-RR	RYD	0.002076
211	H3	S	MIN	0.783083
212	H3	S	RYD	0.000419
213	H3	PX	RYD	0.000025
214	H3	PY	RYD	0.000607
215	H3	PZ	RYD	0.000030
216	H5	S	MIN	0.806803
217	H5	S	RYD	0.001421
218	H5	PX	RYD	0.000176
219	H5	PY	RYD	0.000059
220	H5	PZ	RYD	0.000484
221	H7	S	MIN	0.806803
222	H7	S	RYD	0.001421
223	H7	PX	RYD	0.000176
224	H7	PY	RYD	0.000059
225	H7	PZ	RYD	0.000484

Total MIN occupancy: 83.713120

Total RYD occupancy: 0.286880

Total occupancy: 84.000000

Natural Atomic Populations and Charges

Atom	Occupancy	Charge
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H1	0.761656	0.238344
C1	6.357838	-0.357838
C2	6.219092	-0.219092
C3	6.094699	-0.094699
C4	5.602160	0.397840
C5	6.227136	-0.227136
C6	5.726786	0.273214
C7	6.220977	-0.220977
O1	8.605530	-0.605530
H4	0.750640	0.249360
N1	7.513248	-0.513248
H6	0.750114	0.249886
C8	5.897425	0.102575
H8	0.763672	0.236328
C10	6.314904	-0.314904
H16	0.784041	0.215959
H18	0.767560	0.232440
C9	6.240471	-0.240471
H3	0.784165	0.215835
H5	0.808943	0.191057
H7	0.808943	0.191057

Total Charge = 0.000000

Q-minus(NAO) = -0.6055

Q-plus(NAO) = 0.2499

Reason for exit: Normal completion

Wall Time: 000:00:00

CPU Time: 000:00:00

TITAN Properties Program: (PC/x86)

Release 6.0.2

Closed-Shell Molecular Orbital Coefficients

MO:		1	2	3	4	5
Eigenvalues:		-20.60019	-15.54147	-11.31105	-11.28860	-11.27098
(ev):		-560.55981	-422.90511	-307.78945	-307.17847	-306.69918
		A	A	A	A	A
1 H1	S	-0.00001	-0.00005	0.00007	0.00003	-0.00006
2 H1	S	-0.00020	-0.00039	-0.00029	0.00013	-0.00068
3 H1	PX	0.00001	0.00000	-0.00013	-0.00001	0.00000
4 H1	PY	0.00002	0.00001	0.00003	0.00002	0.00004
5 H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

6	C1	S	0.00002	0.00003	0.00919	0.00000	0.00007
7	C1	S	0.00013	0.00012	0.00016	0.00016	0.00031
8	C1	PX	0.00001	-0.00003	0.00008	0.00000	-0.00008
9	C1	PY	-0.00003	-0.00001	0.00005	-0.00012	-0.00006
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.00169	-0.00136	0.00161	-0.00311	-0.00240
12	C1	PX	0.00083	0.00120	-0.00013	0.00049	0.00174
13	C1	PY	-0.00028	0.00004	0.00003	0.00039	0.00018
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00002	0.00000	-0.00037	0.00004	-0.00005
16	C1	DYY	-0.00010	0.00002	-0.00038	-0.00013	-0.00006
17	C1	DZZ	0.00002	0.00006	-0.00002	0.00001	0.00014
18	C1	DXY	0.00005	0.00000	-0.00004	0.00002	0.00002
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00001	-0.00002	-0.00026	0.00004	-0.01405
22	C2	S	0.00003	-0.00005	-0.00052	0.00016	-0.00066
23	C2	PX	0.00001	-0.00001	-0.00007	0.00001	0.00014
24	C2	PY	0.00000	0.00004	-0.00004	-0.00006	-0.00001
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.00023	0.00058	0.00426	-0.00241	-0.00107
27	C2	PX	0.00007	0.00032	0.00295	-0.00124	-0.00053
28	C2	PY	-0.00030	-0.00064	0.00034	-0.00086	-0.00083
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.00013	0.00005	0.00000	0.00055
31	C2	DYY	0.00001	0.00003	0.00018	-0.00003	0.00055
32	C2	DZZ	0.00001	-0.00002	-0.00021	0.00005	0.00010
33	C2	DXY	-0.00001	-0.00002	0.00001	-0.00002	-0.00027
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.00001	-0.00040	-0.00002	-0.01165
37	C3	S	0.00000	0.00002	-0.00014	-0.00006	-0.00028
38	C3	PX	0.00002	-0.00003	0.00012	0.00001	-0.00004
39	C3	PY	0.00000	-0.00003	-0.00019	-0.00007	-0.00002
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00012	0.00005	-0.00315	-0.00002	-0.00731
42	C3	PX	-0.00034	-0.00120	-0.00315	0.00013	0.00169
43	C3	PY	0.00070	0.00083	0.00468	0.00225	0.00292
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.00002	0.00005	-0.00005	0.00047
46	C3	DYY	0.00001	-0.00006	0.00009	0.00005	0.00036
47	C3	DZZ	0.00000	0.00001	-0.00004	-0.00003	0.00018
48	C3	DXY	0.00002	0.00005	0.00000	0.00003	0.00020
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00001	-0.00001	0.99568	0.00071	-0.00010
52	C4	S	0.00031	-0.00007	0.02680	-0.00021	-0.00015
53	C4	PX	0.00000	0.00000	-0.00004	-0.00014	-0.00002
54	C4	PY	0.00033	-0.00001	0.00124	-0.00006	-0.00004
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00105	0.00170	-0.00590	0.00034	0.00314
57	C4	PX	0.00094	0.00008	0.00006	0.00309	0.00002
58	C4	PY	-0.00073	-0.00055	0.00413	0.00151	-0.00112
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

60	C4	DXX	0.00001	0.00001	-0.00131	0.00006	0.00006
61	C4	DYY	-0.00011	0.00002	-0.00063	0.00024	0.00008
62	C4	DZZ	-0.00009	-0.00002	-0.00235	-0.00006	-0.00002
63	C4	DXY	-0.00002	0.00000	-0.00018	0.00003	0.00001
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00001	0.00002	0.00599	0.00001	0.00044
67	C5	S	0.00003	0.00007	0.00048	-0.00021	0.00044
68	C5	PX	0.00000	0.00003	-0.00002	0.00004	0.00009
69	C5	PY	0.00002	-0.00003	-0.00003	0.00009	-0.00011
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00061	-0.00036	0.00017	0.00393	-0.00080
72	C5	PX	-0.00022	-0.00077	0.00025	0.00137	-0.00177
73	C5	PY	-0.00018	0.00028	0.00074	-0.00141	0.00094
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00005	0.00001	-0.00051	-0.00001	-0.00005
76	C5	DYY	-0.00003	0.00002	-0.00044	0.00004	-0.00013
77	C5	DZZ	-0.00002	0.00005	-0.00008	-0.00007	0.00016
78	C5	DXY	-0.00005	-0.00002	-0.00028	0.00002	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00005	-0.00005	-0.00003	-0.99550
82	C6	S	0.00002	-0.00028	0.00015	-0.00005	-0.02755
83	C6	PX	-0.00001	-0.00002	-0.00003	-0.00002	-0.00007
84	C6	PY	0.00001	-0.00011	0.00004	-0.00001	0.00016
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.00016	-0.00438	-0.00240	0.00110	0.00835
87	C6	PX	0.00011	-0.00032	0.00124	0.00018	0.00333
88	C6	PY	-0.00030	0.00147	-0.00380	0.00049	0.00370
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.00003	0.00000	0.00003	0.00176
91	C6	DYY	0.00000	0.00065	-0.00007	-0.00002	0.00099
92	C6	DZZ	0.00001	0.00003	0.00001	-0.00001	0.00243
93	C6	DXY	0.00000	0.00001	0.00001	-0.00004	0.00018
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	-0.00002	-0.00009	-0.00001	0.00121
97	C7	S	-0.00003	-0.00006	-0.00035	-0.00006	-0.00028
98	C7	PX	0.00000	-0.00004	-0.00003	0.00000	0.00006
99	C7	PY	0.00002	-0.00004	0.00006	0.00005	-0.00002
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00078	0.00171	0.00671	0.00146	0.00615
102	C7	PX	-0.00038	-0.00124	-0.00256	-0.00093	-0.00422
103	C7	PY	0.00008	0.00079	0.00184	0.00008	0.00002
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00001	-0.00001	0.00002	-0.00010
106	C7	DYY	0.00001	0.00000	0.00007	0.00000	-0.00004
107	C7	DZZ	-0.00001	-0.00001	-0.00012	-0.00001	-0.00016
108	C7	DXY	0.00000	0.00002	0.00001	-0.00001	0.00008
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.99462	0.00000	0.00000	-0.00011	0.00001
112	O1	S	0.02130	0.00002	0.00116	0.00043	0.00006
113	O1	PX	0.00106	0.00001	0.00000	0.00027	0.00001

114	O1	PY	-0.00076	-0.00001	-0.00026	0.00004	-0.00002
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00409	-0.00009	-0.00476	-0.00013	-0.00018
117	O1	PX	-0.00088	-0.00003	0.00023	-0.00118	-0.00003
118	O1	PY	0.00026	0.00009	0.00320	0.00029	0.00022
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00419	0.00002	0.00051	-0.00058	0.00005
121	O1	DYY	-0.00417	-0.00001	-0.00067	-0.00018	-0.00002
122	O1	DZZ	-0.00394	0.00002	0.00080	0.00025	0.00005
123	O1	DXY	-0.00007	0.00000	-0.00015	-0.00032	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00002	-0.00006	-0.00007	0.00008	-0.00012
127	H4	S	-0.00019	-0.00028	-0.00006	0.00042	-0.00085
128	H4	PX	-0.00001	0.00000	0.00006	0.00001	0.00003
129	H4	PY	0.00003	0.00002	-0.00005	0.00002	0.00002
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	-0.99524	0.00001	-0.00001	0.00032
132	N1	S	0.00000	-0.02514	0.00002	-0.00002	-0.00071
133	N1	PX	0.00000	-0.00166	0.00001	-0.00002	0.00008
134	N1	PY	0.00000	-0.00131	-0.00003	0.00001	-0.00007
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.00010	0.00724	-0.00108	0.00018	0.00525
137	N1	PX	0.00005	0.00263	0.00009	0.00010	0.00106
138	N1	PY	-0.00005	0.00147	-0.00026	0.00001	0.00232
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00001	0.00291	0.00005	0.00000	0.00014
141	N1	DYY	0.00000	0.00252	0.00003	0.00000	0.00013
142	N1	DZZ	0.00000	0.00308	-0.00001	-0.00002	-0.00047
143	N1	DXY	0.00000	-0.00012	-0.00001	0.00000	0.00004
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00001	-0.00001	0.00008	-0.00003	-0.00007
147	H6	S	0.00001	0.00002	0.00096	-0.00035	-0.00021
148	H6	PX	0.00000	0.00002	-0.00001	0.00000	-0.00010
149	H6	PY	0.00001	0.00005	0.00002	0.00002	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.00001	0.00004	0.00000	-0.00040
152	C8	S	0.00002	-0.00038	0.00013	0.00000	0.00030
153	C8	PX	0.00000	0.00016	-0.00006	0.00000	0.00010
154	C8	PY	0.00000	-0.00008	0.00005	-0.00003	0.00005
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.00029	-0.00284	-0.00122	-0.00071	-0.00342
157	C8	PX	-0.00006	0.00211	0.00006	-0.00023	0.00031
158	C8	PY	-0.00023	-0.00161	-0.00227	0.00013	-0.00500
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00001	0.00030	-0.00001	-0.00001	-0.00018
161	C8	DYY	0.00000	0.00009	-0.00001	0.00000	-0.00009
162	C8	DZZ	0.00001	0.00009	0.00004	0.00000	0.00005
163	C8	DXY	-0.00001	-0.00014	-0.00003	-0.00001	0.00009
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00001	0.00007	-0.00003	0.00003	0.00016
167	H8	S	0.00009	0.00039	0.00053	0.00027	0.00119

168	H8	PX	0.00000	-0.00001	0.00000	0.00000	-0.00002
169	H8	PY	0.00000	-0.00002	-0.00006	0.00000	0.00001
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	-0.00001	-0.00001	0.00000	0.00000
172	C10	S	0.00000	0.00000	0.00000	-0.00002	-0.00003
173	C10	PX	0.00000	0.00000	-0.00003	-0.00001	0.00006
174	C10	PY	0.00000	0.00000	-0.00006	0.00001	-0.00008
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.00007	-0.00063	-0.00124	0.00036	-0.00255
177	C10	PX	0.00007	-0.00071	0.00049	0.00006	0.00015
178	C10	PY	-0.00001	-0.00027	-0.00027	0.00019	-0.00075
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.00002	-0.00003	0.00000	-0.00007
181	C10	DYY	0.00000	-0.00005	-0.00001	0.00001	0.00002
182	C10	DZZ	0.00000	0.00001	-0.00002	0.00000	-0.00003
183	C10	DXY	0.00000	-0.00011	0.00000	0.00000	0.00002
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.00001	0.00005	-0.00004	-0.00002	0.00006
187	H16	S	-0.00003	0.00029	-0.00008	-0.00003	0.00008
188	H16	PX	0.00000	0.00001	-0.00001	0.00000	-0.00003
189	H16	PY	0.00000	0.00000	0.00000	0.00000	0.00001
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00001	-0.00003	0.00006	0.00000	-0.00001
192	H18	S	0.00002	-0.00020	0.00020	0.00004	0.00009
193	H18	PX	0.00000	0.00003	0.00001	0.00000	0.00002
194	H18	PY	0.00000	0.00002	0.00001	0.00000	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00000	-0.00071	0.99583	-0.00002
197	C9	S	0.00025	0.00001	-0.00018	0.02763	0.00000
198	C9	PX	-0.00038	-0.00001	-0.00004	-0.00097	-0.00001
199	C9	PY	-0.00017	0.00000	-0.00001	-0.00069	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00016	-0.00002	-0.00022	-0.01224	-0.00003
202	C9	PX	0.00021	0.00001	0.00029	-0.00044	0.00004
203	C9	PY	-0.00015	-0.00001	-0.00074	0.00088	-0.00009
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00008	0.00000	0.00002	-0.00138	-0.00001
206	C9	DYY	0.00004	0.00001	0.00020	-0.00148	0.00001
207	C9	DZZ	0.00003	0.00001	0.00005	-0.00156	0.00001
208	C9	DXY	0.00005	0.00000	0.00015	0.00006	0.00001
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.00001	0.00000	0.00009	-0.00007	0.00001
212	H3	S	-0.00004	0.00000	0.00025	0.00182	0.00005
213	H3	PX	0.00003	0.00000	0.00004	-0.00001	0.00000
214	H3	PY	0.00007	0.00000	0.00006	0.00014	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00007	0.00000	-0.00009	0.00013	-0.00001
217	H5	S	-0.00013	0.00001	-0.00001	0.00251	0.00002
218	H5	PX	0.00004	0.00000	-0.00003	0.00007	0.00000
219	H5	PY	0.00002	0.00000	0.00005	-0.00007	0.00000
220	H5	PZ	-0.00004	0.00000	-0.00001	-0.00006	0.00000
221	H7	S	-0.00007	0.00000	-0.00009	0.00013	-0.00001

222	H7	S	-0.00013	0.00001	-0.00001	0.00251	0.00002
223	H7	PX	0.00004	0.00000	-0.00003	0.00007	0.00000
224	H7	PY	0.00002	0.00000	0.00005	-0.00007	0.00000
225	H7	PZ	0.00004	0.00000	0.00001	0.00006	0.00000

MO:		6	7	8	9	10
Eigenvalues:		-11.25727	-11.24891	-11.24274	-11.24199	-11.23919
(ev):		-306.32603	-306.09843	-305.93066	-305.91030	-305.83416

		A	A	A	A	A	
1	H1	S	0.00007	-0.00007	0.00000	-0.00004	-0.00004
2	H1	S	0.00072	-0.00076	0.00002	-0.00079	-0.00029
3	H1	PX	0.00000	-0.00001	0.00000	-0.00003	-0.00010
4	H1	PY	-0.00003	-0.00002	0.00001	-0.00001	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00006	0.00151	0.00001	-0.00018	0.03839
7	C1	S	-0.00015	0.00042	-0.00005	0.00039	0.00120
8	C1	PX	0.00004	-0.00004	0.00000	0.00000	0.00005
9	C1	PY	0.00004	-0.00004	0.00000	0.00004	0.00022
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00158	-0.00395	0.00045	-0.00657	0.00164
12	C1	PX	-0.00210	0.00227	-0.00015	0.00303	0.00048
13	C1	PY	0.00055	0.00105	-0.00017	0.00130	-0.00106
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	-0.00013	-0.00001	-0.00008	-0.00045
16	C1	DYY	-0.00006	-0.00012	0.00002	-0.00008	-0.00082
17	C1	DZZ	-0.00007	0.00014	-0.00002	0.00012	-0.00022
18	C1	DXY	-0.00001	0.00004	0.00000	-0.00002	-0.00017
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00024	-0.11731	0.00107	0.98857	0.00315
22	C2	S	0.00012	-0.00312	0.00003	0.02750	-0.00008
23	C2	PX	0.00003	0.00003	0.00001	0.00033	-0.00004
24	C2	PY	-0.00007	0.00016	-0.00001	0.00003	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.00051	-0.00008	0.00000	-0.01013	0.00102
27	C2	PX	-0.00074	0.00054	-0.00001	-0.00046	0.00065
28	C2	PY	-0.00083	-0.00066	-0.00026	-0.00021	0.00034
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00001	0.00064	0.00000	-0.00155	0.00008
31	C2	DYY	0.00004	0.00054	0.00001	-0.00141	0.00006
32	C2	DZZ	0.00006	0.00032	0.00000	-0.00246	-0.00006
33	C2	DXY	0.00003	0.00000	-0.00001	0.00013	-0.00002
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00036	0.00037	0.00043	-0.00331	0.98854
37	C3	S	0.00009	-0.00006	0.00007	-0.00020	0.02762
38	C3	PX	-0.00005	-0.00001	0.00001	0.00007	-0.00019
39	C3	PY	-0.00006	-0.00003	0.00004	-0.00013	0.00005
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00293	0.00105	-0.00167	-0.00070	-0.01350
42	C3	PX	0.00324	-0.00119	-0.00021	-0.00124	0.00071
43	C3	PY	0.00072	0.00328	0.00050	0.00582	0.00114

44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00003	0.00001	0.00001	0.00007	-0.00182
46	C3	DYY	0.00020	0.00006	-0.00004	0.00007	-0.00118
47	C3	DZZ	0.00009	0.00001	0.00001	-0.00001	-0.00234
48	C3	DXY	-0.00007	0.00001	0.00000	0.00004	-0.00015
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00622	0.00001	0.00089	-0.00001
52	C4	S	0.00012	-0.00010	0.00004	-0.00028	-0.00027
53	C4	PX	0.00000	-0.00008	0.00000	0.00001	0.00002
54	C4	PY	0.00000	-0.00004	0.00000	0.00000	0.00003
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.00268	-0.00152	-0.00021	0.00195	0.00081
57	C4	PX	-0.00053	0.00173	-0.00004	0.00153	0.00006
58	C4	PY	0.00130	-0.00142	0.00038	-0.00268	-0.00131
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00067	0.00001	0.00012	0.00006
61	C4	DYY	-0.00001	0.00025	0.00001	0.00003	0.00008
62	C4	DZZ	0.00004	0.00006	0.00001	-0.00007	-0.00007
63	C4	DXY	0.00000	0.00002	0.00000	0.00003	-0.00005
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00014	-0.98859	-0.00008	-0.11796	0.00004
67	C5	S	-0.00014	-0.02735	-0.00001	-0.00346	0.00003
68	C5	PX	-0.00002	-0.00029	0.00001	0.00004	-0.00004
69	C5	PY	0.00005	0.00001	0.00001	0.00018	0.00003
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00160	0.01017	0.00029	0.00455	-0.00095
72	C5	PX	0.00073	0.00075	0.00002	-0.00013	-0.00026
73	C5	PY	-0.00113	0.00058	-0.00020	-0.00038	0.00058
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.00177	0.00000	-0.00019	-0.00005
76	C5	DYY	-0.00002	0.00140	0.00000	-0.00025	-0.00004
77	C5	DZZ	-0.00006	0.00246	0.00000	0.00025	-0.00002
78	C5	DXY	-0.00001	-0.00007	0.00000	0.00005	0.00001
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00046	0.00136	-0.00006	-0.01430	-0.01185
82	C6	S	-0.00039	0.00028	-0.00006	-0.00024	-0.00022
83	C6	PX	-0.00005	-0.00001	-0.00004	0.00008	-0.00007
84	C6	PY	-0.00008	0.00009	0.00004	0.00003	0.00002
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00492	-0.00025	-0.00007	0.00468	0.00478
87	C6	PX	0.00336	0.00005	0.00043	0.00014	0.00194
88	C6	PY	-0.00061	-0.00310	-0.00001	-0.00259	-0.00091
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00008	0.00005	-0.00001	-0.00041	-0.00057
91	C6	DYY	0.00015	-0.00004	-0.00001	-0.00039	-0.00024
92	C6	DZZ	-0.00010	0.00007	-0.00003	-0.00006	-0.00010
93	C6	DXY	-0.00004	0.00004	0.00003	0.00020	-0.00004
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.01480	-0.00004	0.00235	-0.00009	0.11103
97	C7	S	0.00054	-0.00009	0.00008	-0.00020	0.00281

98	C7	PX	0.00005	0.00000	0.00004	-0.00004	0.00015
99	C7	PY	0.00007	0.00003	-0.00005	0.00009	-0.00016
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00392	0.00270	0.00149	0.00542	0.00391
102	C7	PX	-0.00076	-0.00124	-0.00096	-0.00256	-0.00115
103	C7	PY	-0.00278	0.00045	0.00045	0.00076	0.00108
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00062	0.00001	-0.00005	0.00005	-0.00074
106	C7	DYY	-0.00041	0.00001	-0.00009	0.00002	-0.00049
107	C7	DZZ	-0.00014	-0.00003	-0.00002	-0.00005	-0.00037
108	C7	DXY	-0.00023	0.00001	-0.00007	-0.00001	0.00008
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00005	0.00001	-0.00005	-0.00003
112	O1	S	0.00000	-0.00010	0.00003	-0.00021	-0.00013
113	O1	PX	-0.00001	-0.00001	0.00000	0.00003	0.00000
114	O1	PY	0.00001	0.00001	0.00000	0.00001	0.00002
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.00015	0.00130	-0.00025	0.00160	0.00086
117	O1	PX	0.00009	-0.00005	0.00001	-0.00033	-0.00004
118	O1	PY	-0.00003	-0.00029	0.00007	-0.00043	-0.00027
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.00020	0.00002	-0.00015	-0.00010
121	O1	DYY	0.00002	-0.00018	0.00002	-0.00013	-0.00008
122	O1	DZZ	-0.00001	-0.00006	0.00002	-0.00010	-0.00008
123	O1	DXY	-0.00001	-0.00007	0.00000	0.00004	-0.00001
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00006	0.00021	0.00000	0.00002	-0.00001
127	H4	S	0.00042	-0.00187	0.00004	-0.00042	-0.00012
128	H4	PX	0.00000	0.00017	0.00000	0.00010	0.00001
129	H4	PY	0.00000	-0.00014	0.00000	-0.00016	-0.00002
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00011	0.00004	-0.00004	0.00007	0.00009
132	N1	S	0.00073	0.00017	0.00001	0.00016	0.00025
133	N1	PX	0.00005	-0.00001	-0.00001	0.00005	0.00006
134	N1	PY	-0.00010	0.00000	-0.00004	-0.00001	0.00002
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.00348	-0.00217	0.00092	-0.00301	-0.00300
137	N1	PX	-0.00214	0.00016	0.00018	-0.00010	-0.00081
138	N1	PY	-0.00012	-0.00084	0.00014	-0.00087	-0.00048
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00050	0.00011	-0.00014	0.00019	0.00020
141	N1	DYY	-0.00003	0.00003	-0.00012	0.00017	0.00021
142	N1	DZZ	0.00041	0.00008	-0.00002	0.00007	0.00018
143	N1	DXY	0.00011	0.00003	0.00009	0.00001	0.00003
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.00004	0.00001	-0.00001	-0.00030	0.00002
147	H6	S	-0.00034	0.00004	-0.00003	0.00177	0.00031
148	H6	PX	0.00000	-0.00010	0.00000	-0.00026	0.00000
149	H6	PY	-0.00001	-0.00008	0.00001	-0.00007	-0.00002
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.99379	-0.00007	0.05930	-0.00027	-0.00132

152	C8	S	0.02729	0.00007	0.00197	0.00013	-0.00008
153	C8	PX	-0.00029	-0.00003	0.00000	-0.00007	-0.00002
154	C8	PY	0.00028	0.00001	-0.00020	0.00005	0.00006
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.01057	-0.00080	-0.00566	-0.00118	0.00029
157	C8	PX	-0.00396	-0.00008	-0.00014	-0.00048	-0.00103
158	C8	PY	-0.00032	-0.00072	0.00107	-0.00160	-0.00039
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00159	0.00000	0.00027	-0.00001	0.00002
161	C8	DYY	-0.00110	0.00001	0.00023	0.00004	0.00014
162	C8	DZZ	-0.00236	0.00003	-0.00003	0.00006	0.00003
163	C8	DXY	-0.00028	-0.00001	0.00000	-0.00004	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00007	0.00001	0.00004	0.00002	-0.00003
167	H8	S	-0.00030	0.00031	0.00033	0.00060	0.00017
168	H8	PX	-0.00009	0.00000	-0.00001	0.00002	-0.00011
169	H8	PY	0.00011	0.00000	-0.00003	-0.00001	0.00001
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.05863	-0.00006	-0.99390	0.00105	0.00061
172	C10	S	0.00135	0.00000	-0.02744	0.00004	0.00001
173	C10	PX	0.00004	-0.00002	-0.00010	-0.00002	-0.00002
174	C10	PY	-0.00025	-0.00001	-0.00004	-0.00004	-0.00005
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00315	-0.00028	0.01163	-0.00076	-0.00023
177	C10	PX	0.00125	0.00025	-0.00017	0.00053	0.00066
178	C10	PY	0.00174	-0.00008	0.00101	-0.00018	0.00009
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.00058	-0.00001	0.00167	-0.00002	-0.00001
181	C10	DYY	-0.00050	0.00000	0.00145	-0.00002	-0.00002
182	C10	DZZ	-0.00023	0.00000	0.00256	0.00000	-0.00001
183	C10	DXY	0.00008	0.00001	0.00008	0.00002	0.00005
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.00010	-0.00002	0.00027	-0.00004	-0.00006
187	H16	S	-0.00052	-0.00010	-0.00197	-0.00017	-0.00019
188	H16	PX	-0.00012	0.00000	-0.00028	0.00000	-0.00001
189	H16	PY	0.00009	0.00000	0.00003	0.00000	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00012	0.00003	0.00022	0.00006	0.00006
192	H18	S	0.00066	0.00006	-0.00194	0.00016	0.00027
193	H18	PX	0.00006	0.00000	0.00020	0.00000	-0.00001
194	H18	PY	0.00013	0.00000	0.00011	0.00000	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00005	0.00000	0.00001	0.00000
197	C9	S	0.00000	0.00002	0.00000	0.00005	-0.00004
198	C9	PX	0.00001	-0.00001	0.00000	-0.00001	0.00000
199	C9	PY	-0.00001	-0.00001	0.00000	-0.00003	0.00002
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.00001	-0.00025	0.00001	-0.00014	0.00014
202	C9	PX	-0.00001	-0.00009	0.00002	-0.00010	-0.00002
203	C9	PY	0.00011	0.00020	-0.00003	0.00021	-0.00017
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	0.00006	0.00000	0.00004	0.00000

206	C9	DYY	0.00000	0.00001	0.00000	0.00002	-0.00001
207	C9	DZZ	0.00000	0.00000	0.00000	0.00002	-0.00002
208	C9	DXY	-0.00001	0.00002	0.00000	0.00001	0.00001
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.00001	0.00000	0.00000	-0.00001	0.00001
212	H3	S	-0.00006	-0.00009	0.00002	-0.00011	0.00007
213	H3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
214	H3	PY	0.00000	0.00000	0.00000	0.00001	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00002	0.00002	0.00000	0.00002	-0.00001
217	H5	S	-0.00003	0.00011	-0.00001	0.00010	0.00000
218	H5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
219	H5	PY	0.00000	0.00000	0.00000	-0.00001	0.00000
220	H5	PZ	0.00000	0.00001	0.00000	0.00001	0.00000
221	H7	S	0.00002	0.00002	0.00000	0.00002	-0.00001
222	H7	S	-0.00003	0.00011	-0.00001	0.00010	0.00000
223	H7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
224	H7	PY	0.00000	0.00000	0.00000	-0.00001	0.00000
225	H7	PZ	0.00000	-0.00001	0.00000	-0.00001	0.00000

MO:	11	12	13	14	15
Eigenvalues:	-11.23182	-11.22847	-1.43013	-1.27321	-1.13071
(ev):	-305.63346	-305.54247	-38.91592	-34.64594	-30.76832

		A	A	A	A	A	
1	H1	S	0.00004	0.00025	-0.00620	0.00452	0.03571
2	H1	S	0.00044	-0.00209	0.00026	-0.00754	0.00369
3	H1	PX	0.00000	-0.00024	0.00118	-0.00045	-0.00376
4	H1	PY	-0.00001	-0.00011	0.00036	-0.00001	-0.00122
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01493	-0.99466	0.01629	-0.01587	-0.09051
7	C1	S	0.00030	-0.02771	-0.02953	0.03274	0.17011
8	C1	PX	0.00004	0.00027	0.01457	-0.00998	-0.06321
9	C1	PY	0.00002	0.00013	-0.01860	-0.01397	-0.00228
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00308	0.00839	-0.02690	-0.00274	0.09795
12	C1	PX	-0.00160	0.00032	0.00492	0.01936	-0.00169
13	C1	PY	-0.00057	0.00105	-0.01783	-0.00115	0.00566
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00007	0.00150	0.00002	0.00012	0.00462
16	C1	DYY	-0.00021	0.00163	-0.00312	0.00256	0.00524
17	C1	DZZ	-0.00010	0.00249	0.00146	-0.00087	-0.00738
18	C1	DXY	-0.00004	0.00009	0.00393	0.00058	-0.00291
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00031	-0.00033	0.00256	-0.02948	-0.08909
22	C2	S	0.00012	-0.00029	-0.00706	0.05458	0.17204
23	C2	PX	-0.00001	0.00005	-0.00277	0.02450	0.04652
24	C2	PY	0.00003	-0.00002	-0.00338	-0.01624	0.05474
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.00244	0.00483	0.00008	0.03863	0.08974
27	C2	PX	-0.00140	0.00247	0.01110	0.00772	-0.01030
28	C2	PY	-0.00106	-0.00004	-0.00488	-0.01343	-0.00243

29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.00004	0.00008	-0.00007	0.00156	0.00155
31	C2	DYY	0.00003	0.00005	-0.00005	0.00376	0.00721
32	C2	DZZ	0.00003	-0.00007	-0.00031	-0.00322	-0.00693
33	C2	DXY	-0.00003	0.00000	-0.00047	-0.00380	0.00224
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.11120	0.04025	0.00262	-0.06081	-0.06079
37	C3	S	0.00351	0.00113	-0.00583	0.11327	0.11797
38	C3	PX	0.00001	0.00004	0.00150	-0.02790	-0.01432
39	C3	PY	-0.00020	0.00001	-0.00420	-0.04467	0.05041
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00954	-0.00620	-0.01975	0.05279	0.06226
42	C3	PX	0.00027	-0.00058	-0.01921	-0.01945	0.00744
43	C3	PY	0.00106	0.00426	0.01976	0.00554	0.01982
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00009	0.00021	0.00003	0.00621	0.00201
46	C3	DYY	0.00034	0.00062	-0.00099	0.00544	0.00821
47	C3	DZZ	-0.00013	0.00005	0.00004	-0.00594	-0.00520
48	C3	DXY	0.00003	0.00010	0.00034	0.00283	0.00006
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.00010	0.00979	0.07671	-0.00875	-0.09414
52	C4	S	0.00013	0.00030	-0.14337	0.01608	0.18693
53	C4	PX	-0.00002	0.00016	-0.01128	-0.00036	-0.01194
54	C4	PY	0.00001	-0.00012	-0.10579	-0.01437	-0.08564
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.00204	-0.00203	-0.00534	0.03740	0.10198
57	C4	PX	-0.00040	-0.00140	0.01211	0.00012	0.00151
58	C4	PY	0.00162	-0.00055	0.03856	-0.01100	-0.03074
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00003	0.00039	0.00849	0.00163	0.01181
61	C4	DYY	0.00000	0.00039	-0.02244	0.00001	-0.00152
62	C4	DZZ	0.00004	0.00000	0.01138	-0.00082	-0.00812
63	C4	DXY	0.00002	-0.00005	-0.00331	-0.00037	-0.00328
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00004	-0.00133	0.01436	-0.01301	-0.10698
67	C5	S	-0.00005	0.00027	-0.02680	0.02757	0.20249
68	C5	PX	0.00000	0.00008	-0.01793	0.00457	0.03794
69	C5	PY	-0.00001	0.00000	-0.01060	-0.01386	-0.05080
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00202	-0.00240	-0.00784	0.00593	0.15158
72	C5	PX	0.00032	-0.00137	-0.00575	-0.01547	0.01217
73	C5	PY	-0.00118	0.00156	-0.01311	0.00578	-0.01329
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00001	-0.00012	-0.00409	-0.00003	0.00572
76	C5	DYY	0.00000	-0.00004	-0.00071	0.00136	0.00726
77	C5	DZZ	-0.00001	0.00009	0.00146	-0.00051	-0.00943
78	C5	DXY	-0.00001	0.00001	-0.00365	0.00022	0.00413
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00267	-0.00050	0.00171	-0.11298	-0.02907
82	C6	S	-0.00013	0.00015	-0.00276	0.21798	0.05602

83	C6	PX	-0.00004	-0.00001	-0.00060	0.02423	-0.00469
84	C6	PY	0.00001	0.00014	-0.00137	-0.10599	0.10320
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00150	0.00047	-0.01626	0.04154	0.05675
87	C6	PX	0.00097	0.00268	0.00330	0.00929	0.00983
88	C6	PY	0.00274	-0.00412	-0.00979	0.02919	0.03149
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00024	-0.00004	-0.00030	-0.00093	0.00938
91	C6	DYY	-0.00012	-0.00003	-0.00066	0.01852	-0.00252
92	C6	DZZ	-0.00007	0.00004	0.00020	-0.01225	-0.00267
93	C6	DXY	0.00001	0.00000	-0.00006	-0.00149	-0.00214
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.98929	-0.01065	0.00025	-0.05284	-0.00585
97	C7	S	-0.02771	-0.00053	-0.00260	0.09704	0.00965
98	C7	PX	0.00026	0.00004	0.00025	-0.05402	0.00238
99	C7	PY	-0.00001	0.00008	0.00009	0.00090	0.03699
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.01463	0.00635	0.03172	0.06360	0.02502
102	C7	PX	-0.00326	-0.00311	-0.01214	-0.01692	-0.01040
103	C7	PY	0.00031	0.00055	0.00919	0.01369	-0.00322
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00121	-0.00007	0.00014	0.00522	-0.00156
106	C7	DYY	0.00169	-0.00002	0.00045	0.00391	0.00025
107	C7	DZZ	0.00232	-0.00004	-0.00033	-0.00547	-0.00026
108	C7	DXY	0.00024	0.00007	-0.00012	0.00088	-0.00416
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00001	-0.00005	0.19869	0.00610	0.03367
112	O1	S	0.00007	-0.00013	-0.43672	-0.01326	-0.07932
113	O1	PX	-0.00001	-0.00001	-0.05646	-0.00299	-0.04093
114	O1	PY	-0.00001	0.00001	0.05701	-0.00238	-0.06206
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.00060	0.00126	-0.45294	-0.01548	-0.07702
117	O1	PX	0.00007	0.00023	-0.03808	-0.00205	-0.02420
118	O1	PY	0.00012	-0.00008	0.04337	0.00032	-0.03702
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00004	-0.00012	-0.00896	-0.00038	-0.00789
121	O1	DYY	0.00005	-0.00026	-0.01538	-0.00006	0.00450
122	O1	DZZ	0.00003	-0.00007	0.00485	0.00019	-0.00161
123	O1	DXY	-0.00001	0.00005	-0.00400	-0.00025	-0.00312
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00002	-0.00009	-0.00615	0.00287	0.04607
127	H4	S	0.00020	-0.00069	-0.00063	-0.00699	0.00907
128	H4	PX	0.00000	-0.00001	-0.00097	0.00033	0.00345
129	H4	PY	0.00002	-0.00003	0.00046	-0.00018	-0.00369
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00008	0.00006	0.00049	-0.14549	0.05153
132	N1	S	-0.00023	0.00021	-0.00168	0.28830	-0.10701
133	N1	PX	0.00001	0.00002	-0.00032	0.08535	-0.04046
134	N1	PY	-0.00003	-0.00006	-0.00059	0.08472	0.00234
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00327	-0.00292	0.00139	0.33063	-0.10288

137	N1	PX	0.00044	-0.00049	0.00147	0.05264	-0.02143
138	N1	PY	0.00095	-0.00055	0.00072	0.03942	0.00698
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00022	0.00013	-0.00005	0.00447	-0.00525
141	N1	DYY	-0.00011	0.00008	-0.00005	0.00748	-0.00007
142	N1	DZZ	-0.00015	0.00010	-0.00022	-0.01361	0.00365
143	N1	DXY	-0.00001	-0.00002	-0.00001	0.00218	0.00139
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.00005	0.00000	-0.00002	0.01078	0.03504
147	H6	S	-0.00043	0.00055	0.00450	0.00123	-0.00140
148	H6	PX	0.00001	-0.00003	0.00003	0.00127	0.00362
149	H6	PY	0.00002	0.00001	0.00018	0.00060	0.00163
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.01523	0.00019	0.00037	-0.08657	0.04650
152	C8	S	0.00033	0.00018	-0.00010	0.16516	-0.09069
153	C8	PX	0.00006	-0.00007	0.00006	-0.06111	0.03221
154	C8	PY	0.00006	0.00003	-0.00020	0.05161	0.00531
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.00503	-0.00176	-0.00653	0.04241	-0.05469
157	C8	PX	-0.00077	-0.00095	0.00048	0.02983	-0.01517
158	C8	PY	-0.00239	-0.00232	-0.00929	0.00402	-0.00435
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00033	0.00003	-0.00015	0.01251	-0.00509
161	C8	DYY	0.00057	0.00002	-0.00020	0.00756	-0.00204
162	C8	DZZ	0.00011	0.00006	0.00013	-0.00981	0.00444
163	C8	DXY	0.00018	-0.00004	-0.00006	-0.00913	0.00457
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00049	0.00007	-0.00026	0.01424	0.00347
167	H8	S	-0.00110	0.00077	0.00245	0.00462	0.00370
168	H8	PX	-0.00036	-0.00003	0.00009	-0.00138	-0.00046
169	H8	PY	0.00000	0.00001	-0.00017	-0.00018	0.00056
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00143	-0.00002	0.00003	-0.02468	0.02710
172	C10	S	0.00003	0.00000	-0.00018	0.04663	-0.05226
173	C10	PX	0.00006	-0.00003	-0.00009	-0.01004	0.00901
174	C10	PY	-0.00002	-0.00004	-0.00026	0.02935	-0.02506
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.00028	-0.00098	-0.00477	0.03307	-0.03464
177	C10	PX	-0.00002	0.00079	0.00194	-0.01486	0.00625
178	C10	PY	-0.00018	-0.00022	-0.00076	0.00286	0.00008
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.00006	-0.00002	-0.00007	-0.00126	0.00081
181	C10	DYY	-0.00013	-0.00001	0.00001	0.00197	-0.00249
182	C10	DZZ	0.00005	-0.00001	-0.00005	-0.00183	0.00207
183	C10	DXY	0.00006	0.00003	-0.00001	-0.00274	0.00181
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00006	-0.00005	-0.00016	0.00850	-0.01175
187	H16	S	0.00001	-0.00027	-0.00027	0.00476	-0.00310
188	H16	PX	-0.00002	0.00000	-0.00003	-0.00078	0.00114
189	H16	PY	0.00002	0.00000	-0.00002	0.00028	-0.00063
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

191	H18	S	-0.00002	0.00008	0.00017	0.00916	-0.01342
192	H18	S	-0.00014	0.00023	0.00102	-0.00391	0.00033
193	H18	PX	0.00001	0.00000	0.00003	0.00107	-0.00102
194	H18	PY	-0.00001	0.00000	0.00003	0.00109	-0.00138
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	-0.00003	0.06057	0.00287	0.03593
197	C9	S	-0.00001	0.00002	-0.11069	-0.00537	-0.06957
198	C9	PX	0.00000	0.00003	0.07509	0.00328	0.03080
199	C9	PY	0.00001	-0.00001	0.04254	0.00138	0.00749
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00004	-0.00022	-0.02784	-0.00226	-0.03599
202	C9	PX	0.00004	0.00017	-0.00235	0.00007	-0.00330
203	C9	PY	-0.00004	0.00017	-0.00033	-0.00076	0.00027
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.00001	-0.00001	-0.01393	-0.00062	-0.00515
206	C9	DYY	0.00000	0.00001	0.00142	0.00009	0.00097
207	C9	DZZ	0.00000	0.00002	0.00915	0.00038	0.00296
208	C9	DXY	0.00000	-0.00002	-0.01446	-0.00049	-0.00386
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.00000	-0.02125	-0.00125	-0.02164
212	H3	S	0.00002	-0.00005	-0.00603	0.00011	-0.00638
213	H3	PX	0.00000	-0.00001	0.00019	-0.00001	-0.00031
214	H3	PY	0.00000	0.00000	0.00400	0.00017	0.00229
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00000	0.00004	-0.02188	-0.00118	-0.01661
217	H5	S	-0.00004	-0.00001	-0.00422	0.00004	-0.00287
218	H5	PX	0.00000	0.00000	0.00241	0.00011	0.00152
219	H5	PY	0.00000	-0.00002	-0.00055	-0.00003	-0.00060
220	H5	PZ	0.00000	0.00000	-0.00304	-0.00013	-0.00166
221	H7	S	0.00000	0.00004	-0.02188	-0.00118	-0.01661
222	H7	S	-0.00004	-0.00001	-0.00422	0.00004	-0.00287
223	H7	PX	0.00000	0.00000	0.00241	0.00011	0.00152
224	H7	PY	0.00000	-0.00002	-0.00055	-0.00003	-0.00060
225	H7	PZ	0.00000	0.00000	0.00304	0.00013	0.00166

MO:	16	17	18	19	20
Eigenvalues:	-1.06874	-1.03349	-1.00471	-0.96765	-0.89142
(ev):	-29.08200	-28.12281	-27.33952	-26.33104	-24.25674

		A	A	A	A	A	
1	H1	S	-0.04210	0.01786	-0.04039	-0.06499	-0.00852
2	H1	S	-0.01383	0.00887	-0.00197	-0.01493	-0.00424
3	H1	PX	0.00398	-0.00135	0.00444	0.00585	0.00065
4	H1	PY	0.00158	-0.00071	0.00072	0.00116	0.00080
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.07406	-0.02515	0.07305	0.09554	0.01529
7	C1	S	-0.13894	0.04709	-0.14070	-0.18394	-0.03015
8	C1	PX	0.01375	0.01260	0.04749	0.03366	-0.01256
9	C1	PY	0.03033	-0.04594	-0.06411	-0.03314	0.05262
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.10548	0.04857	-0.07061	-0.11440	-0.02504
12	C1	PX	0.00868	-0.00658	-0.01914	-0.01788	0.00119
13	C1	PY	0.00295	-0.00908	-0.01871	-0.02534	0.01669

14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.00087	-0.00111	-0.00387	-0.00633	0.00248
16	C1	DYY	-0.00823	0.00563	-0.00039	-0.00062	-0.00588
17	C1	DZZ	0.00647	-0.00258	0.00474	0.00678	0.00153
18	C1	DXY	0.00069	0.00336	0.00638	0.00214	-0.00466
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08246	0.02774	-0.09790	0.00232	0.04365
22	C2	S	0.15676	-0.05306	0.18836	-0.00284	-0.08880
23	C2	PX	0.02391	0.00966	0.02017	-0.00768	-0.04680
24	C2	PY	0.00839	-0.06620	0.04172	0.01446	0.14008
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.12242	-0.03097	0.13035	-0.02274	-0.06017
27	C2	PX	0.00801	0.00359	-0.00838	-0.01270	0.00605
28	C2	PY	0.00275	-0.01357	0.00664	-0.00316	0.02929
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00128	0.00307	0.00186	-0.00083	-0.00993
31	C2	DYY	0.00842	-0.00340	0.00601	-0.00019	0.00270
32	C2	DZZ	-0.00691	0.00165	-0.00767	0.00079	0.00380
33	C2	DXY	-0.00190	-0.00558	0.00075	0.00087	0.01084
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.10009	-0.07534	-0.03584	-0.02340	0.03607
37	C3	S	-0.19116	0.14579	0.06960	0.04539	-0.07381
38	C3	PX	-0.06446	-0.01048	0.00687	0.02385	0.07246
39	C3	PY	0.02480	-0.01744	-0.08078	-0.13091	-0.05911
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.13955	0.08624	0.04585	0.03588	-0.04157
42	C3	PX	-0.00474	-0.00050	0.01066	0.01765	0.01209
43	C3	PY	-0.00201	0.00225	-0.03767	-0.07364	-0.01970
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00319	0.00490	0.00389	0.00233	-0.00786
46	C3	DYY	-0.01407	0.00479	-0.00257	-0.00365	0.00230
47	C3	DZZ	0.00777	-0.00603	-0.00234	-0.00109	0.00267
48	C3	DXY	0.00606	0.00143	-0.00489	-0.00611	-0.00516
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01915	0.04241	0.09287	0.01058	-0.04032
52	C4	S	-0.03924	-0.08424	-0.18426	-0.02082	0.08445
53	C4	PX	-0.06425	0.05901	-0.06431	-0.11439	-0.08331
54	C4	PY	0.02846	-0.01373	-0.00175	0.14497	-0.05958
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.01231	-0.05705	-0.14550	-0.04625	0.07676
57	C4	PX	-0.00858	0.00443	-0.01657	-0.00839	-0.02950
58	C4	PY	-0.00505	0.02019	0.03417	0.02762	-0.02442
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00149	-0.00505	-0.00060	-0.00740	0.01418
61	C4	DYY	-0.00035	-0.00171	-0.00758	0.01285	-0.01064
62	C4	DZZ	0.00092	0.00469	0.00873	-0.00205	-0.00220
63	C4	DXY	0.00628	-0.00210	0.00988	0.00503	0.00403
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.05449	0.07105	-0.04742	-0.02129	-0.09399
67	C5	S	0.10618	-0.13717	0.08843	0.04100	0.18596

68	C5	PX	-0.02075	-0.01317	-0.07005	-0.00444	0.01754
69	C5	PY	-0.04882	0.00589	-0.09736	0.02996	0.05515
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.06178	-0.10294	0.07806	0.06084	0.14998
72	C5	PX	-0.00868	-0.00217	-0.00144	0.00623	-0.01152
73	C5	PY	0.00568	-0.00409	-0.01902	-0.00023	0.02319
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00295	-0.00383	-0.00947	0.00045	0.00858
76	C5	DYY	0.00677	-0.00387	0.01009	0.00201	-0.00020
77	C5	DZZ	-0.00374	0.00580	-0.00339	-0.00188	-0.00720
78	C5	DXY	0.00138	-0.00328	-0.00065	0.00205	0.00149
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.05846	-0.05665	-0.01611	0.00017	0.08238
82	C6	S	0.11672	0.11208	0.03037	-0.00213	-0.16801
83	C6	PX	-0.10105	0.04247	-0.00888	0.03609	0.04351
84	C6	PY	-0.05468	-0.02278	0.12031	0.00382	-0.10466
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.05427	0.07607	0.04038	0.00952	-0.15586
87	C6	PX	-0.00989	0.02773	-0.00307	0.00614	0.00376
88	C6	PY	0.01425	0.00081	0.03840	0.01213	-0.04409
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00950	0.00538	0.01190	0.00519	-0.00949
91	C6	DYY	0.01352	0.00131	-0.00637	-0.00347	0.00187
92	C6	DZZ	-0.00549	-0.00541	-0.00112	-0.00019	0.00574
93	C6	DXY	-0.00533	0.00539	-0.00673	-0.00106	-0.00014
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.10899	-0.01574	-0.06771	-0.07718	-0.04742
97	C7	S	-0.20858	0.02800	0.12946	0.15018	0.09490
98	C7	PX	0.04975	-0.01677	-0.02469	-0.03633	-0.01753
99	C7	PY	-0.03090	0.08636	0.01157	0.02668	-0.02715
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.14186	0.04091	0.07915	0.07371	0.06056
102	C7	PX	-0.00078	-0.00750	0.00987	0.02125	0.00901
103	C7	PY	-0.00169	0.01019	-0.00508	-0.00640	-0.00450
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00351	0.00044	0.00293	0.00501	0.00471
106	C7	DYY	-0.00810	-0.00168	0.00368	0.00166	0.00027
107	C7	DZZ	0.00854	-0.00113	-0.00535	-0.00583	-0.00360
108	C7	DXY	0.00232	-0.00946	-0.00242	-0.00366	0.00391
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00797	-0.00234	-0.00686	-0.04673	0.04112
112	O1	S	0.01796	0.00772	0.01881	0.10638	-0.09460
113	O1	PX	-0.00868	0.05693	0.07601	-0.13342	0.02023
114	O1	PY	0.01052	0.06591	0.14423	-0.09973	0.00248
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.02469	-0.00402	0.00769	0.14318	-0.13116
117	O1	PX	-0.00243	0.03086	0.04507	-0.07107	0.01175
118	O1	PY	0.00579	0.03772	0.07919	-0.05112	-0.00212
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00035	0.00729	0.01271	-0.01248	0.00306
121	O1	DYY	-0.00086	-0.00486	-0.01019	0.00779	0.00021

122	O1	DZZ	0.00042	0.00066	0.00150	0.00184	-0.00141
123	O1	DXY	0.00173	0.00153	0.00728	-0.00076	0.00214
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.02906	-0.04457	0.02521	0.02729	0.08672
127	H4	S	0.00241	-0.00994	0.01067	0.01194	0.02585
128	H4	PX	0.00183	-0.00322	0.00083	0.00224	0.00532
129	H4	PY	-0.00252	0.00303	-0.00309	-0.00097	-0.00524
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.06702	-0.00328	0.06555	0.02414	-0.03575
132	N1	S	0.13832	0.00596	-0.13818	-0.05106	0.07607
133	N1	PX	-0.02349	-0.03238	-0.01885	0.00495	0.07469
134	N1	PY	0.07420	0.08935	-0.02218	0.01545	-0.05274
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.16746	0.00156	-0.14612	-0.06134	0.08604
137	N1	PX	0.00039	-0.01893	-0.01302	-0.00285	0.03419
138	N1	PY	0.03087	0.03535	-0.00426	0.00495	-0.02637
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.00761	-0.00893	-0.00016	0.00055	0.01050
141	N1	DYY	0.00750	0.00658	-0.00235	-0.00059	-0.00728
142	N1	DZZ	-0.00315	-0.00020	0.00329	0.00064	-0.00290
143	N1	DXY	0.00098	0.00835	-0.00050	0.00364	-0.00058
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.04633	-0.01489	0.05690	-0.00062	-0.03520
147	H6	S	0.01240	-0.00417	0.01188	-0.00387	-0.00777
148	H6	PX	0.00469	-0.00134	0.00534	-0.00021	-0.00326
149	H6	PY	0.00139	-0.00115	0.00226	0.00024	0.00074
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.05973	0.10478	-0.01926	0.01109	-0.02550
152	C8	S	-0.11672	-0.20539	0.03641	-0.02222	0.05363
153	C8	PX	-0.07948	-0.01887	0.08573	0.04075	-0.04871
154	C8	PY	0.00525	0.12952	-0.01034	0.09575	0.13389
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.08468	-0.13950	0.03957	-0.00105	0.03907
157	C8	PX	-0.00881	-0.01790	0.00793	0.00678	0.00446
158	C8	PY	-0.01597	0.00308	0.01253	0.03017	0.03801
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00492	0.00294	-0.00696	0.00099	0.01245
161	C8	DYY	-0.01086	-0.00793	0.00722	0.00223	-0.00402
162	C8	DZZ	0.00463	0.00764	-0.00094	0.00035	-0.00341
163	C8	DXY	-0.00916	0.00292	0.00844	0.00765	0.00234
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.05559	0.00114	0.03915	0.04244	0.03237
167	H8	S	-0.01066	-0.00105	0.00736	0.00452	0.00864
168	H8	PX	0.00555	-0.00013	-0.00361	-0.00376	-0.00267
169	H8	PY	-0.00071	0.00103	0.00042	0.00073	-0.00004
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.04977	0.13180	-0.02938	0.05405	0.08586
172	C10	S	-0.09534	-0.25340	0.05621	-0.10445	-0.16694
173	C10	PX	-0.00260	0.01903	0.01004	0.01497	-0.00764
174	C10	PY	-0.04046	-0.08618	0.01815	-0.01754	0.01281
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

176	C10	S	-0.07753	-0.19722	0.05074	-0.07824	-0.14095
177	C10	PX	0.00018	0.00367	0.00118	-0.00318	-0.01098
178	C10	PY	-0.00530	-0.00781	0.00394	0.00082	0.00971
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00191	0.00226	-0.00078	-0.00046	-0.00317
181	C10	DYY	-0.00490	-0.01141	0.00261	-0.00354	-0.00292
182	C10	DZZ	0.00404	0.01095	-0.00248	0.00465	0.00737
183	C10	DXY	-0.00035	0.00357	0.00105	0.00202	-0.00036
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.02971	-0.07442	0.02251	-0.03185	-0.07407
187	H16	S	-0.00679	-0.01773	0.00739	-0.00737	-0.02687
188	H16	PX	0.00307	0.00723	-0.00218	0.00296	0.00624
189	H16	PY	-0.00157	-0.00354	0.00108	-0.00121	-0.00228
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.02219	-0.07399	0.01282	-0.03976	-0.06985
192	H18	S	-0.00166	-0.01477	0.00181	-0.01426	-0.02854
193	H18	PX	-0.00159	-0.00532	0.00099	-0.00275	-0.00488
194	H18	PY	-0.00165	-0.00608	0.00077	-0.00303	-0.00409
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.00118	-0.04517	-0.08845	0.12012	-0.06968
197	C9	S	0.00234	0.08810	0.17312	-0.23432	0.13590
198	C9	PX	-0.00501	-0.01422	-0.02448	-0.02404	0.06104
199	C9	PY	0.00266	-0.00259	0.01003	-0.00903	0.02942
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.00068	0.06283	0.12898	-0.20316	0.14302
202	C9	PX	-0.00068	0.00555	0.00903	-0.02062	0.01919
203	C9	PY	0.00106	-0.00085	0.00358	0.00222	0.00355
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00058	0.00285	0.00472	0.00109	-0.00698
206	C9	DYY	-0.00023	-0.00083	-0.00202	0.00059	0.00053
207	C9	DZZ	-0.00043	-0.00170	-0.00309	0.00005	0.00316
208	C9	DXY	0.00027	0.00162	0.00153	0.00197	-0.00610
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00205	0.03072	0.06738	-0.08951	0.06349
212	H3	S	0.00067	0.00995	0.02200	-0.03100	0.02471
213	H3	PX	0.00000	0.00060	0.00130	-0.00211	0.00171
214	H3	PY	-0.00015	-0.00297	-0.00616	0.00806	-0.00511
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00108	0.02810	0.05452	-0.09218	0.06522
217	H5	S	0.00009	0.00627	0.01354	-0.02619	0.02274
218	H5	PX	-0.00012	-0.00171	-0.00338	0.00418	-0.00220
219	H5	PY	0.00009	0.00076	0.00173	-0.00222	0.00178
220	H5	PZ	0.00004	0.00228	0.00454	-0.00688	0.00460
221	H7	S	-0.00108	0.02810	0.05452	-0.09218	0.06522
222	H7	S	0.00009	0.00627	0.01354	-0.02619	0.02274
223	H7	PX	-0.00012	-0.00171	-0.00338	0.00418	-0.00220
224	H7	PY	0.00009	0.00076	0.00173	-0.00222	0.00178
225	H7	PZ	-0.00004	-0.00228	-0.00454	0.00688	-0.00460

MO:	21	22	23	24	25
Eigenvalues:	-0.80914	-0.78893	-0.75398	-0.71283	-0.69053
(ev):	-22.01776	-21.46801	-20.51684	-19.39700	-18.79033

		A	A	A	A	A	
1	H1	S	0.08957	-0.05558	0.07055	-0.04284	-0.00203
2	H1	S	0.04411	-0.02156	0.04148	-0.02747	-0.00689
3	H1	PX	-0.00692	0.00301	-0.00388	0.00241	-0.00103
4	H1	PY	-0.00120	0.00339	-0.00259	0.00033	0.00274
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.05475	0.04801	-0.01669	-0.01564	-0.00206
7	C1	S	0.10543	-0.09677	0.03415	0.02966	0.00110
8	C1	PX	0.05386	-0.07982	0.11873	-0.09988	-0.06175
9	C1	PY	0.10514	0.15356	-0.04132	-0.01112	0.17702
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.11926	-0.06094	0.03315	0.03347	0.01070
12	C1	PX	0.01633	-0.04176	0.04066	-0.03564	-0.01654
13	C1	PY	0.03258	0.03364	-0.00567	-0.01127	0.06613
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00437	0.00142	-0.00080	0.00462	0.00494
16	C1	DYY	-0.00178	-0.00825	0.00314	-0.00438	-0.00786
17	C1	DZZ	-0.00363	0.00350	-0.00093	-0.00080	-0.00035
18	C1	DXY	-0.00543	-0.01001	0.00294	-0.00336	-0.00905
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.08677	0.00552	0.01176	0.03219	0.01285
22	C2	S	0.17335	-0.00641	-0.02397	-0.06559	-0.02867
23	C2	PX	-0.08573	0.06374	-0.08517	0.10132	-0.03896
24	C2	PY	-0.02692	-0.14145	-0.00890	-0.02329	0.15879
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.14700	-0.03489	0.00329	-0.06238	-0.01868
27	C2	PX	-0.04706	0.00282	-0.01539	0.05109	-0.00232
28	C2	PY	-0.00619	-0.03559	0.00434	0.00754	0.04006
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00310	0.00641	-0.00306	-0.00264	-0.00819
31	C2	DYY	0.00183	-0.00347	0.00365	0.00262	0.00465
32	C2	DZZ	-0.00583	0.00041	0.00104	0.00152	0.00086
33	C2	DXY	0.00195	-0.00792	0.00017	-0.00297	0.00615
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.06495	0.05277	-0.00785	0.04330	0.01990
37	C3	S	-0.13054	-0.10537	0.01616	-0.08859	-0.04169
38	C3	PX	0.11679	-0.06392	0.17277	0.01088	-0.06959
39	C3	PY	0.01272	-0.12025	-0.00358	0.09313	-0.14481
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.10078	-0.09288	0.03403	-0.07563	-0.05787
42	C3	PX	0.03608	-0.00105	0.06218	-0.00631	-0.02028
43	C3	PY	-0.01317	-0.07611	-0.00745	0.02362	-0.03704
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.00900	0.00559	-0.00449	-0.00187	0.00071
46	C3	DYY	0.00316	-0.00850	0.00196	0.00138	-0.00022
47	C3	DZZ	0.00481	0.00352	0.00067	0.00243	0.00047
48	C3	DXY	-0.00529	-0.00419	-0.00412	-0.00196	0.00095
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00925	-0.08006	0.01292	-0.00553	-0.00382
52	C4	S	-0.01960	0.17103	-0.02669	0.01005	0.00766

53	C4	PX	0.18642	0.01816	-0.05263	-0.06064	0.16597
54	C4	PY	0.01598	0.03798	0.07079	-0.22342	-0.09874
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.03915	0.10340	-0.01725	0.04564	0.00743
57	C4	PX	0.04726	0.00254	-0.01340	-0.02839	0.03589
58	C4	PY	0.01664	0.00290	0.00728	-0.03596	-0.01443
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.00605	0.00042	0.00217	0.01233	0.00604
61	C4	DYY	0.00315	0.00401	0.00046	-0.01830	-0.00934
62	C4	DZZ	0.00088	-0.00653	0.00032	0.00326	0.00138
63	C4	DXY	-0.00418	0.00082	-0.00031	-0.00251	0.00290
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.04337	0.04204	-0.02829	-0.01478	-0.03001
67	C5	S	-0.08825	-0.08315	0.05896	0.03039	0.05897
68	C5	PX	-0.09147	0.11815	-0.06156	0.11508	-0.10411
69	C5	PY	-0.12087	0.04637	0.09576	0.02166	-0.07418
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.07723	-0.06213	0.04892	0.00785	0.05566
72	C5	PX	-0.00871	0.04251	-0.03190	0.03758	-0.04391
73	C5	PY	-0.04097	-0.00713	0.04805	0.00764	-0.02159
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00975	0.00682	0.00182	0.00702	-0.00351
76	C5	DYY	0.00429	-0.00572	-0.00016	-0.00497	0.00247
77	C5	DZZ	0.00379	0.00251	-0.00160	-0.00120	-0.00152
78	C5	DXY	0.00204	0.00282	-0.00153	-0.00259	-0.00301
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.04005	-0.06350	0.00675	-0.01563	-0.00295
82	C6	S	-0.08214	0.13213	-0.01212	0.03434	0.00679
83	C6	PX	-0.15669	-0.06580	-0.09797	-0.09750	0.12714
84	C6	PY	-0.01206	0.01108	-0.18498	-0.05396	-0.11850
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.06085	0.13298	-0.01740	0.01348	-0.01426
87	C6	PX	-0.05989	-0.02020	-0.02049	-0.03847	0.06205
88	C6	PY	-0.00008	0.02213	-0.06419	-0.01505	-0.03838
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00534	0.00236	-0.01119	-0.01153	-0.00134
91	C6	DYY	0.00252	-0.00004	0.00633	0.00733	0.00217
92	C6	DZZ	0.00294	-0.00448	-0.00040	-0.00145	-0.00154
93	C6	DXY	-0.01156	-0.00323	0.00766	0.00336	0.00276
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.05975	-0.04770	-0.04055	-0.03791	-0.00135
97	C7	S	0.12092	0.09513	0.08175	0.07494	0.00146
98	C7	PX	0.05970	0.01987	0.11954	0.14927	-0.10850
99	C7	PY	-0.07849	-0.08329	0.12687	-0.10779	-0.01879
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.08796	0.05525	0.06831	0.09473	0.00882
102	C7	PX	0.03556	0.03066	0.05591	0.06012	-0.04932
103	C7	PY	-0.02341	-0.03746	0.02237	-0.03399	-0.00892
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00371	0.00590	-0.00092	0.00503	0.00258
106	C7	DYY	0.00121	-0.00202	-0.00065	-0.00228	-0.00197

107	C7	DZZ	-0.00401	-0.00340	-0.00176	-0.00261	-0.00069
108	C7	DXY	0.00813	0.00333	-0.01065	0.00645	-0.00009
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00541	0.04426	0.00584	-0.02226	0.00513
112	O1	S	0.01188	-0.10397	-0.01222	0.05353	-0.01420
113	O1	PX	0.06890	0.00467	-0.05016	-0.00042	0.21744
114	O1	PY	-0.02850	-0.19951	-0.04677	0.29547	0.08164
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.01818	-0.15403	-0.02418	0.07983	-0.01290
117	O1	PX	0.04114	0.00203	-0.03197	0.00150	0.14548
118	O1	PY	-0.01433	-0.12203	-0.02600	0.18172	0.05038
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00119	-0.00452	-0.00221	0.00575	0.01171
121	O1	DYY	-0.00049	0.01087	0.00249	-0.00987	-0.00837
122	O1	DZZ	-0.00132	-0.00399	0.00071	0.00385	-0.00357
123	O1	DXY	-0.00756	-0.00832	0.00058	0.01379	-0.00643
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.04954	-0.06252	0.08480	-0.01972	0.03901
127	H4	S	-0.01702	-0.02932	0.03826	-0.00679	0.01855
128	H4	PX	-0.00394	-0.00252	0.00412	-0.00007	0.00027
129	H4	PY	0.00118	0.00464	-0.00375	0.00160	-0.00414
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01439	0.03597	-0.04039	-0.01554	0.01599
132	N1	S	0.03282	-0.07719	0.09163	0.03367	-0.03699
133	N1	PX	-0.00625	-0.06884	-0.13401	-0.08359	0.03669
134	N1	PY	-0.03887	0.12500	0.13249	0.08354	0.12583
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.03989	-0.11124	0.08277	0.04434	-0.06203
137	N1	PX	0.00397	-0.03214	-0.06974	-0.03831	0.01673
138	N1	PY	-0.02651	0.04992	0.04588	0.03391	0.06315
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00390	-0.00955	-0.01764	-0.00992	-0.00170
141	N1	DYY	-0.00366	0.00924	0.01311	0.00686	0.00398
142	N1	DZZ	0.00036	0.00153	0.00161	0.00069	-0.00252
143	N1	DXY	-0.00649	0.00592	0.00319	0.00066	0.01396
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.11992	-0.01204	0.03260	-0.07956	-0.02152
147	H6	S	0.04952	-0.01087	0.02257	-0.03823	-0.01236
148	H6	PX	0.00886	-0.00057	0.00194	-0.00454	-0.00174
149	H6	PY	0.00299	-0.00244	0.00028	-0.00291	0.00202
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.03640	0.00944	0.08766	0.00605	0.03379
152	C8	S	0.07441	-0.02089	-0.18051	-0.01317	-0.06862
153	C8	PX	0.03213	0.14963	0.01922	0.10082	0.04747
154	C8	PY	0.06173	0.02944	-0.03744	-0.00111	0.12865
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.06839	-0.00284	-0.15129	-0.00691	-0.07104
157	C8	PX	0.01900	0.03259	-0.00919	0.02725	0.00967
158	C8	PY	0.03559	0.02045	-0.01817	0.00076	0.02575
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00683	-0.00707	-0.00244	0.00107	-0.00193

161	C8	DYY	-0.00332	0.00628	-0.00082	-0.00283	0.00626
162	C8	DZZ	-0.00266	0.00170	0.00665	0.00127	0.00174
163	C8	DXY	0.00667	0.00750	-0.00135	0.00350	-0.00082
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.08653	0.05824	0.09587	0.12486	-0.05693
167	H8	S	0.03852	0.02286	0.04879	0.07261	-0.03202
168	H8	PX	-0.00667	-0.00413	-0.00695	-0.00819	0.00382
169	H8	PY	-0.00018	-0.00067	0.00255	-0.00091	-0.00080
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.05192	-0.01064	-0.05708	0.00604	-0.02713
172	C10	S	-0.10200	0.01987	0.11249	-0.01285	0.05210
173	C10	PX	0.00208	0.06116	0.04399	0.06295	0.09375
174	C10	PY	0.06241	-0.00790	-0.15352	0.02728	-0.16326
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.08971	0.02822	0.11725	-0.01580	0.06940
177	C10	PX	-0.00741	0.01659	0.01818	0.02292	0.03725
178	C10	PY	0.02447	0.00099	-0.05084	0.01391	-0.05476
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.00513	0.00128	0.01152	-0.00048	0.01134
181	C10	DYY	0.00164	-0.00044	-0.00572	0.00058	-0.00806
182	C10	DZZ	0.00447	-0.00095	-0.00508	0.00033	-0.00275
183	C10	DXY	-0.00110	0.00189	0.00366	-0.00100	0.00361
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.05446	0.03989	0.10396	0.02270	0.10798
187	H16	S	-0.02343	0.02356	0.05900	0.01768	0.06922
188	H16	PX	0.00428	-0.00247	-0.00687	-0.00088	-0.00630
189	H16	PY	-0.00069	0.00122	0.00105	0.00126	0.00027
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.06636	-0.01030	0.09104	-0.04051	0.05047
192	H18	S	-0.03287	-0.00614	0.05154	-0.02072	0.03195
193	H18	PX	-0.00431	0.00011	0.00595	-0.00160	0.00414
194	H18	PY	-0.00296	-0.00113	0.00284	-0.00178	-0.00030
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.02926	-0.03874	-0.00927	0.01533	0.01918
197	C9	S	-0.05871	0.07420	0.01713	-0.02633	-0.03735
198	C9	PX	-0.03235	0.13325	0.05313	-0.17538	-0.12929
199	C9	PY	-0.05540	0.00220	0.01202	0.07437	-0.11180
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.06870	0.10817	0.03389	-0.06400	-0.08003
202	C9	PX	-0.00637	0.03780	0.01404	-0.05771	-0.03032
203	C9	PY	-0.02072	-0.00694	-0.00011	0.04212	-0.04303
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00438	-0.01421	-0.00535	0.01404	0.01436
206	C9	DYY	-0.00043	0.00262	0.00042	0.00007	-0.00332
207	C9	DZZ	-0.00169	0.00838	0.00336	-0.01199	-0.00728
208	C9	DXY	0.00595	-0.00714	-0.00433	0.00437	0.01453
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.04945	0.02519	0.01046	0.04028	-0.07055
212	H3	S	-0.02146	0.00978	0.00501	0.02649	-0.03946
213	H3	PX	-0.00103	0.00167	0.00066	-0.00138	-0.00209
214	H3	PY	0.00317	-0.00211	-0.00063	-0.00172	0.00346

215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.02453	0.06819	0.02233	-0.07585	-0.04082
217	H5	S	-0.01074	0.03130	0.01166	-0.04388	-0.02506
218	H5	PX	0.00085	-0.00085	-0.00008	0.00020	-0.00021
219	H5	PY	-0.00131	0.00132	0.00045	-0.00031	-0.00208
220	H5	PZ	-0.00183	0.00428	0.00130	-0.00447	-0.00243
221	H7	S	-0.02453	0.06819	0.02233	-0.07585	-0.04082
222	H7	S	-0.01074	0.03130	0.01166	-0.04388	-0.02506
223	H7	PX	0.00085	-0.00085	-0.00008	0.00020	-0.00021
224	H7	PY	-0.00131	0.00132	0.00045	-0.00031	-0.00208
225	H7	PZ	0.00183	-0.00428	-0.00130	0.00447	0.00243

MO:	26	27	28	29	30
Eigenvalues:	-0.66680	-0.66574	-0.63677	-0.61061	-0.59333
(ev):	-18.14466	-18.11570	-17.32740	-16.61563	-16.14528

		A	A	A	A	A	
1	H1	S	0.00000	0.13519	0.06131	0.16822	0.09789
2	H1	S	0.00000	0.08301	0.04297	0.12321	0.07031
3	H1	PX	0.00000	-0.00715	-0.00233	-0.00856	-0.00547
4	H1	PY	0.00000	-0.00302	-0.00140	-0.00269	0.00038
5	H1	PZ	-0.00145	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	-0.04170	0.01101	-0.02142	-0.00632
7	C1	S	0.00000	0.08374	-0.02000	0.03999	0.00888
8	C1	PX	0.00000	0.16674	0.12658	0.21386	0.08818
9	C1	PY	0.00000	-0.01534	-0.04094	0.08491	0.19323
10	C1	PZ	-0.05881	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	0.07304	-0.04885	0.06053	0.02433
12	C1	PX	0.00000	0.08496	0.06698	0.09687	0.04890
13	C1	PY	0.00000	0.01004	0.00426	0.03108	0.08471
14	C1	PZ	-0.03466	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.00447	0.00025	0.01035	0.01028
16	C1	DYY	0.00000	-0.00242	0.00115	-0.00872	-0.01192
17	C1	DZZ	0.00000	-0.00242	0.00024	-0.00153	-0.00056
18	C1	DXY	0.00000	0.01134	0.00836	0.00611	-0.00346
19	C1	DXZ	0.00515	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.00387	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.02483	0.02784	-0.01871	0.01434
22	C2	S	0.00000	-0.05255	-0.05625	0.03853	-0.02919
23	C2	PX	0.00000	-0.02340	0.24902	0.17614	0.04900
24	C2	PY	0.00000	-0.04401	0.11732	0.10838	-0.15818
25	C2	PZ	-0.01899	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.00956	-0.06198	0.04061	-0.01048
27	C2	PX	0.00000	0.01845	0.13053	0.07601	0.03636
28	C2	PY	0.00000	-0.00076	0.05073	0.03111	-0.04679
29	C2	PZ	-0.00761	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.00025	-0.01116	-0.00614	0.00445
31	C2	DYY	0.00000	0.00125	0.00887	0.00495	-0.00162
32	C2	DZZ	0.00000	0.00107	0.00205	-0.00051	0.00058
33	C2	DXY	0.00000	-0.00676	-0.00735	0.00157	-0.01135
34	C2	DXZ	-0.00106	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	-0.00157	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.01524	0.00693	0.03949	0.02437
37	C3	S	0.00000	-0.03105	-0.01414	-0.08142	-0.05195

38	C3	PX	0.00000	-0.09255	-0.02838	0.01088	-0.01001
39	C3	PY	0.00000	0.06981	0.04774	-0.06355	-0.18005
40	C3	PZ	-0.02055	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	-0.02589	0.02313	-0.10820	-0.04050
42	C3	PX	0.00000	-0.03488	-0.01707	-0.00244	-0.01752
43	C3	PY	0.00000	0.04573	0.02619	-0.02309	-0.06511
44	C3	PZ	-0.00619	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00076	0.00832	0.00053	0.00632
46	C3	DYY	0.00000	0.00206	-0.00783	-0.00275	-0.00741
47	C3	DZZ	0.00000	0.00017	0.00047	0.00136	0.00103
48	C3	DXY	0.00000	0.01448	0.00358	0.00296	-0.00337
49	C3	DXZ	0.00014	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00123	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.03909	0.03787	0.01496	-0.00783
52	C4	S	0.00000	-0.08616	-0.08146	-0.03314	0.01776
53	C4	PX	0.00000	-0.02548	-0.02913	-0.05564	0.01922
54	C4	PY	0.00000	0.06051	0.08757	0.04116	-0.06621
55	C4	PZ	-0.14054	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.04797	-0.06978	-0.01869	0.03370
57	C4	PX	0.00000	-0.00960	-0.00873	-0.01469	-0.00347
58	C4	PY	0.00000	-0.00222	-0.00947	0.01352	-0.01020
59	C4	PZ	-0.06533	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.00372	-0.00016	0.00074	0.01488
61	C4	DYY	0.00000	-0.00266	0.00532	-0.00010	-0.01804
62	C4	DZZ	0.00000	0.00193	0.00033	0.00060	0.00163
63	C4	DXY	0.00000	-0.00566	0.01529	-0.00019	-0.00279
64	C4	DXZ	-0.00273	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.01386	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.02036	-0.03819	0.00153	-0.00927
67	C5	S	0.00000	0.04320	0.07866	-0.00158	0.01766
68	C5	PX	0.00000	-0.11545	-0.02276	0.09343	-0.01734
69	C5	PY	0.00000	0.14895	-0.07374	-0.19609	0.18518
70	C5	PZ	-0.03835	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.02123	0.05903	-0.02064	0.02221
72	C5	PX	0.00000	-0.06628	-0.03035	0.04806	-0.02201
73	C5	PY	0.00000	0.08495	0.00055	-0.07576	0.07919
74	C5	PZ	-0.02128	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	-0.00057	-0.00840	-0.00898	0.00592
76	C5	DYY	0.00000	0.00112	0.00762	0.00522	-0.00255
77	C5	DZZ	0.00000	-0.00130	-0.00183	0.00062	-0.00105
78	C5	DXY	0.00000	-0.00884	-0.00556	0.00726	-0.01062
79	C5	DXZ	-0.00358	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00042	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.04351	-0.02974	0.00329	-0.04001
82	C6	S	0.00000	0.09570	0.06321	-0.00804	0.08713
83	C6	PX	0.00000	0.02407	-0.00947	-0.01638	-0.04887
84	C6	PY	0.00000	-0.05608	0.05784	0.05462	0.06813
85	C6	PZ	-0.01278	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	0.07597	0.04900	-0.02451	0.08668
87	C6	PX	0.00000	0.01651	-0.00829	0.00400	-0.02435
88	C6	PY	0.00000	-0.02847	0.01162	0.01299	0.00720
89	C6	PZ	-0.00787	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.00066	-0.00685	-0.00291	0.00750
91	C6	DYY	0.00000	-0.00011	0.00641	0.00556	-0.00803

92	C6	DZZ	0.00000	-0.00285	-0.00098	0.00001	-0.00113
93	C6	DXY	0.00000	0.00447	0.00206	-0.01299	-0.00685
94	C6	DXZ	-0.00030	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.00030	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.03415	-0.00399	-0.00791	-0.01884
97	C7	S	0.00000	-0.06875	0.00725	0.01652	0.03988
98	C7	PX	0.00000	-0.08398	0.14560	-0.05993	-0.03999
99	C7	PY	0.00000	-0.16399	-0.00943	-0.04447	0.05441
100	C7	PZ	-0.00764	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	-0.05357	0.01357	0.02305	0.01352
102	C7	PX	0.00000	-0.05195	0.06623	-0.03156	0.00282
103	C7	PY	0.00000	-0.05271	-0.00241	-0.00941	0.03247
104	C7	PZ	-0.00432	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	-0.00300	0.00386	0.00310	0.00132
106	C7	DYY	0.00000	0.00550	-0.00339	-0.00155	-0.00185
107	C7	DZZ	0.00000	0.00133	-0.00025	-0.00094	-0.00070
108	C7	DXY	0.00000	0.01187	-0.00176	0.00432	-0.00506
109	C7	DXZ	0.00074	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.00074	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00756	0.00643	-0.01749	0.00779
112	O1	S	0.00000	0.01892	-0.01958	0.04467	-0.01633
113	O1	PX	0.00000	-0.09240	0.18061	-0.21438	0.03483
114	O1	PY	0.00000	0.02412	-0.08231	0.02150	0.10904
115	O1	PZ	-0.40066	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	0.02772	-0.00779	0.05747	-0.03823
117	O1	PX	0.00000	-0.06477	0.12437	-0.15219	0.02360
118	O1	PY	0.00000	0.01820	-0.05386	0.01879	0.07307
119	O1	PZ	-0.26458	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.00295	0.00939	-0.01144	0.00424
121	O1	DYY	0.00000	-0.00030	-0.00746	0.00604	-0.00188
122	O1	DZZ	0.00000	0.00250	-0.00474	0.00546	0.00043
123	O1	DXY	0.00000	0.00365	-0.00887	0.00698	0.00362
124	O1	DXZ	-0.01809	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.01235	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	0.13156	0.01793	-0.12666	0.10417
127	H4	S	0.00000	0.07609	-0.00697	-0.08246	0.07454
128	H4	PX	0.00000	0.00569	0.00006	-0.00436	0.00437
129	H4	PY	0.00000	-0.00489	-0.00219	0.00466	-0.00239
130	H4	PZ	-0.00090	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	0.03760	-0.01122	0.00350	0.03446
132	N1	S	0.00000	-0.08240	0.02469	-0.00945	-0.07499
133	N1	PX	0.00000	-0.01417	-0.03453	0.08633	-0.01322
134	N1	PY	0.00000	0.16044	-0.01297	-0.03641	0.01407
135	N1	PZ	-0.00802	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	-0.13827	0.03907	-0.00074	-0.12222
137	N1	PX	0.00000	-0.00337	-0.01888	0.05132	-0.00277
138	N1	PY	0.00000	0.07456	-0.00609	-0.01214	0.00163
139	N1	PZ	-0.00394	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.00493	-0.00449	0.00887	-0.00089
141	N1	DYY	0.00000	0.00909	0.00187	-0.00752	0.00504
142	N1	DZZ	0.00000	-0.00071	0.00119	-0.00186	0.00055
143	N1	DXY	0.00000	0.00939	-0.00324	0.00145	-0.00174
144	N1	DXZ	-0.00051	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	-0.00072	0.00000	0.00000	0.00000	0.00000

146	H6	S	0.00000	-0.00642	-0.19416	-0.10381	-0.01513
147	H6	S	0.00000	0.00360	-0.11850	-0.07692	-0.00542
148	H6	PX	0.00000	-0.00060	-0.01016	-0.00520	-0.00053
149	H6	PY	0.00000	-0.00072	-0.00314	-0.00073	-0.00263
150	H6	PZ	-0.00042	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.04177	0.00160	0.00538	-0.00529
152	C8	S	0.00000	0.08657	-0.00444	-0.00936	0.00937
153	C8	PX	0.00000	0.18515	-0.00806	-0.04445	-0.00859
154	C8	PY	0.00000	-0.00779	-0.09522	0.17134	-0.06158
155	C8	PZ	-0.00458	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	0.07050	-0.00373	-0.00003	0.02351
157	C8	PX	0.00000	0.05415	-0.00534	-0.00432	0.02303
158	C8	PY	0.00000	0.00093	-0.02199	0.03904	0.00259
159	C8	PZ	-0.00212	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.00946	0.00021	0.00821	-0.01125
161	C8	DYY	0.00000	0.00784	-0.00346	-0.00259	0.00995
162	C8	DZZ	0.00000	-0.00113	0.00037	-0.00075	0.00012
163	C8	DXY	0.00000	-0.00136	-0.00119	0.00239	0.01080
164	C8	DXZ	0.00018	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	-0.00028	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	-0.07637	0.09307	-0.02312	-0.00696
167	H8	S	0.00000	-0.04162	0.06353	-0.01120	-0.01302
168	H8	PX	0.00000	0.00483	-0.00519	0.00155	0.00020
169	H8	PY	0.00000	-0.00262	0.00054	-0.00061	0.00109
170	H8	PZ	-0.00012	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	0.01053	0.00420	0.00059	-0.00487
172	C10	S	0.00000	-0.02199	-0.00787	-0.00230	0.01124
173	C10	PX	0.00000	0.13466	-0.03838	0.03337	-0.30449
174	C10	PY	0.00000	0.16030	0.07629	-0.17309	-0.00037
175	C10	PZ	-0.00175	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	-0.02631	-0.01314	0.00075	0.01931
177	C10	PX	0.00000	0.05809	-0.01576	0.01162	-0.15249
178	C10	PY	0.00000	0.06366	0.03014	-0.07018	-0.01334
179	C10	PZ	-0.00081	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.00640	-0.00471	0.00959	-0.00932
181	C10	DYY	0.00000	0.00344	0.00374	-0.00698	0.00777
182	C10	DZZ	0.00000	0.00122	0.00052	-0.00066	0.00024
183	C10	DXY	0.00000	-0.00628	-0.00158	0.00394	0.01363
184	C10	DXZ	0.00005	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	-0.00022	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.02940	-0.04099	0.05634	-0.18132
187	H16	S	0.00000	0.01771	-0.02779	0.04442	-0.13822
188	H16	PX	0.00000	-0.00087	0.00227	-0.00294	0.00770
189	H16	PY	0.00000	0.00295	0.00034	-0.00139	-0.00388
190	H16	PZ	-0.00004	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	-0.13134	-0.01873	0.05740	0.14597
192	H18	S	0.00000	-0.08414	-0.01246	0.04162	0.09397
193	H18	PX	0.00000	-0.00548	-0.00145	0.00339	0.00413
194	H18	PY	0.00000	-0.00465	0.00046	-0.00008	0.00646
195	H18	PZ	-0.00004	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00245	0.00335	0.00561	0.00515
197	C9	S	0.00000	-0.00663	-0.00854	-0.01329	-0.00970
198	C9	PX	0.00000	0.03067	0.02408	0.04930	-0.08657
199	C9	PY	0.00000	0.02472	-0.23187	0.14276	0.03471

200	C9	PZ	-0.31445	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	0.00704	-0.02188	0.01224	-0.02238
202	C9	PX	0.00000	0.00553	0.02415	0.00381	-0.03306
203	C9	PY	0.00000	0.00290	-0.10782	0.05543	0.01463
204	C9	PZ	-0.12903	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	-0.00249	0.00726	-0.00848	0.00461
206	C9	DYY	0.00000	-0.00038	-0.01059	0.00530	0.00232
207	C9	DZZ	0.00000	0.00170	0.00480	0.00096	-0.00614
208	C9	DXY	0.00000	-0.00466	0.01104	-0.01184	0.00200
209	C9	DXZ	-0.00428	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.01540	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.00879	-0.14637	0.07842	0.02524
212	H3	S	0.00000	0.00782	-0.10136	0.06080	0.02305
213	H3	PX	0.00000	0.00039	-0.00122	0.00119	-0.00077
214	H3	PY	0.00000	-0.00024	0.00652	-0.00314	-0.00106
215	H3	PZ	-0.00480	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.14889	0.00619	0.03925	-0.00724	-0.03672
217	H5	S	0.11158	0.00611	0.02785	-0.00212	-0.02704
218	H5	PX	-0.00577	0.00040	-0.00090	0.00125	0.00019
219	H5	PY	0.00255	0.00017	-0.00244	0.00138	-0.00041
220	H5	PZ	0.00469	0.00020	0.00240	-0.00075	-0.00227
221	H7	S	-0.14889	0.00619	0.03925	-0.00724	-0.03672
222	H7	S	-0.11158	0.00611	0.02785	-0.00212	-0.02704
223	H7	PX	0.00577	0.00040	-0.00090	0.00125	0.00019
224	H7	PY	-0.00255	0.00017	-0.00244	0.00138	-0.00041
225	H7	PZ	0.00469	-0.00020	-0.00240	0.00075	0.00227

MO:		31	32	33	34	35
Eigenvalues:		-0.57233	-0.56064	-0.55923	-0.53266	-0.51654
(ev):		-15.57390	-15.25578	-15.21754	-14.49451	-14.05566

		A	A	A	A	A	
1	H1	S	0.04066	0.02166	0.00000	0.01612	0.00000
2	H1	S	0.03337	0.02542	0.00000	0.00751	0.00000
3	H1	PX	-0.00136	0.00013	0.00000	-0.00138	0.00000
4	H1	PY	-0.00070	-0.00078	0.00000	0.00018	0.00000
5	H1	PZ	0.00000	0.00000	0.00224	0.00000	0.00123
6	C1	S	0.01459	-0.00550	0.00000	0.00864	0.00000
7	C1	S	-0.03071	0.00835	0.00000	-0.01836	0.00000
8	C1	PX	0.08661	0.03933	0.00000	0.02380	0.00000
9	C1	PY	0.00860	-0.09128	0.00000	0.08984	0.00000
10	C1	PZ	0.00000	0.00000	0.11241	0.00000	0.08591
11	C1	S	-0.03155	0.04429	0.00000	-0.04476	0.00000
12	C1	PX	0.03014	0.00546	0.00000	0.01952	0.00000
13	C1	PY	0.01873	-0.04365	0.00000	0.06011	0.00000
14	C1	PZ	0.00000	0.00000	0.06295	0.00000	0.05449
15	C1	DXX	0.00449	0.00273	0.00000	0.00046	0.00000
16	C1	DYY	-0.00431	-0.00134	0.00000	-0.00149	0.00000
17	C1	DZZ	0.00050	-0.00068	0.00000	-0.00010	0.00000
18	C1	DXY	-0.00297	0.00811	0.00000	-0.00398	0.00000
19	C1	DXZ	0.00000	0.00000	-0.00728	0.00000	-0.00831
20	C1	DYZ	0.00000	0.00000	-0.00255	0.00000	0.00653
21	C2	S	-0.00651	-0.00326	0.00000	0.00112	0.00000
22	C2	S	0.01665	0.00398	0.00000	0.00149	0.00000

23	C2	PX	0.03659	-0.03078	0.00000	0.12026	0.00000
24	C2	PY	-0.05283	-0.22527	0.00000	-0.13517	0.00000
25	C2	PZ	0.00000	0.00000	0.12140	0.00000	0.01884
26	C2	S	-0.00409	0.03703	0.00000	-0.01399	0.00000
27	C2	PX	-0.00288	-0.00748	0.00000	0.05935	0.00000
28	C2	PY	-0.02948	-0.08480	0.00000	-0.05696	0.00000
29	C2	PZ	0.00000	0.00000	0.06650	0.00000	0.01421
30	C2	DXX	0.00008	0.01252	0.00000	0.00307	0.00000
31	C2	DYY	0.00075	-0.00921	0.00000	-0.00209	0.00000
32	C2	DZZ	0.00033	-0.00112	0.00000	0.00061	0.00000
33	C2	DXY	0.00396	-0.00428	0.00000	-0.01425	0.00000
34	C2	DXZ	0.00000	0.00000	0.00814	0.00000	-0.00036
35	C2	DYZ	0.00000	0.00000	0.00129	0.00000	0.00595
36	C3	S	-0.01603	0.01705	0.00000	-0.00527	0.00000
37	C3	S	0.03403	-0.03629	0.00000	0.01069	0.00000
38	C3	PX	0.23169	-0.02858	0.00000	0.01230	0.00000
39	C3	PY	-0.14982	0.11103	0.00000	-0.09141	0.00000
40	C3	PZ	0.00000	0.00000	0.18426	0.00000	-0.03999
41	C3	S	0.00533	-0.06184	0.00000	0.02838	0.00000
42	C3	PX	0.10726	-0.02247	0.00000	0.01124	0.00000
43	C3	PY	-0.02204	0.03115	0.00000	-0.00909	0.00000
44	C3	PZ	0.00000	0.00000	0.10895	0.00000	-0.02610
45	C3	DXX	-0.01131	-0.00328	0.00000	0.00651	0.00000
46	C3	DYY	0.00578	0.00404	0.00000	-0.00749	0.00000
47	C3	DZZ	0.00005	0.00009	0.00000	0.00011	0.00000
48	C3	DXY	-0.01069	0.00320	0.00000	-0.00722	0.00000
49	C3	DXZ	0.00000	0.00000	-0.00302	0.00000	0.00117
50	C3	DYZ	0.00000	0.00000	-0.00712	0.00000	0.00822
51	C4	S	-0.01829	0.01035	0.00000	-0.00822	0.00000
52	C4	S	0.04460	-0.02068	0.00000	0.01936	0.00000
53	C4	PX	-0.16130	-0.16175	0.00000	0.08116	0.00000
54	C4	PY	-0.07228	-0.06828	0.00000	0.06201	0.00000
55	C4	PZ	0.00000	0.00000	0.10870	0.00000	0.19874
56	C4	S	0.04197	-0.00872	0.00000	-0.00379	0.00000
57	C4	PX	-0.06314	-0.07348	0.00000	0.04058	0.00000
58	C4	PY	-0.00641	-0.01219	0.00000	0.00964	0.00000
59	C4	PZ	0.00000	0.00000	0.06189	0.00000	0.11993
60	C4	DXX	0.01233	0.01055	0.00000	0.00137	0.00000
61	C4	DYY	-0.01171	-0.00995	0.00000	-0.00253	0.00000
62	C4	DZZ	0.00098	0.00187	0.00000	-0.00103	0.00000
63	C4	DXY	0.01355	0.00369	0.00000	0.00137	0.00000
64	C4	DXZ	0.00000	0.00000	0.00135	0.00000	0.00154
65	C4	DYZ	0.00000	0.00000	-0.00484	0.00000	0.00936
66	C5	S	-0.01223	0.00577	0.00000	-0.00035	0.00000
67	C5	S	0.02552	-0.01204	0.00000	-0.00481	0.00000
68	C5	PX	0.21234	0.11376	0.00000	-0.08685	0.00000
69	C5	PY	-0.01547	0.19828	0.00000	0.14101	0.00000
70	C5	PZ	0.00000	0.00000	0.10056	0.00000	0.07776
71	C5	S	0.05167	-0.00920	0.00000	0.03710	0.00000
72	C5	PX	0.09896	0.03868	0.00000	-0.04960	0.00000
73	C5	PY	-0.03274	0.07049	0.00000	0.06010	0.00000
74	C5	PZ	0.00000	0.00000	0.06193	0.00000	0.05099
75	C5	DXX	0.00747	0.01091	0.00000	-0.00008	0.00000
76	C5	DYY	-0.00532	-0.00714	0.00000	0.00365	0.00000

77	C5	DZZ	-0.00037	-0.00035	0.00000	-0.00110	0.00000
78	C5	DXY	0.00873	-0.00294	0.00000	-0.01280	0.00000
79	C5	DXZ	0.00000	0.00000	0.00304	0.00000	0.00591
80	C5	DYZ	0.00000	0.00000	-0.00664	0.00000	0.00071
81	C6	S	0.02335	0.01064	0.00000	-0.00294	0.00000
82	C6	S	-0.05049	-0.02494	0.00000	0.00055	0.00000
83	C6	PX	-0.15797	-0.06450	0.00000	-0.06108	0.00000
84	C6	PY	-0.06518	0.14022	0.00000	0.23011	0.00000
85	C6	PZ	0.00000	0.00000	0.23109	0.00000	-0.09462
86	C6	S	-0.02883	-0.03142	0.00000	0.04742	0.00000
87	C6	PX	-0.05509	-0.02183	0.00000	-0.02895	0.00000
88	C6	PY	-0.03155	0.04223	0.00000	0.06963	0.00000
89	C6	PZ	0.00000	0.00000	0.13526	0.00000	-0.05806
90	C6	DXX	-0.00140	0.00664	0.00000	0.01048	0.00000
91	C6	DYY	0.00035	-0.00543	0.00000	-0.00745	0.00000
92	C6	DZZ	0.00062	0.00102	0.00000	0.00183	0.00000
93	C6	DXY	-0.00547	-0.01106	0.00000	-0.00980	0.00000
94	C6	DXZ	0.00000	0.00000	0.00405	0.00000	-0.00217
95	C6	DYZ	0.00000	0.00000	-0.01115	0.00000	0.01007
96	C7	S	0.00216	-0.00513	0.00000	-0.00188	0.00000
97	C7	S	-0.00176	0.01073	0.00000	0.00321	0.00000
98	C7	PX	-0.23428	-0.02754	0.00000	0.01257	0.00000
99	C7	PY	0.18743	-0.14480	0.00000	0.10914	0.00000
100	C7	PZ	0.00000	0.00000	0.14676	0.00000	-0.06559
101	C7	S	-0.00762	0.03647	0.00000	0.02433	0.00000
102	C7	PX	-0.11571	-0.02435	0.00000	0.00151	0.00000
103	C7	PY	0.06761	-0.04735	0.00000	0.03407	0.00000
104	C7	PZ	0.00000	0.00000	0.08504	0.00000	-0.04196
105	C7	DXX	-0.01737	0.00436	0.00000	0.00107	0.00000
106	C7	DYY	0.01502	-0.00241	0.00000	-0.00167	0.00000
107	C7	DZZ	0.00103	-0.00072	0.00000	0.00022	0.00000
108	C7	DXY	-0.00694	0.01202	0.00000	-0.00697	0.00000
109	C7	DXZ	0.00000	0.00000	-0.01161	0.00000	0.00517
110	C7	DYZ	0.00000	0.00000	0.00410	0.00000	0.00074
111	O1	S	0.00879	-0.00154	0.00000	0.02192	0.00000
112	O1	S	-0.01860	0.00361	0.00000	-0.05224	0.00000
113	O1	PX	0.11260	0.04803	0.00000	0.14085	0.00000
114	O1	PY	0.07338	0.11186	0.00000	-0.08666	0.00000
115	O1	PZ	0.00000	0.00000	0.03953	0.00000	0.32398
116	O1	S	-0.04372	0.00352	0.00000	-0.08718	0.00000
117	O1	PX	0.08256	0.03338	0.00000	0.10492	0.00000
118	O1	PY	0.05250	0.08318	0.00000	-0.07372	0.00000
119	O1	PZ	0.00000	0.00000	0.02839	0.00000	0.25348
120	O1	DXX	0.00974	0.00977	0.00000	0.00235	0.00000
121	O1	DYY	-0.00551	-0.01150	0.00000	0.00695	0.00000
122	O1	DZZ	-0.00060	0.00071	0.00000	-0.00493	0.00000
123	O1	DXY	0.00348	0.00489	0.00000	-0.00518	0.00000
124	O1	DXZ	0.00000	0.00000	-0.00157	0.00000	0.00353
125	O1	DYZ	0.00000	0.00000	-0.00479	0.00000	-0.01659
126	H4	S	-0.09283	0.03431	0.00000	0.11186	0.00000
127	H4	S	-0.07059	0.02911	0.00000	0.08315	0.00000
128	H4	PX	-0.00219	0.00292	0.00000	0.00326	0.00000
129	H4	PY	0.00433	0.00138	0.00000	-0.00314	0.00000
130	H4	PZ	0.00000	0.00000	0.00189	0.00000	0.00180

131	N1	S	-0.00766	0.00315	0.00000	-0.02493	0.00000
132	N1	S	0.01924	-0.00879	0.00000	0.05666	0.00000
133	N1	PX	-0.10779	0.10458	0.00000	0.01363	0.00000
134	N1	PY	0.03147	-0.13595	0.00000	-0.25312	0.00000
135	N1	PZ	0.00000	0.00000	0.23856	0.00000	-0.13762
136	N1	S	0.00387	0.01388	0.00000	0.09168	0.00000
137	N1	PX	-0.06260	0.06300	0.00000	-0.00413	0.00000
138	N1	PY	0.00436	-0.06446	0.00000	-0.13757	0.00000
139	N1	PZ	0.00000	0.00000	0.15075	0.00000	-0.09338
140	N1	DXX	-0.00706	0.01522	0.00000	0.00864	0.00000
141	N1	DYY	0.00540	-0.01426	0.00000	-0.01423	0.00000
142	N1	DZZ	0.00191	-0.00132	0.00000	0.00283	0.00000
143	N1	DXY	-0.00547	-0.00407	0.00000	-0.01431	0.00000
144	N1	DXZ	0.00000	0.00000	0.01594	0.00000	-0.00966
145	N1	DYZ	0.00000	0.00000	0.01698	0.00000	-0.00806
146	H6	S	-0.00209	0.07041	0.00000	-0.05128	0.00000
147	H6	S	-0.00742	0.05763	0.00000	-0.03642	0.00000
148	H6	PX	0.00007	0.00358	0.00000	-0.00164	0.00000
149	H6	PY	-0.00154	-0.00158	0.00000	-0.00276	0.00000
150	H6	PZ	0.00000	0.00000	0.00253	0.00000	0.00031
151	C8	S	-0.00921	-0.01004	0.00000	0.00733	0.00000
152	C8	S	0.01765	0.02352	0.00000	-0.01555	0.00000
153	C8	PX	0.06034	-0.06236	0.00000	-0.13646	0.00000
154	C8	PY	-0.08868	0.25146	0.00000	0.01034	0.00000
155	C8	PZ	0.00000	0.00000	0.17383	0.00000	-0.11704
156	C8	S	0.00400	0.05138	0.00000	-0.01885	0.00000
157	C8	PX	0.00683	-0.00820	0.00000	-0.08929	0.00000
158	C8	PY	-0.02742	0.05587	0.00000	-0.00779	0.00000
159	C8	PZ	0.00000	0.00000	0.10041	0.00000	-0.07198
160	C8	DXX	-0.01127	0.01652	0.00000	0.01423	0.00000
161	C8	DYY	0.00879	-0.01064	0.00000	-0.01385	0.00000
162	C8	DZZ	0.00057	-0.00183	0.00000	-0.00099	0.00000
163	C8	DXY	-0.00184	0.00677	0.00000	-0.00689	0.00000
164	C8	DXZ	0.00000	0.00000	-0.00511	0.00000	0.00305
165	C8	DYZ	0.00000	0.00000	0.00415	0.00000	-0.00065
166	H8	S	-0.16984	-0.00207	0.00000	0.00787	0.00000
167	H8	S	-0.13204	0.00377	0.00000	0.01032	0.00000
168	H8	PX	0.00800	0.00038	0.00000	-0.00005	0.00000
169	H8	PY	0.00219	-0.00235	0.00000	0.00156	0.00000
170	H8	PZ	0.00000	0.00000	0.00307	0.00000	-0.00135
171	C10	S	-0.00731	0.01534	0.00000	0.00810	0.00000
172	C10	S	0.01532	-0.03248	0.00000	-0.01709	0.00000
173	C10	PX	0.07475	0.05110	0.00000	0.21538	0.00000
174	C10	PY	0.13040	-0.22192	0.00000	-0.00968	0.00000
175	C10	PZ	0.00000	0.00000	0.08709	0.00000	-0.06724
176	C10	S	0.01645	-0.04722	0.00000	-0.02362	0.00000
177	C10	PX	0.03884	0.02205	0.00000	0.12001	0.00000
178	C10	PY	0.05516	-0.09712	0.00000	0.01015	0.00000
179	C10	PZ	0.00000	0.00000	0.05071	0.00000	-0.04299
180	C10	DXX	-0.00442	0.01177	0.00000	0.00880	0.00000
181	C10	DYY	0.00208	-0.00808	0.00000	-0.00712	0.00000
182	C10	DZZ	0.00006	-0.00001	0.00000	-0.00014	0.00000
183	C10	DXY	-0.00684	0.00441	0.00000	-0.01439	0.00000
184	C10	DXZ	0.00000	0.00000	-0.00196	0.00000	0.00143

185	C10	DYZ	0.00000	0.00000	0.00938	0.00000	-0.00665
186	H16	S	0.02297	0.06613	0.00000	0.13848	0.00000
187	H16	S	0.01098	0.05923	0.00000	0.11797	0.00000
188	H16	PX	-0.00113	-0.00304	0.00000	-0.00550	0.00000
189	H16	PY	0.00216	-0.00201	0.00000	0.00232	0.00000
190	H16	PZ	0.00000	0.00000	0.00185	0.00000	-0.00143
191	H18	S	-0.08520	0.05870	0.00000	-0.11287	0.00000
192	H18	S	-0.06447	0.05088	0.00000	-0.07810	0.00000
193	H18	PX	-0.00358	0.00333	0.00000	-0.00349	0.00000
194	H18	PY	-0.00177	-0.00084	0.00000	-0.00420	0.00000
195	H18	PZ	0.00000	0.00000	0.00190	0.00000	-0.00146
196	C9	S	-0.00163	-0.00289	0.00000	-0.00125	0.00000
197	C9	S	0.00514	0.00473	0.00000	0.00553	0.00000
198	C9	PX	-0.05583	0.02765	0.00000	-0.12200	0.00000
199	C9	PY	-0.10152	-0.21429	0.00000	0.13169	0.00000
200	C9	PZ	0.00000	0.00000	-0.12387	0.00000	-0.28302
201	C9	S	-0.01335	-0.00125	0.00000	-0.00775	0.00000
202	C9	PX	-0.01244	0.02102	0.00000	-0.04919	0.00000
203	C9	PY	-0.04501	-0.10844	0.00000	0.07342	0.00000
204	C9	PZ	0.00000	0.00000	-0.05825	0.00000	-0.13154
205	C9	DXX	0.00860	0.01085	0.00000	-0.00302	0.00000
206	C9	DYY	-0.00613	-0.01752	0.00000	0.01614	0.00000
207	C9	DZZ	-0.00138	0.00623	0.00000	-0.01088	0.00000
208	C9	DXY	0.00673	0.00480	0.00000	0.00516	0.00000
209	C9	DXZ	0.00000	0.00000	-0.00906	0.00000	-0.03027
210	C9	DYZ	0.00000	0.00000	0.00305	0.00000	0.00408
211	H3	S	-0.05990	-0.14589	0.00000	0.10972	0.00000
212	H3	S	-0.04805	-0.11726	0.00000	0.09249	0.00000
213	H3	PX	-0.00132	-0.00122	0.00000	-0.00016	0.00000
214	H3	PY	0.00236	0.00591	0.00000	-0.00457	0.00000
215	H3	PZ	0.00000	0.00000	-0.00206	0.00000	-0.00492
216	H5	S	-0.00023	0.04886	0.06856	-0.06616	0.17248
217	H5	S	-0.00051	0.04198	0.05712	-0.06193	0.16182
218	H5	PX	-0.00075	-0.00106	-0.00214	0.00016	-0.00480
219	H5	PY	-0.00149	-0.00217	0.00136	0.00078	0.00324
220	H5	PZ	0.00005	0.00290	0.00190	-0.00375	0.00457
221	H7	S	-0.00023	0.04886	-0.06856	-0.06616	-0.17248
222	H7	S	-0.00051	0.04198	-0.05712	-0.06193	-0.16182
223	H7	PX	-0.00075	-0.00106	0.00214	0.00016	0.00480
224	H7	PY	-0.00149	-0.00217	-0.00136	0.00078	-0.00324
225	H7	PZ	-0.00005	-0.00290	0.00190	0.00375	0.00457

MO:	36	37	38	39	40
Eigenvalues:	-0.50639	-0.49379	-0.42839	-0.41333	-0.39930
(ev):	-13.77952	-13.43683	-11.65714	-11.24742	-10.86560

		A	A	A	A	A	
1	H1	S	-0.02589	-0.11153	0.00000	0.06460	0.00000
2	H1	S	-0.03694	-0.09881	0.00000	0.06995	0.00000
3	H1	PX	0.00198	0.00337	0.00000	-0.00208	0.00000
4	H1	PY	-0.00312	0.00209	0.00000	-0.00037	0.00000
5	H1	PZ	0.00000	0.00000	-0.00331	0.00000	-0.00580
6	C1	S	-0.00310	-0.01853	0.00000	0.00878	0.00000
7	C1	S	0.00972	0.03815	0.00000	-0.01944	0.00000

8	C1	PX	0.04148	-0.18460	0.00000	0.07912	0.00000
9	C1	PY	-0.21580	-0.01188	0.00000	0.04487	0.00000
10	C1	PZ	0.00000	0.00000	-0.13795	0.00000	-0.23812
11	C1	S	-0.01783	0.06703	0.00000	-0.05137	0.00000
12	C1	PX	0.02876	-0.11732	0.00000	0.04597	0.00000
13	C1	PY	-0.06753	-0.02635	0.00000	0.05947	0.00000
14	C1	PZ	0.00000	0.00000	-0.10950	0.00000	-0.18530
15	C1	DXX	-0.00763	-0.01040	0.00000	0.00658	0.00000
16	C1	DYY	0.00996	0.00798	0.00000	-0.00712	0.00000
17	C1	DZZ	-0.00059	-0.00034	0.00000	-0.00024	0.00000
18	C1	DXY	0.00549	-0.01021	0.00000	0.00841	0.00000
19	C1	DXZ	0.00000	0.00000	0.00830	0.00000	0.00889
20	C1	DYZ	0.00000	0.00000	-0.00166	0.00000	0.00446
21	C2	S	-0.00056	-0.00202	0.00000	0.01898	0.00000
22	C2	S	0.00414	0.00590	0.00000	-0.03822	0.00000
23	C2	PX	0.04536	0.18199	0.00000	-0.11150	0.00000
24	C2	PY	0.00123	0.00542	0.00000	0.07809	0.00000
25	C2	PZ	0.00000	0.00000	-0.22060	0.00000	0.19298
26	C2	S	-0.00963	0.01018	0.00000	-0.10901	0.00000
27	C2	PX	0.01685	0.12395	0.00000	-0.06783	0.00000
28	C2	PY	-0.00483	0.00585	0.00000	0.02450	0.00000
29	C2	PZ	0.00000	0.00000	-0.16704	0.00000	0.14320
30	C2	DXX	-0.00368	-0.01093	0.00000	0.00546	0.00000
31	C2	DYY	0.00289	0.01039	0.00000	-0.00616	0.00000
32	C2	DZZ	0.00058	0.00001	0.00000	0.00068	0.00000
33	C2	DXY	-0.00124	-0.01475	0.00000	0.00892	0.00000
34	C2	DXZ	0.00000	0.00000	-0.00846	0.00000	0.00697
35	C2	DYZ	0.00000	0.00000	-0.01369	0.00000	0.00447
36	C3	S	-0.00120	-0.00233	0.00000	-0.02013	0.00000
37	C3	S	0.00119	0.00448	0.00000	0.04055	0.00000
38	C3	PX	0.07399	0.14134	0.00000	-0.21264	0.00000
39	C3	PY	0.19322	0.03215	0.00000	-0.05395	0.00000
40	C3	PZ	0.00000	0.00000	-0.05267	0.00000	-0.24781
41	C3	S	0.01587	-0.03082	0.00000	0.11885	0.00000
42	C3	PX	0.05592	0.06233	0.00000	-0.11493	0.00000
43	C3	PY	0.08986	0.02228	0.00000	0.02323	0.00000
44	C3	PZ	0.00000	0.00000	-0.04530	0.00000	-0.18030
45	C3	DXX	-0.01285	-0.01426	0.00000	0.00758	0.00000
46	C3	DYY	0.01406	0.01336	0.00000	-0.00457	0.00000
47	C3	DZZ	-0.00018	0.00046	0.00000	-0.00023	0.00000
48	C3	DXY	0.00571	-0.01227	0.00000	0.00546	0.00000
49	C3	DXZ	0.00000	0.00000	0.00284	0.00000	-0.01220
50	C3	DYZ	0.00000	0.00000	-0.00780	0.00000	0.00127
51	C4	S	-0.00087	0.01738	0.00000	0.00147	0.00000
52	C4	S	0.00270	-0.03919	0.00000	-0.00227	0.00000
53	C4	PX	-0.07401	0.20849	0.00000	-0.06244	0.00000
54	C4	PY	0.15577	-0.03219	0.00000	0.01568	0.00000
55	C4	PZ	0.00000	0.00000	-0.10133	0.00000	-0.09542
56	C4	S	-0.02465	-0.05831	0.00000	-0.02101	0.00000
57	C4	PX	-0.00572	0.07100	0.00000	-0.03715	0.00000
58	C4	PY	0.00113	0.02807	0.00000	-0.00014	0.00000
59	C4	PZ	0.00000	0.00000	-0.06501	0.00000	-0.06861
60	C4	DXX	-0.00849	-0.01052	0.00000	0.00309	0.00000
61	C4	DYY	0.01304	0.00871	0.00000	-0.00317	0.00000

62	C4	DZZ	-0.00307	0.00099	0.00000	-0.00002	0.00000
63	C4	DXY	0.01691	-0.01861	0.00000	0.00470	0.00000
64	C4	DXZ	0.00000	0.00000	0.00196	0.00000	-0.01495
65	C4	DYZ	0.00000	0.00000	0.02356	0.00000	0.01326
66	C5	S	-0.01104	0.00529	0.00000	-0.00507	0.00000
67	C5	S	0.02223	-0.01290	0.00000	0.00676	0.00000
68	C5	PX	0.02062	-0.20312	0.00000	0.04669	0.00000
69	C5	PY	-0.00461	-0.02000	0.00000	-0.02053	0.00000
70	C5	PZ	0.00000	0.00000	-0.23534	0.00000	0.13043
71	C5	S	0.05499	-0.03530	0.00000	0.04164	0.00000
72	C5	PX	-0.00060	-0.10627	0.00000	0.03840	0.00000
73	C5	PY	0.00380	0.00580	0.00000	-0.04131	0.00000
74	C5	PZ	0.00000	0.00000	-0.17241	0.00000	0.10373
75	C5	DXX	-0.00091	-0.00966	0.00000	0.00221	0.00000
76	C5	DYY	0.00210	0.00857	0.00000	-0.00226	0.00000
77	C5	DZZ	-0.00043	-0.00012	0.00000	-0.00109	0.00000
78	C5	DXY	0.00308	-0.01677	0.00000	0.00776	0.00000
79	C5	DXZ	0.00000	0.00000	-0.00291	0.00000	-0.00509
80	C5	DYZ	0.00000	0.00000	0.01519	0.00000	-0.01151
81	C6	S	0.00920	0.01605	0.00000	0.01984	0.00000
82	C6	S	-0.01972	-0.03737	0.00000	-0.05634	0.00000
83	C6	PX	-0.11097	-0.21494	0.00000	0.16778	0.00000
84	C6	PY	-0.05438	0.05338	0.00000	0.09514	0.00000
85	C6	PZ	0.00000	0.00000	-0.04713	0.00000	0.15686
86	C6	S	-0.02215	-0.03596	0.00000	0.03956	0.00000
87	C6	PX	-0.04009	-0.09489	0.00000	0.06261	0.00000
88	C6	PY	-0.01190	-0.01770	0.00000	-0.02026	0.00000
89	C6	PZ	0.00000	0.00000	-0.02859	0.00000	0.11016
90	C6	DXX	-0.00768	-0.00440	0.00000	0.01137	0.00000
91	C6	DYY	0.00690	0.00360	0.00000	-0.01043	0.00000
92	C6	DZZ	-0.00065	0.00084	0.00000	0.00181	0.00000
93	C6	DXY	-0.00172	-0.00280	0.00000	0.03310	0.00000
94	C6	DXZ	0.00000	0.00000	0.00412	0.00000	-0.01541
95	C6	DYZ	0.00000	0.00000	-0.01423	0.00000	-0.01149
96	C7	S	-0.00043	-0.02306	0.00000	-0.01279	0.00000
97	C7	S	0.00540	0.05016	0.00000	0.02577	0.00000
98	C7	PX	-0.09658	-0.18438	0.00000	-0.06143	0.00000
99	C7	PY	-0.15961	-0.02947	0.00000	-0.14457	0.00000
100	C7	PZ	0.00000	0.00000	0.04953	0.00000	-0.21888
101	C7	S	-0.00514	0.09121	0.00000	0.09684	0.00000
102	C7	PX	-0.05858	-0.10228	0.00000	-0.03381	0.00000
103	C7	PY	-0.06707	-0.01611	0.00000	-0.09782	0.00000
104	C7	PZ	0.00000	0.00000	0.03997	0.00000	-0.17271
105	C7	DXX	-0.00628	-0.01194	0.00000	0.00280	0.00000
106	C7	DYY	0.00655	0.01070	0.00000	0.00053	0.00000
107	C7	DZZ	0.00038	-0.00009	0.00000	0.00025	0.00000
108	C7	DXY	0.01496	0.00761	0.00000	0.00143	0.00000
109	C7	DXZ	0.00000	0.00000	-0.00362	0.00000	0.01005
110	C7	DYZ	0.00000	0.00000	-0.00734	0.00000	-0.01124
111	O1	S	0.02868	-0.02215	0.00000	0.00250	0.00000
112	O1	S	-0.07026	0.05219	0.00000	-0.00685	0.00000
113	O1	PX	0.27489	-0.18061	0.00000	0.01936	0.00000
114	O1	PY	-0.22849	0.03889	0.00000	-0.00249	0.00000
115	O1	PZ	0.00000	0.00000	0.29100	0.00000	0.11367

116	O1	S	-0.10269	0.08847	0.00000	-0.00686	0.00000
117	O1	PX	0.21289	-0.13929	0.00000	0.01551	0.00000
118	O1	PY	-0.18687	0.04229	0.00000	-0.00741	0.00000
119	O1	PZ	0.00000	0.00000	0.24980	0.00000	0.10141
120	O1	DXX	0.00581	-0.00785	0.00000	0.00042	0.00000
121	O1	DYY	0.00904	-0.00239	0.00000	0.00057	0.00000
122	O1	DZZ	-0.00909	0.00448	0.00000	-0.00092	0.00000
123	O1	DXY	-0.00832	-0.00194	0.00000	0.00128	0.00000
124	O1	DXZ	0.00000	0.00000	0.00746	0.00000	0.00246
125	O1	DYZ	0.00000	0.00000	-0.00584	0.00000	-0.00052
126	H4	S	-0.00602	0.09612	0.00000	-0.03681	0.00000
127	H4	S	-0.03225	0.09644	0.00000	-0.03133	0.00000
128	H4	PX	-0.00083	0.00188	0.00000	-0.00052	0.00000
129	H4	PY	-0.00069	-0.00343	0.00000	0.00073	0.00000
130	H4	PZ	0.00000	0.00000	-0.00467	0.00000	0.00299
131	N1	S	0.00764	-0.02227	0.00000	-0.06294	0.00000
132	N1	S	-0.01804	0.04936	0.00000	0.13584	0.00000
133	N1	PX	-0.01908	-0.16375	0.00000	-0.40913	0.00000
134	N1	PY	0.08491	-0.05837	0.00000	-0.22161	0.00000
135	N1	PZ	0.00000	0.00000	0.09663	0.00000	0.21210
136	N1	S	-0.01938	0.07957	0.00000	0.24386	0.00000
137	N1	PX	-0.00211	-0.10387	0.00000	-0.32214	0.00000
138	N1	PY	0.04379	-0.05054	0.00000	-0.18013	0.00000
139	N1	PZ	0.00000	0.00000	0.07260	0.00000	0.17022
140	N1	DXX	-0.00060	-0.00620	0.00000	-0.02185	0.00000
141	N1	DYY	0.00160	-0.00242	0.00000	-0.00646	0.00000
142	N1	DZZ	-0.00089	0.00379	0.00000	0.01056	0.00000
143	N1	DXY	0.00234	-0.01035	0.00000	-0.00989	0.00000
144	N1	DXZ	0.00000	0.00000	0.01029	0.00000	0.00820
145	N1	DYZ	0.00000	0.00000	-0.00135	0.00000	0.01531
146	H6	S	-0.03105	-0.12763	0.00000	0.04963	0.00000
147	H6	S	-0.02997	-0.09725	0.00000	0.07588	0.00000
148	H6	PX	-0.00118	-0.00428	0.00000	0.00145	0.00000
149	H6	PY	-0.00073	-0.00252	0.00000	0.00113	0.00000
150	H6	PZ	0.00000	0.00000	-0.00447	0.00000	0.00441
151	C8	S	-0.02017	-0.00814	0.00000	0.02728	0.00000
152	C8	S	0.04202	0.01508	0.00000	-0.06687	0.00000
153	C8	PX	0.10740	0.10309	0.00000	0.18952	0.00000
154	C8	PY	0.14664	0.09950	0.00000	0.00175	0.00000
155	C8	PZ	0.00000	0.00000	0.20478	0.00000	-0.01817
156	C8	S	0.06965	0.04263	0.00000	-0.05179	0.00000
157	C8	PX	0.07069	0.04120	0.00000	0.02986	0.00000
158	C8	PY	0.05245	0.00741	0.00000	-0.02319	0.00000
159	C8	PZ	0.00000	0.00000	0.14212	0.00000	-0.00699
160	C8	DXX	-0.00133	-0.00062	0.00000	0.00252	0.00000
161	C8	DYY	0.00291	-0.00013	0.00000	-0.00712	0.00000
162	C8	DZZ	-0.00032	0.00060	0.00000	0.00183	0.00000
163	C8	DXY	0.01244	0.01602	0.00000	0.02389	0.00000
164	C8	DXZ	0.00000	0.00000	-0.00024	0.00000	-0.01443
165	C8	DYZ	0.00000	0.00000	-0.00719	0.00000	-0.00194
166	H8	S	-0.06280	-0.10831	0.00000	-0.01887	0.00000
167	H8	S	-0.05322	-0.10528	0.00000	-0.02476	0.00000
168	H8	PX	0.00231	0.00400	0.00000	0.00144	0.00000
169	H8	PY	-0.00238	-0.00103	0.00000	-0.00251	0.00000

170	H8	PZ	0.00000	0.00000	0.00101	0.00000	-0.00511
171	C10	S	0.00692	0.00711	0.00000	0.00836	0.00000
172	C10	S	-0.01491	-0.01490	0.00000	-0.01930	0.00000
173	C10	PX	-0.09582	-0.02588	0.00000	-0.01723	0.00000
174	C10	PY	-0.10031	-0.06729	0.00000	-0.02924	0.00000
175	C10	PZ	0.00000	0.00000	0.16060	0.00000	-0.01725
176	C10	S	-0.01748	-0.04217	0.00000	-0.05445	0.00000
177	C10	PX	-0.06122	-0.01516	0.00000	-0.00022	0.00000
178	C10	PY	-0.05487	-0.03967	0.00000	-0.00078	0.00000
179	C10	PZ	0.00000	0.00000	0.12153	0.00000	-0.01554
180	C10	DXX	-0.00052	0.00028	0.00000	-0.00165	0.00000
181	C10	DYY	0.00151	0.00059	0.00000	0.00329	0.00000
182	C10	DZZ	0.00030	0.00018	0.00000	-0.00045	0.00000
183	C10	DXY	0.01215	0.00705	0.00000	0.00837	0.00000
184	C10	DXZ	0.00000	0.00000	-0.00259	0.00000	-0.00119
185	C10	DYZ	0.00000	0.00000	0.01315	0.00000	-0.00168
186	H16	S	-0.05338	-0.01414	0.00000	-0.02113	0.00000
187	H16	S	-0.04549	-0.01374	0.00000	-0.01911	0.00000
188	H16	PX	0.00184	0.00001	0.00000	-0.00002	0.00000
189	H16	PY	-0.00241	-0.00121	0.00000	-0.00032	0.00000
190	H16	PZ	0.00000	0.00000	0.00354	0.00000	-0.00059
191	H18	S	0.09160	0.04198	0.00000	0.02638	0.00000
192	H18	S	0.07419	0.04471	0.00000	0.06381	0.00000
193	H18	PX	0.00330	0.00121	0.00000	-0.00015	0.00000
194	H18	PY	0.00162	0.00068	0.00000	0.00120	0.00000
195	H18	PZ	0.00000	0.00000	0.00347	0.00000	-0.00008
196	C9	S	-0.00985	0.00514	0.00000	0.00052	0.00000
197	C9	S	0.02521	-0.01368	0.00000	-0.00037	0.00000
198	C9	PX	-0.15200	0.12712	0.00000	-0.02082	0.00000
199	C9	PY	0.11852	-0.02805	0.00000	0.00633	0.00000
200	C9	PZ	0.00000	0.00000	-0.08512	0.00000	-0.01142
201	C9	S	0.00800	0.00112	0.00000	-0.00306	0.00000
202	C9	PX	-0.05535	0.04860	0.00000	-0.01054	0.00000
203	C9	PY	0.07529	-0.01766	0.00000	0.00356	0.00000
204	C9	PZ	0.00000	0.00000	-0.02852	0.00000	0.00720
205	C9	DXX	-0.00461	-0.00236	0.00000	0.00036	0.00000
206	C9	DYY	0.02049	-0.00804	0.00000	0.00164	0.00000
207	C9	DZZ	-0.01288	0.00876	0.00000	-0.00145	0.00000
208	C9	DXY	0.01160	-0.00791	0.00000	0.00062	0.00000
209	C9	DXZ	0.00000	0.00000	-0.01782	0.00000	-0.00573
210	C9	DYZ	0.00000	0.00000	-0.00080	0.00000	-0.00043
211	H3	S	0.11986	-0.04371	0.00000	0.00787	0.00000
212	H3	S	0.10113	-0.03898	0.00000	0.00798	0.00000
213	H3	PX	-0.00020	0.00103	0.00000	-0.00024	0.00000
214	H3	PY	-0.00519	0.00206	0.00000	-0.00025	0.00000
215	H3	PZ	0.00000	0.00000	-0.00170	0.00000	-0.00032
216	H5	S	-0.07307	0.04665	0.06815	-0.00830	0.01620
217	H5	S	-0.07698	0.04645	0.08774	-0.00746	0.03569
218	H5	PX	-0.00059	0.00051	-0.00141	0.00004	-0.00044
219	H5	PY	0.00095	0.00052	0.00096	-0.00035	-0.00020
220	H5	PZ	-0.00381	0.00252	0.00165	-0.00046	0.00044
221	H7	S	-0.07307	0.04665	-0.06815	-0.00830	-0.01620
222	H7	S	-0.07698	0.04645	-0.08774	-0.00746	-0.03569
223	H7	PX	-0.00059	0.00051	0.00141	0.00004	0.00044

224	H7	PY	0.00095	0.00052	-0.00096	-0.00035	0.00020
225	H7	PZ	0.00381	-0.00252	0.00165	0.00046	0.00044

MO:		41	42	43	44	45
Eigenvalues:		-0.32668	-0.28259	0.04162	0.17416	0.20872
(ev):		-8.88935	-7.68968	1.13250	4.73911	5.67969

		A	A	A	A	A
1	H1	S	0.00000	0.00000	0.00000	0.00000
2	H1	S	0.00000	0.00000	0.00000	0.00000
3	H1	PX	0.00000	0.00000	0.00000	0.00000
4	H1	PY	0.00000	0.00000	0.00000	0.00000
5	H1	PZ	0.00027	-0.00692	0.00366	0.01010
6	C1	S	0.00000	0.00000	0.00000	0.00000
7	C1	S	0.00000	0.00000	0.00000	0.00000
8	C1	PX	0.00000	0.00000	0.00000	0.00000
9	C1	PY	0.00000	0.00000	0.00000	0.00000
10	C1	PZ	0.00513	-0.26612	0.11129	0.21402
11	C1	S	0.00000	0.00000	0.00000	0.00000
12	C1	PX	0.00000	0.00000	0.00000	0.00000
13	C1	PY	0.00000	0.00000	0.00000	0.00000
14	C1	PZ	-0.00684	-0.25860	0.15890	0.42522
15	C1	DXX	0.00000	0.00000	0.00000	0.00000
16	C1	DYY	0.00000	0.00000	0.00000	0.00000
17	C1	DZZ	0.00000	0.00000	0.00000	0.00000
18	C1	DXY	0.00000	0.00000	0.00000	0.00000
19	C1	DXZ	0.00263	0.01395	0.00334	0.00782
20	C1	DYZ	-0.00741	-0.01552	-0.01204	0.01153
21	C2	S	0.00000	0.00000	0.00000	0.00000
22	C2	S	0.00000	0.00000	0.00000	0.00000
23	C2	PX	0.00000	0.00000	0.00000	0.00000
24	C2	PY	0.00000	0.00000	0.00000	0.00000
25	C2	PZ	-0.11942	0.17099	0.14818	0.29353
26	C2	S	0.00000	0.00000	0.00000	0.00000
27	C2	PX	0.00000	0.00000	0.00000	0.00000
28	C2	PY	0.00000	0.00000	0.00000	0.00000
29	C2	PZ	-0.10910	0.14903	0.22670	0.54919
30	C2	DXX	0.00000	0.00000	0.00000	0.00000
31	C2	DYY	0.00000	0.00000	0.00000	0.00000
32	C2	DZZ	0.00000	0.00000	0.00000	0.00000
33	C2	DXY	0.00000	0.00000	0.00000	0.00000
34	C2	DXZ	0.00070	0.00344	0.00713	-0.00840
35	C2	DYZ	-0.01817	0.00847	-0.01507	-0.00783
36	C3	S	0.00000	0.00000	0.00000	0.00000
37	C3	S	0.00000	0.00000	0.00000	0.00000
38	C3	PX	0.00000	0.00000	0.00000	0.00000
39	C3	PY	0.00000	0.00000	0.00000	0.00000
40	C3	PZ	0.13961	0.16922	0.12553	-0.21038
41	C3	S	0.00000	0.00000	0.00000	0.00000
42	C3	PX	0.00000	0.00000	0.00000	0.00000
43	C3	PY	0.00000	0.00000	0.00000	0.00000
44	C3	PZ	0.11812	0.16547	0.15524	-0.38075
45	C3	DXX	0.00000	0.00000	0.00000	0.00000
46	C3	DYY	0.00000	0.00000	0.00000	0.00000

47	C3	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
48	C3	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
49	C3	DXZ	-0.00581	0.00727	-0.01383	0.01423	-0.01313
50	C3	DYZ	-0.00461	-0.02533	0.01634	0.00929	-0.02113
51	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
52	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
53	C4	PX	0.00000	0.00000	0.00000	0.00000	0.00000
54	C4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
55	C4	PZ	-0.08024	-0.22400	-0.16130	-0.08844	0.34258
56	C4	S	0.00000	0.00000	0.00000	0.00000	0.00000
57	C4	PX	0.00000	0.00000	0.00000	0.00000	0.00000
58	C4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
59	C4	PZ	-0.05219	-0.19200	-0.17043	-0.16732	0.58402
60	C4	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
61	C4	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
62	C4	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
63	C4	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
64	C4	DXZ	0.00756	-0.01753	0.01479	0.02904	0.00401
65	C4	DYZ	0.00778	0.01829	0.00149	-0.00121	0.00332
66	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
67	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
68	C5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
69	C5	PY	0.00000	0.00000	0.00000	0.00000	0.00000
70	C5	PZ	-0.20954	0.09769	-0.18409	-0.19910	-0.20184
71	C5	S	0.00000	0.00000	0.00000	0.00000	0.00000
72	C5	PX	0.00000	0.00000	0.00000	0.00000	0.00000
73	C5	PY	0.00000	0.00000	0.00000	0.00000	0.00000
74	C5	PZ	-0.17959	0.10648	-0.25284	-0.41246	-0.40746
75	C5	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
76	C5	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
77	C5	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
78	C5	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
79	C5	DXZ	-0.00191	-0.01026	-0.00887	-0.01403	0.02083
80	C5	DYZ	0.00848	-0.01222	-0.01149	-0.02125	0.00585
81	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
82	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
83	C6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
84	C6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
85	C6	PZ	0.21093	-0.01530	0.17335	-0.12048	0.25817
86	C6	S	0.00000	0.00000	0.00000	0.00000	0.00000
87	C6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
88	C6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
89	C6	PZ	0.17581	-0.02564	0.17898	-0.18729	0.46859
90	C6	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
91	C6	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
92	C6	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
93	C6	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
94	C6	DXZ	0.00706	0.00432	-0.00204	-0.02435	-0.00940
95	C6	DYZ	-0.01503	0.02087	0.02387	0.00433	0.00987
96	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
97	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
98	C7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
99	C7	PY	0.00000	0.00000	0.00000	0.00000	0.00000
100	C7	PZ	-0.00309	0.27311	-0.21089	0.09618	0.15049

101	C7	S	0.00000	0.00000	0.00000	0.00000	0.00000
102	C7	PX	0.00000	0.00000	0.00000	0.00000	0.00000
103	C7	PY	0.00000	0.00000	0.00000	0.00000	0.00000
104	C7	PZ	-0.00479	0.25381	-0.26918	0.21400	0.31348
105	C7	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
106	C7	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
107	C7	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
108	C7	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
109	C7	DXZ	-0.00125	-0.00977	0.00279	0.00355	0.00334
110	C7	DYZ	0.01474	0.01023	0.00682	-0.01767	-0.01250
111	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
112	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
113	O1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
114	O1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
115	O1	PZ	0.09876	0.16033	0.08997	0.06019	-0.11936
116	O1	S	0.00000	0.00000	0.00000	0.00000	0.00000
117	O1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
118	O1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
119	O1	PZ	0.08931	0.15819	0.09326	0.08020	-0.16892
120	O1	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
121	O1	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
122	O1	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
123	O1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
124	O1	DXZ	0.00345	0.00396	0.00526	0.00748	-0.00390
125	O1	DYZ	-0.00001	0.00293	0.00572	0.00300	-0.01615
126	H4	S	0.00000	0.00000	0.00000	0.00000	0.00000
127	H4	S	0.00000	0.00000	0.00000	0.00000	0.00000
128	H4	PX	0.00000	0.00000	0.00000	0.00000	0.00000
129	H4	PY	0.00000	0.00000	0.00000	0.00000	0.00000
130	H4	PZ	-0.00478	0.00240	-0.00617	-0.00811	-0.00938
131	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
132	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
133	N1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
134	N1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
135	N1	PZ	0.16889	-0.22253	-0.19390	0.00111	-0.18178
136	N1	S	0.00000	0.00000	0.00000	0.00000	0.00000
137	N1	PX	0.00000	0.00000	0.00000	0.00000	0.00000
138	N1	PY	0.00000	0.00000	0.00000	0.00000	0.00000
139	N1	PZ	0.15004	-0.20173	-0.21764	0.01862	-0.30439
140	N1	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
141	N1	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
142	N1	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
143	N1	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
144	N1	DXZ	0.00175	-0.01066	-0.01315	0.00351	-0.01200
145	N1	DYZ	0.02184	-0.00769	0.00163	-0.00817	0.01206
146	H6	S	0.00000	0.00000	0.00000	0.00000	0.00000
147	H6	S	0.00000	0.00000	0.00000	0.00000	0.00000
148	H6	PX	0.00000	0.00000	0.00000	0.00000	0.00000
149	H6	PY	0.00000	0.00000	0.00000	0.00000	0.00000
150	H6	PZ	-0.00259	0.00424	0.00436	0.01246	0.00053
151	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
152	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
153	C8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
154	C8	PY	0.00000	0.00000	0.00000	0.00000	0.00000

155	C8	PZ	-0.24885	-0.03916	-0.08851	0.17224	-0.04798
156	C8	S	0.00000	0.00000	0.00000	0.00000	0.00000
157	C8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
158	C8	PY	0.00000	0.00000	0.00000	0.00000	0.00000
159	C8	PZ	-0.19579	-0.04032	-0.13599	0.23399	-0.07956
160	C8	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
161	C8	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
162	C8	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
163	C8	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
164	C8	DXZ	-0.01301	0.01692	0.00655	0.00418	0.02098
165	C8	DYZ	0.02377	0.00932	-0.02649	0.01025	0.00357
166	H8	S	0.00000	0.00000	0.00000	0.00000	0.00000
167	H8	S	0.00000	0.00000	0.00000	0.00000	0.00000
168	H8	PX	0.00000	0.00000	0.00000	0.00000	0.00000
169	H8	PY	0.00000	0.00000	0.00000	0.00000	0.00000
170	H8	PZ	-0.00036	0.00699	-0.00733	0.00449	0.00718
171	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
172	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
173	C10	PX	0.00000	0.00000	0.00000	0.00000	0.00000
174	C10	PY	0.00000	0.00000	0.00000	0.00000	0.00000
175	C10	PZ	-0.29828	-0.05634	0.26317	-0.16804	0.03159
176	C10	S	0.00000	0.00000	0.00000	0.00000	0.00000
177	C10	PX	0.00000	0.00000	0.00000	0.00000	0.00000
178	C10	PY	0.00000	0.00000	0.00000	0.00000	0.00000
179	C10	PZ	-0.26390	-0.05066	0.37306	-0.30374	0.07443
180	C10	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
181	C10	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
182	C10	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
183	C10	DXY	0.00000	0.00000	0.00000	0.00000	0.00000
184	C10	DXZ	0.00259	0.00281	0.00098	-0.00145	0.00575
185	C10	DYZ	-0.01893	-0.00256	-0.00244	0.01199	-0.00231
186	H16	S	0.00000	0.00000	0.00000	0.00000	0.00000
187	H16	S	0.00000	0.00000	0.00000	0.00000	0.00000
188	H16	PX	0.00000	0.00000	0.00000	0.00000	0.00000
189	H16	PY	0.00000	0.00000	0.00000	0.00000	0.00000
190	H16	PZ	-0.00710	-0.00102	0.00867	-0.00722	0.00243
191	H18	S	0.00000	0.00000	0.00000	0.00000	0.00000
192	H18	S	0.00000	0.00000	0.00000	0.00000	0.00000
193	H18	PX	0.00000	0.00000	0.00000	0.00000	0.00000
194	H18	PY	0.00000	0.00000	0.00000	0.00000	0.00000
195	H18	PZ	-0.00657	-0.00174	0.00831	-0.00738	0.00055
196	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
197	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
198	C9	PX	0.00000	0.00000	0.00000	0.00000	0.00000
199	C9	PY	0.00000	0.00000	0.00000	0.00000	0.00000
200	C9	PZ	-0.01648	0.00190	-0.00200	-0.02571	-0.04464
201	C9	S	0.00000	0.00000	0.00000	0.00000	0.00000
202	C9	PX	0.00000	0.00000	0.00000	0.00000	0.00000
203	C9	PY	0.00000	0.00000	0.00000	0.00000	0.00000
204	C9	PZ	-0.00055	0.03193	0.02738	-0.04912	-0.17572
205	C9	DXX	0.00000	0.00000	0.00000	0.00000	0.00000
206	C9	DYY	0.00000	0.00000	0.00000	0.00000	0.00000
207	C9	DZZ	0.00000	0.00000	0.00000	0.00000	0.00000
208	C9	DXY	0.00000	0.00000	0.00000	0.00000	0.00000

209	C9	DXZ	-0.00576	-0.00774	-0.00645	-0.00633	0.00945
210	C9	DYZ	-0.00071	-0.00067	-0.00116	-0.00186	-0.00122
211	H3	S	0.00000	0.00000	0.00000	0.00000	0.00000
212	H3	S	0.00000	0.00000	0.00000	0.00000	0.00000
213	H3	PX	0.00000	0.00000	0.00000	0.00000	0.00000
214	H3	PY	0.00000	0.00000	0.00000	0.00000	0.00000
215	H3	PZ	-0.00042	-0.00017	-0.00028	-0.00055	-0.00123
216	H5	S	0.01770	0.01653	0.01498	0.01802	-0.02033
217	H5	S	0.02831	0.06204	0.04534	-0.04716	-0.21259
218	H5	PX	-0.00021	-0.00045	0.00015	0.00114	-0.00006
219	H5	PY	0.00030	-0.00061	0.00063	0.00191	0.00027
220	H5	PZ	0.00037	0.00051	0.00015	-0.00062	-0.00042
221	H7	S	-0.01770	-0.01653	-0.01498	-0.01802	0.02033
222	H7	S	-0.02831	-0.06204	-0.04534	0.04716	0.21259
223	H7	PX	0.00021	0.00045	-0.00015	-0.00114	0.00006
224	H7	PY	-0.00030	0.00061	-0.00063	-0.00191	-0.00027
225	H7	PZ	0.00037	0.00051	0.00015	-0.00062	-0.00042

MO:	46	47	48	49	50
Eigenvalues:	0.24034	0.26187	0.27027	0.28712	0.28819
(ev):	6.53990	7.12597	7.35443	7.81290	7.84201

		A	A	A	A	A	
1	H1	S	-0.00619	0.03893	0.02832	0.00000	-0.03004
2	H1	S	1.08684	0.20809	0.66057	0.00000	-0.85845
3	H1	PX	-0.00260	0.00192	-0.00132	0.00000	0.00245
4	H1	PY	0.00254	-0.00148	-0.00673	0.00000	0.00480
5	H1	PZ	0.00000	0.00000	0.00000	0.00401	0.00000
6	C1	S	0.05094	0.01548	0.01412	0.00000	-0.01494
7	C1	S	-0.09647	-0.02132	0.01187	0.00000	-0.01147
8	C1	PX	-0.11575	-0.00380	-0.06031	0.00000	0.09776
9	C1	PY	-0.05439	0.00687	-0.03961	0.00000	0.03417
10	C1	PZ	0.00000	0.00000	0.00000	0.03752	0.00000
11	C1	S	-0.57641	-0.10038	-0.51255	0.00000	0.59910
12	C1	PX	-0.68766	0.03191	-0.27120	0.00000	0.29158
13	C1	PY	-0.20704	-0.17457	-0.28345	0.00000	0.50676
14	C1	PZ	0.00000	0.00000	0.00000	0.20662	0.00000
15	C1	DXX	-0.00170	0.01614	0.01332	0.00000	-0.01069
16	C1	DYY	-0.00101	-0.00600	-0.01096	0.00000	0.00874
17	C1	DZZ	0.00082	-0.00324	0.00234	0.00000	-0.00267
18	C1	DXY	0.00190	0.00092	-0.00032	0.00000	-0.00140
19	C1	DXZ	0.00000	0.00000	0.00000	0.00830	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00573	0.00000
21	C2	S	0.01054	0.04900	0.01417	0.00000	0.01593
22	C2	S	-0.02742	-0.06174	-0.01166	0.00000	-0.01555
23	C2	PX	0.01756	0.13624	0.04484	0.00000	0.09234
24	C2	PY	-0.00273	0.03270	-0.00946	0.00000	0.03848
25	C2	PZ	0.00000	0.00000	0.00000	0.04340	0.00000
26	C2	S	-0.19832	-0.90900	-0.36237	0.00000	-0.32974
27	C2	PX	0.12896	0.53309	0.05994	0.00000	0.40415
28	C2	PY	-0.01499	0.41024	-0.06562	0.00000	0.29295
29	C2	PZ	0.00000	0.00000	0.00000	0.14642	0.00000
30	C2	DXX	0.00150	0.01467	-0.00216	0.00000	0.00623
31	C2	DYY	-0.00118	-0.01093	0.00084	0.00000	-0.00457

32	C2	DZZ	-0.00258	-0.00003	0.00021	0.00000	0.00090
33	C2	DXY	0.00127	0.01071	0.00380	0.00000	0.00547
34	C2	DXZ	0.00000	0.00000	0.00000	-0.00932	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00260	0.00000
36	C3	S	-0.00308	0.02750	0.00517	0.00000	-0.01280
37	C3	S	0.01417	-0.06468	0.00531	0.00000	-0.00644
38	C3	PX	-0.00424	0.02618	-0.01320	0.00000	0.09111
39	C3	PY	0.03231	0.00581	-0.07439	0.00000	0.02315
40	C3	PZ	0.00000	0.00000	0.00000	-0.08611	0.00000
41	C3	S	-0.28257	-0.11029	-0.55799	0.00000	0.79586
42	C3	PX	0.05252	-0.28012	0.17599	0.00000	0.21015
43	C3	PY	0.10233	-0.10052	0.14321	0.00000	-0.02272
44	C3	PZ	0.00000	0.00000	0.00000	-0.30890	0.00000
45	C3	DXX	-0.00139	0.01128	-0.01130	0.00000	0.00919
46	C3	DYY	-0.00402	-0.00749	0.00683	0.00000	-0.00404
47	C3	DZZ	0.00119	-0.00352	-0.00166	0.00000	-0.00170
48	C3	DXY	-0.00875	-0.00978	-0.00137	0.00000	-0.00064
49	C3	DXZ	0.00000	0.00000	0.00000	0.02664	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.00417	0.00000
51	C4	S	-0.00321	0.01247	0.00197	0.00000	0.00625
52	C4	S	-0.02486	-0.01750	0.00909	0.00000	-0.03073
53	C4	PX	-0.00618	0.01113	-0.00306	0.00000	0.02019
54	C4	PY	-0.03216	-0.08070	-0.09100	0.00000	0.06727
55	C4	PZ	0.00000	0.00000	0.00000	-0.01878	0.00000
56	C4	S	0.01515	0.06311	0.04453	0.00000	-0.11309
57	C4	PX	-0.02026	-0.04517	0.07317	0.00000	-0.28361
58	C4	PY	0.30425	-0.08013	-0.10468	0.00000	0.19724
59	C4	PZ	0.00000	0.00000	0.00000	-0.11812	0.00000
60	C4	DXX	-0.01474	-0.00938	-0.01108	0.00000	0.00934
61	C4	DYY	0.01511	0.02505	0.02022	0.00000	-0.00988
62	C4	DZZ	-0.00253	-0.00586	-0.00427	0.00000	0.00139
63	C4	DXY	0.00924	0.01180	0.00252	0.00000	0.00850
64	C4	DXZ	0.00000	0.00000	0.00000	0.00409	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00287	0.00000
66	C5	S	0.01515	0.04388	0.01875	0.00000	0.01638
67	C5	S	-0.02142	-0.04567	-0.02363	0.00000	0.00073
68	C5	PX	0.00917	0.11400	0.02734	0.00000	0.09577
69	C5	PY	-0.02867	-0.09987	-0.06392	0.00000	-0.04198
70	C5	PZ	0.00000	0.00000	0.00000	0.01654	0.00000
71	C5	S	-0.17293	-1.00320	-0.20067	0.00000	-0.69296
72	C5	PX	0.04067	0.30822	0.09382	0.00000	0.20899
73	C5	PY	-0.24188	-0.44948	-0.29734	0.00000	-0.20524
74	C5	PZ	0.00000	0.00000	0.00000	-0.02684	0.00000
75	C5	DXX	0.00621	0.00432	0.00769	0.00000	-0.01111
76	C5	DYY	-0.00471	-0.00177	-0.00140	0.00000	0.00290
77	C5	DZZ	0.00111	0.00031	-0.00084	0.00000	0.00392
78	C5	DXY	-0.00911	-0.01916	-0.00988	0.00000	-0.00115
79	C5	DXZ	0.00000	0.00000	0.00000	-0.00585	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.00170	0.00000
81	C6	S	0.00971	0.00361	0.00870	0.00000	-0.00991
82	C6	S	-0.02500	-0.00510	-0.03215	0.00000	0.03227
83	C6	PX	-0.03025	0.03576	-0.03611	0.00000	0.03921
84	C6	PY	-0.00328	0.03687	-0.03602	0.00000	-0.00720
85	C6	PZ	0.00000	0.00000	0.00000	-0.09263	0.00000

86	C6	S	0.02000	-0.03886	0.15318	0.00000	0.10525
87	C6	PX	0.04187	-0.25476	0.03621	0.00000	-0.03187
88	C6	PY	-0.09139	-0.11285	-0.00845	0.00000	-0.14376
89	C6	PZ	0.00000	0.00000	0.00000	-0.26219	0.00000
90	C6	DXX	-0.00279	-0.01897	0.00864	0.00000	-0.01259
91	C6	DYY	0.00744	0.02347	-0.00077	0.00000	0.01290
92	C6	DZZ	-0.00213	-0.00172	-0.00414	0.00000	0.00200
93	C6	DXY	0.00555	-0.00015	-0.00057	0.00000	-0.00521
94	C6	DXZ	0.00000	0.00000	0.00000	-0.01943	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.02113	0.00000
96	C7	S	-0.00025	-0.02390	0.04688	0.00000	-0.00671
97	C7	S	-0.00581	0.04419	-0.06732	0.00000	0.00865
98	C7	PX	-0.01761	0.05800	-0.18041	0.00000	0.07349
99	C7	PY	0.01734	0.02943	0.02840	0.00000	0.01052
100	C7	PZ	0.00000	0.00000	0.00000	0.21306	0.00000
101	C7	S	0.05476	0.26039	-0.70134	0.00000	0.07176
102	C7	PX	-0.15135	0.49960	-1.07502	0.00000	0.42282
103	C7	PY	0.15457	0.31217	0.12646	0.00000	-0.43524
104	C7	PZ	0.00000	0.00000	0.00000	0.62851	0.00000
105	C7	DXX	-0.00207	-0.00375	0.00321	0.00000	-0.01455
106	C7	DYY	0.00087	0.00053	-0.00004	0.00000	0.00978
107	C7	DZZ	-0.00044	0.00051	-0.00032	0.00000	0.00062
108	C7	DXY	0.00186	0.00469	-0.00258	0.00000	-0.00187
109	C7	DXZ	0.00000	0.00000	0.00000	0.02366	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.01682	0.00000
111	O1	S	-0.00429	-0.02637	-0.03259	0.00000	0.03394
112	O1	S	0.00399	0.04905	0.05186	0.00000	-0.04810
113	O1	PX	0.04676	0.03350	0.05065	0.00000	-0.06171
114	O1	PY	-0.02972	-0.06217	-0.04713	0.00000	0.01427
115	O1	PZ	0.00000	0.00000	0.00000	0.01926	0.00000
116	O1	S	-0.00273	0.27781	0.39420	0.00000	-0.47112
117	O1	PX	0.15852	0.07491	0.12333	0.00000	-0.15826
118	O1	PY	0.09908	-0.03163	-0.03626	0.00000	0.04233
119	O1	PZ	0.00000	0.00000	0.00000	0.06273	0.00000
120	O1	DXX	-0.00217	0.00333	-0.00079	0.00000	0.00550
121	O1	DYY	-0.01146	-0.01183	-0.01108	0.00000	0.00523
122	O1	DZZ	0.00134	-0.00646	-0.00975	0.00000	0.01049
123	O1	DXY	-0.00596	-0.00477	0.00132	0.00000	-0.01016
124	O1	DXZ	0.00000	0.00000	0.00000	0.00178	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.00172	0.00000
126	H4	S	0.02096	0.04489	0.02851	0.00000	-0.00783
127	H4	S	0.33185	1.18998	0.52532	0.00000	0.60583
128	H4	PX	-0.00087	0.00049	-0.00219	0.00000	0.00585
129	H4	PY	-0.00111	-0.00283	-0.00144	0.00000	0.00047
130	H4	PZ	0.00000	0.00000	0.00000	0.00116	0.00000
131	N1	S	-0.00046	-0.01114	0.01356	0.00000	-0.00210
132	N1	S	0.01018	0.04777	-0.05357	0.00000	0.02579
133	N1	PX	-0.00043	0.01307	-0.03989	0.00000	0.07087
134	N1	PY	0.02334	0.02993	0.03395	0.00000	0.02181
135	N1	PZ	0.00000	0.00000	0.00000	0.24798	0.00000
136	N1	S	-0.04520	-0.10487	0.08509	0.00000	-0.17155
137	N1	PX	-0.00809	0.00664	0.01086	0.00000	0.04287
138	N1	PY	0.00191	-0.04749	-0.01644	0.00000	-0.05721
139	N1	PZ	0.00000	0.00000	0.00000	0.50593	0.00000

140	N1	DXX	0.00441	0.00517	0.00071	0.00000	-0.00356
141	N1	DYY	-0.00218	-0.00750	-0.00241	0.00000	0.00386
142	N1	DZZ	0.00215	0.00661	-0.00728	0.00000	0.00439
143	N1	DXY	-0.00225	0.00508	-0.00421	0.00000	0.00798
144	N1	DXZ	0.00000	0.00000	0.00000	-0.01260	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.01121	0.00000
146	H6	S	0.00610	0.04324	-0.00559	0.00000	0.02550
147	H6	S	0.22392	1.22351	0.24505	0.00000	0.74365
148	H6	PX	0.00081	0.00260	0.00089	0.00000	0.00162
149	H6	PY	0.00096	0.00003	-0.00013	0.00000	0.00066
150	H6	PZ	0.00000	0.00000	0.00000	0.00306	0.00000
151	C8	S	-0.00745	-0.00367	-0.01191	0.00000	0.01143
152	C8	S	0.01386	-0.01272	0.03365	0.00000	-0.01122
153	C8	PX	-0.00159	0.02899	-0.02810	0.00000	0.03565
154	C8	PY	0.01770	0.01968	0.00538	0.00000	-0.05602
155	C8	PZ	0.00000	0.00000	0.00000	-0.39579	0.00000
156	C8	S	0.13811	0.39890	-0.28415	0.00000	-0.34031
157	C8	PX	0.06333	0.08820	0.21986	0.00000	-0.17930
158	C8	PY	-0.08972	0.24413	-0.21555	0.00000	0.07315
159	C8	PZ	0.00000	0.00000	0.00000	-0.87698	0.00000
160	C8	DXX	-0.00168	0.00249	-0.01443	0.00000	0.01473
161	C8	DYY	0.00157	0.00330	0.00655	0.00000	-0.01119
162	C8	DZZ	0.00061	-0.00142	0.00087	0.00000	-0.00134
163	C8	DXY	-0.00082	-0.00445	0.00515	0.00000	-0.00779
164	C8	DXZ	0.00000	0.00000	0.00000	-0.00292	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	-0.00217	0.00000
166	H8	S	-0.00913	-0.00938	-0.00870	0.00000	-0.03141
167	H8	S	0.13767	-0.63734	1.55074	0.00000	-0.59359
168	H8	PX	-0.00115	0.00224	-0.00654	0.00000	-0.00023
169	H8	PY	0.00156	0.00261	-0.00141	0.00000	-0.00311
170	H8	PZ	0.00000	0.00000	0.00000	0.01426	0.00000
171	C10	S	-0.00350	-0.04121	0.05811	0.00000	0.07719
172	C10	S	0.00971	0.04891	-0.05729	0.00000	-0.09223
173	C10	PX	0.00321	0.06129	-0.10503	0.00000	0.00463
174	C10	PY	-0.00804	-0.05219	0.09314	0.00000	0.12911
175	C10	PZ	0.00000	0.00000	0.00000	0.15426	0.00000
176	C10	S	-0.04562	0.74536	-1.14521	0.00000	-1.11468
177	C10	PX	0.01985	0.20569	-0.47057	0.00000	0.14040
178	C10	PY	-0.09823	-0.25327	0.33936	0.00000	0.63849
179	C10	PZ	0.00000	0.00000	0.00000	0.60369	0.00000
180	C10	DXX	-0.00082	-0.00229	0.00197	0.00000	0.00447
181	C10	DYY	-0.00113	-0.00063	-0.00107	0.00000	0.00536
182	C10	DZZ	0.00077	-0.00217	0.00519	0.00000	0.00297
183	C10	DXY	-0.00045	0.00030	-0.00226	0.00000	0.00714
184	C10	DXZ	0.00000	0.00000	0.00000	0.00697	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	-0.02995	0.00000
186	H16	S	-0.00050	-0.00733	0.00825	0.00000	0.00102
187	H16	S	-0.06089	-0.71531	1.19181	0.00000	0.69927
188	H16	PX	-0.00011	0.00091	-0.00209	0.00000	0.00197
189	H16	PY	-0.00020	-0.00296	0.00482	0.00000	0.00340
190	H16	PZ	0.00000	0.00000	0.00000	0.01044	0.00000
191	H18	S	-0.00066	-0.01014	0.01453	0.00000	0.03636
192	H18	S	-0.05236	-0.31846	0.38882	0.00000	1.20170
193	H18	PX	0.00021	0.00054	-0.00034	0.00000	-0.00039

194	H18	PY	0.00017	-0.00159	0.00213	0.00000	0.00234
195	H18	PZ	0.00000	0.00000	0.00000	0.00941	0.00000
196	C9	S	0.12324	-0.02388	-0.01554	0.00000	0.00859
197	C9	S	-0.08691	0.01342	0.01833	0.00000	-0.01893
198	C9	PX	-0.11757	0.08721	0.07042	0.00000	-0.03007
199	C9	PY	-0.03064	0.01990	0.05310	0.00000	-0.11934
200	C9	PZ	0.00000	0.00000	0.00000	-0.04506	0.00000
201	C9	S	-2.21528	0.50303	0.37139	0.00000	-0.25642
202	C9	PX	-0.36198	0.39307	0.38058	0.00000	-0.28991
203	C9	PY	-0.06116	0.00045	0.22787	0.00000	-0.51874
204	C9	PZ	0.00000	0.00000	0.00000	-0.18214	0.00000
205	C9	DXX	0.00477	-0.00394	-0.00013	0.00000	-0.00374
206	C9	DYY	0.01537	0.00003	-0.00028	0.00000	0.00391
207	C9	DZZ	0.00676	-0.00654	-0.00563	0.00000	0.00495
208	C9	DXY	-0.00217	0.00457	0.00352	0.00000	-0.00256
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00129	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.00103	0.00000
211	H3	S	0.01559	0.01435	0.00409	0.00000	0.00932
212	H3	S	0.89048	-0.08429	-0.30514	0.00000	0.67073
213	H3	PX	-0.00236	0.00264	0.00213	0.00000	-0.00169
214	H3	PY	-0.00060	-0.00059	0.00112	0.00000	-0.00195
215	H3	PZ	0.00000	0.00000	0.00000	-0.00083	0.00000
216	H5	S	-0.00331	-0.01623	-0.01326	0.00154	0.01194
217	H5	S	1.05077	-0.42321	-0.29044	-0.19845	0.06697
218	H5	PX	-0.00182	0.00260	0.00292	0.00081	-0.00272
219	H5	PY	-0.00368	0.00107	0.00039	0.00103	-0.00101
220	H5	PZ	0.00269	-0.00005	0.00072	-0.00102	-0.00105
221	H7	S	-0.00331	-0.01623	-0.01326	-0.00154	0.01194
222	H7	S	1.05077	-0.42321	-0.29044	0.19845	0.06697
223	H7	PX	-0.00182	0.00260	0.00292	-0.00081	-0.00272
224	H7	PY	-0.00368	0.00107	0.00039	-0.00103	-0.00101
225	H7	PZ	-0.00269	0.00005	-0.00072	-0.00102	0.00105

MO:	51	52	53	54	55
Eigenvalues:	0.30343	0.31075	0.31495	0.32001	0.32750
(ev):	8.25679	8.45594	8.57019	8.70780	8.91174

		A	A	A	A	A	
1	H1	S	-0.00467	-0.02783	-0.03848	0.00000	-0.04848
2	H1	S	0.26537	-0.75614	0.07471	0.00000	-0.88657
3	H1	PX	-0.00169	0.00070	-0.00318	0.00000	-0.00135
4	H1	PY	-0.00693	-0.00008	0.00147	0.00000	-0.00127
5	H1	PZ	0.00000	0.00000	0.00000	-0.00586	0.00000
6	C1	S	0.00934	-0.02912	0.01226	0.00000	-0.03780
7	C1	S	-0.02252	0.01516	-0.02113	0.00000	0.03436
8	C1	PX	0.00409	0.08723	-0.00936	0.00000	0.08843
9	C1	PY	0.00966	-0.01104	-0.00592	0.00000	0.04089
10	C1	PZ	0.00000	0.00000	0.00000	0.07258	0.00000
11	C1	S	-0.23505	0.59110	-0.22465	0.00000	0.48640
12	C1	PX	-0.03381	0.40995	-0.04719	0.00000	0.45332
13	C1	PY	-0.32498	0.15931	-0.13183	0.00000	0.16536
14	C1	PZ	0.00000	0.00000	0.00000	-0.05990	0.00000
15	C1	DXX	0.00057	-0.00918	-0.01193	0.00000	-0.01437
16	C1	DYY	-0.00766	-0.00295	0.00292	0.00000	0.00662

17	C1	DZZ	0.00062	0.00178	0.00326	0.00000	-0.00262
18	C1	DXY	-0.01070	-0.00156	-0.00209	0.00000	-0.00717
19	C1	DXZ	0.00000	0.00000	0.00000	-0.01150	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00257	0.00000
21	C2	S	-0.00026	0.02448	-0.03172	0.00000	0.04951
22	C2	S	0.00736	-0.02237	0.06933	0.00000	-0.06261
23	C2	PX	-0.00153	0.08678	0.01159	0.00000	0.13473
24	C2	PY	-0.00393	0.05952	0.01382	0.00000	0.00780
25	C2	PZ	0.00000	0.00000	0.00000	0.01158	0.00000
26	C2	S	-0.05539	-0.53634	0.32967	0.00000	-0.71272
27	C2	PX	-0.09959	0.46174	-0.36177	0.00000	0.98315
28	C2	PY	0.08800	0.24381	0.01640	0.00000	-0.05734
29	C2	PZ	0.00000	0.00000	0.00000	0.06748	0.00000
30	C2	DXX	0.00340	-0.00090	0.00220	0.00000	-0.00244
31	C2	DYY	-0.00464	0.00163	-0.00515	0.00000	0.00528
32	C2	DZZ	0.00116	0.00095	0.00270	0.00000	0.00253
33	C2	DXY	-0.00362	-0.00032	0.00236	0.00000	0.00130
34	C2	DXZ	0.00000	0.00000	0.00000	0.00015	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	-0.00388	0.00000
36	C3	S	0.01435	-0.00064	-0.00750	0.00000	-0.00037
37	C3	S	-0.01617	-0.02716	0.05087	0.00000	0.00202
38	C3	PX	0.04178	-0.00554	0.01624	0.00000	0.04334
39	C3	PY	-0.01582	0.00047	-0.00541	0.00000	-0.02191
40	C3	PZ	0.00000	0.00000	0.00000	-0.05935	0.00000
41	C3	S	-0.30941	0.34857	-0.67024	0.00000	-0.02177
42	C3	PX	0.18064	-0.30051	0.14735	0.00000	0.08548
43	C3	PY	-0.17161	-0.01655	0.38559	0.00000	0.08671
44	C3	PZ	0.00000	0.00000	0.00000	-0.06076	0.00000
45	C3	DXX	0.00901	-0.00131	-0.00413	0.00000	0.00297
46	C3	DYY	-0.01219	0.00758	-0.00455	0.00000	-0.00208
47	C3	DZZ	0.00061	-0.00256	0.00288	0.00000	-0.00122
48	C3	DXY	0.00112	0.00646	0.00936	0.00000	0.00985
49	C3	DXZ	0.00000	0.00000	0.00000	0.00318	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00303	0.00000
51	C4	S	-0.03384	-0.01300	-0.02054	0.00000	0.02250
52	C4	S	0.03910	-0.02604	0.02652	0.00000	-0.05333
53	C4	PX	0.00642	-0.00674	-0.00297	0.00000	0.08417
54	C4	PY	0.00218	0.09694	0.06546	0.00000	0.02855
55	C4	PZ	0.00000	0.00000	0.00000	0.10029	0.00000
56	C4	S	0.43241	0.32887	0.12399	0.00000	0.07629
57	C4	PX	0.22837	-0.13579	0.21081	0.00000	0.04347
58	C4	PY	0.01798	0.20112	0.37996	0.00000	-0.12481
59	C4	PZ	0.00000	0.00000	0.00000	0.15399	0.00000
60	C4	DXX	-0.00989	-0.00237	-0.00138	0.00000	0.01684
61	C4	DYY	-0.00533	-0.01013	-0.00452	0.00000	-0.01172
62	C4	DZZ	0.00110	0.00153	0.00513	0.00000	-0.00217
63	C4	DXY	-0.00582	-0.00147	-0.00844	0.00000	0.00681
64	C4	DXZ	0.00000	0.00000	0.00000	0.00505	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.01407	0.00000
66	C5	S	0.01232	0.01145	0.04184	0.00000	-0.06736
67	C5	S	-0.03371	-0.00149	-0.06707	0.00000	0.09619
68	C5	PX	-0.03056	0.02801	0.03270	0.00000	-0.00781
69	C5	PY	0.01192	-0.05532	-0.06175	0.00000	0.07594
70	C5	PZ	0.00000	0.00000	0.00000	-0.03169	0.00000

71	C5	S	-0.03587	-0.45718	-0.42662	0.00000	0.88318
72	C5	PX	-0.00667	-0.01465	0.52124	0.00000	-0.58837
73	C5	PY	0.00485	-0.19843	-0.25667	0.00000	0.41663
74	C5	PZ	0.00000	0.00000	0.00000	-0.10713	0.00000
75	C5	DXX	0.00533	-0.00771	-0.00614	0.00000	-0.00815
76	C5	DYY	-0.00258	0.00277	0.00767	0.00000	0.00146
77	C5	DZZ	-0.00193	0.00227	0.00029	0.00000	0.00060
78	C5	DXY	0.00180	0.00445	0.00963	0.00000	-0.01144
79	C5	DXZ	0.00000	0.00000	0.00000	0.00580	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	-0.00133	0.00000
81	C6	S	-0.01848	-0.00044	0.01543	0.00000	-0.00319
82	C6	S	0.02313	0.01973	-0.04779	0.00000	0.00813
83	C6	PX	0.04501	-0.01932	0.02959	0.00000	0.02071
84	C6	PY	0.03354	0.00360	0.01761	0.00000	0.05130
85	C6	PZ	0.00000	0.00000	0.00000	0.00305	0.00000
86	C6	S	0.38781	-0.19904	0.24991	0.00000	-0.23927
87	C6	PX	0.12346	-0.33843	0.17007	0.00000	0.10678
88	C6	PY	0.14168	-0.26389	0.08529	0.00000	-0.17563
89	C6	PZ	0.00000	0.00000	0.00000	-0.01107	0.00000
90	C6	DXX	-0.00408	-0.00355	0.00759	0.00000	-0.00101
91	C6	DYY	0.00699	0.00122	0.00640	0.00000	-0.00325
92	C6	DZZ	0.00086	0.00197	-0.00363	0.00000	0.00083
93	C6	DXY	-0.00596	0.00307	-0.00793	0.00000	-0.00394
94	C6	DXZ	0.00000	0.00000	0.00000	-0.00661	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.00243	0.00000
96	C7	S	0.00235	-0.00525	0.06047	0.00000	0.05456
97	C7	S	-0.02271	0.03303	-0.11854	0.00000	-0.07202
98	C7	PX	0.06397	-0.05109	-0.10726	0.00000	-0.08038
99	C7	PY	0.02991	-0.05293	0.03927	0.00000	0.03554
100	C7	PZ	0.00000	0.00000	0.00000	0.05195	0.00000
101	C7	S	0.08644	-0.18843	-0.48964	0.00000	-0.75765
102	C7	PX	0.30663	-0.09239	-0.99134	0.00000	-0.50232
103	C7	PY	-0.00570	0.02841	0.30980	0.00000	0.09398
104	C7	PZ	0.00000	0.00000	0.00000	0.10915	0.00000
105	C7	DXX	-0.01107	0.00750	0.00345	0.00000	0.00290
106	C7	DYY	0.01232	-0.01089	0.01158	0.00000	0.00665
107	C7	DZZ	-0.00315	0.00386	-0.00745	0.00000	-0.00216
108	C7	DXY	0.00211	-0.00134	0.00264	0.00000	0.00365
109	C7	DXZ	0.00000	0.00000	0.00000	0.00513	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.00230	0.00000
111	O1	S	-0.00086	0.04323	0.07180	0.00000	-0.03196
112	O1	S	0.00775	-0.03756	-0.06026	0.00000	0.02165
113	O1	PX	0.05660	-0.04120	-0.11936	0.00000	0.05243
114	O1	PY	0.01156	-0.00684	-0.01998	0.00000	0.06383
115	O1	PZ	0.00000	0.00000	0.00000	-0.11176	0.00000
116	O1	S	0.00016	-0.67365	-1.13329	0.00000	0.51144
117	O1	PX	0.13016	-0.14289	-0.43076	0.00000	0.21801
118	O1	PY	-0.03764	-0.06522	-0.02882	0.00000	0.10914
119	O1	PZ	0.00000	0.00000	0.00000	-0.29008	0.00000
120	O1	DXX	-0.00375	0.00701	0.02176	0.00000	-0.01341
121	O1	DYY	0.00915	0.02135	0.02772	0.00000	-0.01441
122	O1	DZZ	0.00600	0.02537	0.03568	0.00000	-0.01585
123	O1	DXY	0.00877	-0.00069	-0.00028	0.00000	-0.00535
124	O1	DXZ	0.00000	0.00000	0.00000	0.00169	0.00000

125	O1	DYZ	0.00000	0.00000	0.00000	0.01031	0.00000
126	H4	S	0.00808	-0.01497	-0.01429	0.00000	0.00047
127	H4	S	0.01583	0.33830	0.79367	0.00000	-1.12102
128	H4	PX	-0.00275	0.00349	0.00436	0.00000	-0.00059
129	H4	PY	-0.00229	-0.00017	0.00017	0.00000	0.00449
130	H4	PZ	0.00000	0.00000	0.00000	-0.00253	0.00000
131	N1	S	-0.00973	0.01555	-0.01570	0.00000	0.00294
132	N1	S	0.03566	-0.04092	0.02702	0.00000	-0.01034
133	N1	PX	0.05896	-0.06785	-0.01109	0.00000	0.00871
134	N1	PY	-0.02658	0.03072	-0.02390	0.00000	-0.02068
135	N1	PZ	0.00000	0.00000	0.00000	0.01752	0.00000
136	N1	S	-0.01286	-0.12631	0.19796	0.00000	-0.10162
137	N1	PX	0.00915	0.01884	0.01370	0.00000	-0.09563
138	N1	PY	-0.05007	-0.06565	-0.02393	0.00000	-0.01046
139	N1	PZ	0.00000	0.00000	0.00000	0.04109	0.00000
140	N1	DXX	-0.00286	0.00406	0.00561	0.00000	0.00276
141	N1	DYY	-0.00239	0.00007	-0.01382	0.00000	-0.01037
142	N1	DZZ	0.00557	-0.00271	0.00028	0.00000	-0.00055
143	N1	DXY	0.00880	-0.00788	0.00708	0.00000	0.00425
144	N1	DXZ	0.00000	0.00000	0.00000	-0.00284	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00254	0.00000
146	H6	S	0.00340	-0.00459	-0.00915	0.00000	0.01186
147	H6	S	-0.03265	0.79117	-0.43356	0.00000	1.36405
148	H6	PX	-0.00064	0.00277	-0.00202	0.00000	0.00460
149	H6	PY	0.00165	0.00091	-0.00055	0.00000	0.00001
150	H6	PZ	0.00000	0.00000	0.00000	0.00067	0.00000
151	C8	S	0.00182	-0.00246	-0.00834	0.00000	-0.01252
152	C8	S	-0.01423	0.01081	0.01809	0.00000	0.02019
153	C8	PX	0.08544	-0.08901	0.08547	0.00000	0.03502
154	C8	PY	-0.00543	-0.00168	0.07590	0.00000	0.06448
155	C8	PZ	0.00000	0.00000	0.00000	-0.04664	0.00000
156	C8	S	0.07929	-0.03710	-0.04664	0.00000	0.10893
157	C8	PX	-0.10378	0.23776	0.09784	0.00000	-0.04646
158	C8	PY	0.01019	0.12725	-0.22820	0.00000	0.02148
159	C8	PZ	0.00000	0.00000	0.00000	-0.10522	0.00000
160	C8	DXX	0.01542	-0.01720	-0.00304	0.00000	-0.00032
161	C8	DYY	-0.01049	0.01164	-0.00110	0.00000	-0.00004
162	C8	DZZ	-0.00277	0.00280	0.00085	0.00000	0.00091
163	C8	DXY	-0.01520	0.02117	-0.01865	0.00000	-0.01425
164	C8	DXZ	0.00000	0.00000	0.00000	0.00245	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00115	0.00000
166	H8	S	-0.03123	0.02199	0.01337	0.00000	0.02118
167	H8	S	-0.41093	0.22138	1.41897	0.00000	1.01991
168	H8	PX	0.00016	-0.00039	-0.00199	0.00000	-0.00045
169	H8	PY	0.00249	-0.00429	0.00359	0.00000	0.00224
170	H8	PZ	0.00000	0.00000	0.00000	0.00371	0.00000
171	C10	S	0.03012	-0.02285	-0.03237	0.00000	-0.02018
172	C10	S	-0.03611	0.02612	0.03770	0.00000	0.01914
173	C10	PX	0.13513	-0.18803	0.13826	0.00000	0.09905
174	C10	PY	0.07012	-0.07205	-0.02233	0.00000	-0.01424
175	C10	PZ	0.00000	0.00000	0.00000	0.01260	0.00000
176	C10	S	-0.47744	0.43288	0.34659	0.00000	0.31635
177	C10	PX	0.69617	-1.00561	0.69341	0.00000	0.50356
178	C10	PY	0.31519	-0.30749	-0.08371	0.00000	0.01305

179	C10	PZ	0.00000	0.00000	0.00000	0.06870	0.00000
180	C10	DXX	-0.00074	0.00219	-0.00757	0.00000	-0.00538
181	C10	DYY	0.00344	-0.00337	0.00022	0.00000	-0.00017
182	C10	DZZ	0.00084	-0.00066	-0.00067	0.00000	-0.00011
183	C10	DXY	0.00920	-0.01107	0.00919	0.00000	0.00604
184	C10	DXZ	0.00000	0.00000	0.00000	0.00146	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	-0.00368	0.00000
186	H16	S	-0.01216	0.01750	-0.03625	0.00000	-0.02501
187	H16	S	-0.44276	0.81765	-1.08089	0.00000	-0.74860
188	H16	PX	0.00277	-0.00346	0.00088	0.00000	0.00063
189	H16	PY	0.00122	-0.00128	0.00142	0.00000	0.00125
190	H16	PZ	0.00000	0.00000	0.00000	0.00119	0.00000
191	H18	S	0.02726	-0.02938	0.01932	0.00000	0.01237
192	H18	S	1.14026	-1.35200	0.36500	0.00000	0.30606
193	H18	PX	0.00183	-0.00289	0.00387	0.00000	0.00293
194	H18	PY	0.00172	-0.00196	0.00012	0.00000	-0.00029
195	H18	PZ	0.00000	0.00000	0.00000	0.00088	0.00000
196	C9	S	-0.00252	-0.01053	-0.04933	0.00000	0.05010
197	C9	S	0.01139	0.00573	0.04870	0.00000	-0.05856
198	C9	PX	-0.09592	-0.13991	-0.10398	0.00000	0.07226
199	C9	PY	0.25929	0.10619	-0.08105	0.00000	0.00093
200	C9	PZ	0.00000	0.00000	0.00000	0.35397	0.00000
201	C9	S	0.10505	0.11501	0.78685	0.00000	-0.85523
202	C9	PX	-0.37029	-0.81416	-0.69389	0.00000	0.30449
203	C9	PY	1.17120	0.49082	-0.34613	0.00000	0.11343
204	C9	PZ	0.00000	0.00000	0.00000	1.49800	0.00000
205	C9	DXX	0.00455	-0.00129	-0.00372	0.00000	0.00368
206	C9	DYY	-0.00809	-0.00284	0.00802	0.00000	-0.00863
207	C9	DZZ	0.00441	0.01198	0.00994	0.00000	-0.00130
208	C9	DXY	0.00431	0.00034	-0.00859	0.00000	0.00699
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00090	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00821	0.00000
211	H3	S	-0.04890	-0.03196	0.02027	0.00000	-0.03633
212	H3	S	-1.65992	-0.93690	-0.09336	0.00000	0.33069
213	H3	PX	0.00073	-0.00173	-0.00502	0.00000	0.00323
214	H3	PY	0.00587	0.00390	0.00150	0.00000	-0.00055
215	H3	PZ	0.00000	0.00000	0.00000	0.00886	0.00000
216	H5	S	0.01780	0.03698	0.02573	0.03442	0.00253
217	H5	S	0.64376	0.62127	-0.11680	1.65672	0.25596
218	H5	PX	-0.00230	-0.00594	-0.00329	-0.00149	0.00025
219	H5	PY	0.00471	0.00310	-0.00433	-0.00294	0.00463
220	H5	PZ	-0.00005	-0.00189	-0.00183	0.00625	0.00028
221	H7	S	0.01780	0.03698	0.02573	-0.03442	0.00253
222	H7	S	0.64376	0.62127	-0.11680	-1.65672	0.25596
223	H7	PX	-0.00230	-0.00594	-0.00329	0.00149	0.00025
224	H7	PY	0.00471	0.00310	-0.00433	0.00294	0.00463
225	H7	PZ	0.00005	0.00189	0.00183	0.00625	-0.00028

MO:	56	57	58	59	60
Eigenvalues:	0.34257	0.38340	0.40188	0.43117	0.43713
(ev):	9.32173	10.43278	10.93575	11.73272	11.89486

	A	A	A	A	A	
1 H1	S	0.00671	0.00000	-0.06753	0.05645	0.05346

2	H1	S	-1.28388	0.00000	-0.55255	-0.27599	-0.72249
3	H1	PX	0.00563	0.00000	-0.00152	0.00879	0.00623
4	H1	PY	-0.00244	0.00000	-0.00544	-0.00791	0.00193
5	H1	PZ	0.00000	-0.01587	0.00000	0.00000	0.00000
6	C1	S	-0.04912	0.00000	0.01491	-0.02798	-0.04996
7	C1	S	0.07957	0.00000	-0.05400	0.06888	0.01839
8	C1	PX	0.14604	0.00000	0.08031	0.00672	0.03089
9	C1	PY	-0.01368	0.00000	0.02674	-0.12945	-0.03671
10	C1	PZ	0.00000	-0.20358	0.00000	0.00000	0.00000
11	C1	S	0.76353	0.00000	-0.23067	0.46137	1.22731
12	C1	PX	0.73712	0.00000	0.96305	0.22601	0.39842
13	C1	PY	0.29545	0.00000	-1.15381	0.14930	-0.05196
14	C1	PZ	0.00000	-0.66158	0.00000	0.00000	0.00000
15	C1	DXX	0.01065	0.00000	-0.01233	0.02607	0.02156
16	C1	DYY	-0.01190	0.00000	0.00200	-0.02922	-0.02132
17	C1	DZZ	0.00329	0.00000	-0.00113	0.00767	-0.00294
18	C1	DXY	-0.00061	0.00000	-0.02379	0.00366	0.01742
19	C1	DXZ	0.00000	-0.02089	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.00947	0.00000	0.00000	0.00000
21	C2	S	-0.05195	0.00000	0.01755	0.03906	0.03134
22	C2	S	0.08340	0.00000	-0.01232	-0.00821	-0.04726
23	C2	PX	-0.06179	0.00000	-0.08988	-0.00287	-0.06792
24	C2	PY	-0.07166	0.00000	0.05338	-0.00449	0.01292
25	C2	PZ	0.00000	0.19839	0.00000	0.00000	0.00000
26	C2	S	0.62107	0.00000	-0.40399	-1.28135	-0.72267
27	C2	PX	-0.84029	0.00000	-0.68359	-0.11847	-0.07342
28	C2	PY	-0.28830	0.00000	0.78303	0.88753	-0.77940
29	C2	PZ	0.00000	0.63790	0.00000	0.00000	0.00000
30	C2	DXX	0.00294	0.00000	0.01108	-0.01007	-0.01895
31	C2	DYY	-0.00813	0.00000	-0.01263	0.00541	0.01622
32	C2	DZZ	0.00207	0.00000	0.00065	0.00197	-0.00161
33	C2	DXY	0.01297	0.00000	-0.01994	-0.02940	-0.00841
34	C2	DXZ	0.00000	-0.02006	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	-0.00041	0.00000	0.00000	0.00000
36	C3	S	0.00106	0.00000	0.05599	0.02933	0.03172
37	C3	S	0.00188	0.00000	-0.07774	-0.06614	-0.04750
38	C3	PX	-0.00519	0.00000	0.08758	0.04579	-0.18314
39	C3	PY	-0.09408	0.00000	0.03897	-0.13845	-0.04047
40	C3	PZ	0.00000	0.30802	0.00000	0.00000	0.00000
41	C3	S	0.11315	0.00000	-1.67746	0.77700	-0.95378
42	C3	PX	-0.01997	0.00000	-0.29406	0.39121	-1.12370
43	C3	PY	0.11382	0.00000	-0.25585	-0.62175	0.12388
44	C3	PZ	0.00000	0.74766	0.00000	0.00000	0.00000
45	C3	DXX	-0.00882	0.00000	0.02978	-0.01015	-0.01460
46	C3	DYY	0.01422	0.00000	-0.04311	0.03257	0.00523
47	C3	DZZ	-0.00154	0.00000	-0.00125	-0.00718	0.00127
48	C3	DXY	0.01567	0.00000	0.02250	-0.00607	-0.00376
49	C3	DXZ	0.00000	0.01119	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	-0.00559	0.00000	0.00000	0.00000
51	C4	S	0.00914	0.00000	-0.07733	-0.04883	0.01756
52	C4	S	-0.01604	0.00000	0.08618	0.05212	-0.02875
53	C4	PX	-0.03951	0.00000	-0.02449	-0.22215	-0.13135
54	C4	PY	-0.05360	0.00000	-0.04395	-0.09802	-0.06614
55	C4	PZ	0.00000	0.26738	0.00000	0.00000	0.00000

56	C4	S	-0.16725	0.00000	1.99205	1.21439	0.07907
57	C4	PX	-0.06087	0.00000	0.53103	-1.27733	-0.62829
58	C4	PY	-0.02999	0.00000	-0.25431	-0.91970	-0.11918
59	C4	PZ	0.00000	0.59937	0.00000	0.00000	0.00000
60	C4	DXX	-0.00461	0.00000	0.00746	-0.01099	-0.01549
61	C4	DYY	0.00267	0.00000	-0.00877	0.01029	0.02216
62	C4	DZZ	-0.00172	0.00000	0.00727	0.00077	-0.00181
63	C4	DXY	0.00688	0.00000	-0.00746	-0.01086	-0.00262
64	C4	DXZ	0.00000	-0.00226	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00637	0.00000	0.00000	0.00000
66	C5	S	0.03401	0.00000	0.03687	0.04961	-0.00701
67	C5	S	-0.03326	0.00000	-0.05860	-0.01115	0.00367
68	C5	PX	0.14521	0.00000	-0.04954	-0.14403	-0.05725
69	C5	PY	-0.06413	0.00000	0.03626	0.01079	-0.09407
70	C5	PZ	0.00000	-0.19154	0.00000	0.00000	0.00000
71	C5	S	-0.57219	0.00000	-0.67258	-1.64646	0.35518
72	C5	PX	0.80142	0.00000	-0.07837	-1.34242	-0.47419
73	C5	PY	-0.62623	0.00000	0.09741	-0.17276	-0.93968
74	C5	PZ	0.00000	-0.58587	0.00000	0.00000	0.00000
75	C5	DXX	0.00190	0.00000	0.01269	0.02130	0.01170
76	C5	DYY	0.00148	0.00000	-0.01571	-0.02055	-0.00644
77	C5	DZZ	0.00295	0.00000	-0.00182	-0.00112	-0.00431
78	C5	DXY	0.00142	0.00000	0.01732	0.01103	0.00505
79	C5	DXZ	0.00000	0.01055	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	-0.01070	0.00000	0.00000	0.00000
81	C6	S	0.01809	0.00000	-0.08186	-0.05079	0.00542
82	C6	S	-0.02540	0.00000	0.10008	0.09287	-0.05341
83	C6	PX	0.06516	0.00000	0.08743	-0.13896	-0.10589
84	C6	PY	-0.06050	0.00000	0.15878	0.03885	-0.02965
85	C6	PZ	0.00000	-0.32688	0.00000	0.00000	0.00000
86	C6	S	-0.04536	0.00000	1.45262	1.08715	-0.34145
87	C6	PX	0.11487	0.00000	-0.28276	-0.93680	-0.07443
88	C6	PY	0.11467	0.00000	0.53157	0.52225	-0.60720
89	C6	PZ	0.00000	-0.72723	0.00000	0.00000	0.00000
90	C6	DXX	0.01329	0.00000	-0.01263	0.00711	0.01046
91	C6	DYY	-0.00565	0.00000	0.00477	-0.00516	-0.02271
92	C6	DZZ	-0.00104	0.00000	0.00863	0.00780	-0.00148
93	C6	DXY	-0.01567	0.00000	-0.00110	-0.01700	0.01425
94	C6	DXZ	0.00000	0.00384	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00379	0.00000	0.00000	0.00000
96	C7	S	0.00326	0.00000	0.02851	-0.02471	-0.01947
97	C7	S	-0.02107	0.00000	-0.06004	0.06616	0.00674
98	C7	PX	-0.02851	0.00000	0.03834	-0.09123	0.02876
99	C7	PY	-0.02239	0.00000	-0.02232	-0.00335	0.06833
100	C7	PZ	0.00000	-0.05969	0.00000	0.00000	0.00000
101	C7	S	0.18263	0.00000	-0.52008	-0.28196	1.10671
102	C7	PX	-0.31697	0.00000	0.18825	0.02676	0.03522
103	C7	PY	-0.34842	0.00000	1.32622	-1.09910	0.87839
104	C7	PZ	0.00000	-0.40822	0.00000	0.00000	0.00000
105	C7	DXX	0.01254	0.00000	-0.01767	0.00133	0.03343
106	C7	DYY	-0.00138	0.00000	0.01871	-0.00615	-0.02646
107	C7	DZZ	-0.00486	0.00000	-0.00448	0.00257	0.00123
108	C7	DXY	-0.00920	0.00000	0.01925	-0.01009	0.00369
109	C7	DXZ	0.00000	-0.01291	0.00000	0.00000	0.00000

110	C7	DYZ	0.00000	0.02592	0.00000	0.00000	0.00000
111	O1	S	-0.04524	0.00000	0.01174	-0.00555	-0.00582
112	O1	S	0.01644	0.00000	-0.01792	0.00597	0.05016
113	O1	PX	0.14406	0.00000	0.02813	-0.04134	-0.03071
114	O1	PY	0.01949	0.00000	0.09940	-0.06224	-0.10969
115	O1	PZ	0.00000	-0.07103	0.00000	0.00000	0.00000
116	O1	S	0.77098	0.00000	-0.16646	0.17573	-0.09420
117	O1	PX	0.38082	0.00000	0.03091	0.01353	-0.07577
118	O1	PY	0.10125	0.00000	0.27858	-0.24517	-0.23644
119	O1	PZ	0.00000	-0.15183	0.00000	0.00000	0.00000
120	O1	DXX	-0.01385	0.00000	0.00102	-0.00569	0.00629
121	O1	DYY	-0.03491	0.00000	-0.00283	0.00887	0.00612
122	O1	DZZ	-0.02873	0.00000	0.00621	0.00006	0.01445
123	O1	DXY	-0.00291	0.00000	0.00560	0.00849	-0.00068
124	O1	DXZ	0.00000	-0.00313	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	-0.01517	0.00000	0.00000	0.00000
126	H4	S	0.01979	0.00000	-0.03718	-0.02317	-0.00355
127	H4	S	1.38695	0.00000	0.04545	-0.38728	0.23054
128	H4	PX	0.00284	0.00000	-0.00564	-0.00977	-0.00094
129	H4	PY	-0.00326	0.00000	-0.01005	-0.01152	-0.00251
130	H4	PZ	0.00000	-0.01287	0.00000	0.00000	0.00000
131	N1	S	-0.01102	0.00000	-0.00166	0.00739	0.07571
132	N1	S	0.01059	0.00000	-0.03733	-0.00941	-0.09495
133	N1	PX	-0.00351	0.00000	-0.09141	0.05364	-0.10242
134	N1	PY	-0.03362	0.00000	-0.04220	-0.06118	0.03703
135	N1	PZ	0.00000	0.13848	0.00000	0.00000	0.00000
136	N1	S	0.20157	0.00000	0.40943	-0.17547	-1.53284
137	N1	PX	0.06822	0.00000	0.14894	0.23102	-0.67484
138	N1	PY	-0.00410	0.00000	-0.22641	-0.26196	0.17441
139	N1	PZ	0.00000	0.36123	0.00000	0.00000	0.00000
140	N1	DXX	-0.00223	0.00000	-0.00489	-0.00549	0.00849
141	N1	DYY	0.00183	0.00000	-0.01437	0.00949	0.00282
142	N1	DZZ	-0.00404	0.00000	0.00037	0.00068	0.01678
143	N1	DXY	0.00696	0.00000	0.00240	-0.00174	-0.01156
144	N1	DXZ	0.00000	0.00559	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	-0.02108	0.00000	0.00000	0.00000
146	H6	S	0.00555	0.00000	-0.00226	-0.06253	-0.06302
147	H6	S	-1.20794	0.00000	-0.30437	0.39887	-0.18278
148	H6	PX	-0.00395	0.00000	-0.00339	0.00267	0.00425
149	H6	PY	-0.00411	0.00000	0.00925	0.01221	-0.00095
150	H6	PZ	0.00000	0.01433	0.00000	0.00000	0.00000
151	C8	S	0.03307	0.00000	-0.06385	0.07109	-0.08020
152	C8	S	-0.03017	0.00000	0.03498	-0.07064	0.05562
153	C8	PX	0.00612	0.00000	0.14223	-0.07633	-0.14756
154	C8	PY	-0.02278	0.00000	0.04779	-0.00746	-0.01862
155	C8	PZ	0.00000	0.00183	0.00000	0.00000	0.00000
156	C8	S	-0.84729	0.00000	1.80359	-2.42556	2.50362
157	C8	PX	-0.19895	0.00000	1.24924	-0.74681	-0.82917
158	C8	PY	-0.04479	0.00000	-0.09370	0.93923	-0.56754
159	C8	PZ	0.00000	0.01225	0.00000	0.00000	0.00000
160	C8	DXX	-0.00121	0.00000	-0.01094	0.00486	-0.01782
161	C8	DYY	-0.00040	0.00000	0.00450	-0.01902	0.02921
162	C8	DZZ	0.00022	0.00000	-0.00150	-0.00109	0.00438
163	C8	DXY	-0.00413	0.00000	0.01397	0.00771	-0.00370

164	C8	DXZ	0.00000	-0.02041	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	-0.00471	0.00000	0.00000	0.00000
166	H8	S	0.03269	0.00000	-0.05806	-0.00471	0.10550
167	H8	S	0.27638	0.00000	0.05962	0.03589	-0.22852
168	H8	PX	0.00256	0.00000	-0.00382	-0.00022	0.00897
169	H8	PY	-0.00361	0.00000	0.00536	-0.00411	0.00659
170	H8	PZ	0.00000	-0.00744	0.00000	0.00000	0.00000
171	C10	S	-0.02545	0.00000	0.02968	-0.04443	0.04449
172	C10	S	0.01653	0.00000	-0.00211	-0.03220	0.01769
173	C10	PX	0.00878	0.00000	-0.05248	0.04258	0.11738
174	C10	PY	-0.01191	0.00000	-0.02170	-0.02955	0.09225
175	C10	PZ	0.00000	0.00777	0.00000	0.00000	0.00000
176	C10	S	0.54677	0.00000	-0.98231	1.87753	-1.46032
177	C10	PX	0.10742	0.00000	-0.65684	0.14316	0.97466
178	C10	PY	0.17769	0.00000	-0.82302	1.30135	-0.75803
179	C10	PZ	0.00000	-0.00267	0.00000	0.00000	0.00000
180	C10	DXX	0.00100	0.00000	-0.00952	0.01535	-0.00282
181	C10	DYY	0.00031	0.00000	0.00398	-0.00082	-0.01286
182	C10	DZZ	-0.00364	0.00000	0.00568	-0.01297	0.01453
183	C10	DXY	0.00267	0.00000	0.00060	-0.00209	-0.03097
184	C10	DXZ	0.00000	-0.00718	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	-0.00160	0.00000	0.00000	0.00000
186	H16	S	-0.00833	0.00000	-0.01359	0.03327	0.05547
187	H16	S	-0.28533	0.00000	0.64343	-0.39870	-0.50793
188	H16	PX	0.00057	0.00000	-0.00465	0.00363	0.00170
189	H16	PY	0.00085	0.00000	-0.00196	0.00381	-0.01337
190	H16	PZ	0.00000	-0.00100	0.00000	0.00000	0.00000
191	H18	S	0.00538	0.00000	-0.01133	0.02033	-0.10435
192	H18	S	-0.07874	0.00000	-0.54740	0.25181	0.81432
193	H18	PX	0.00009	0.00000	0.00015	-0.00189	0.00088
194	H18	PY	0.00071	0.00000	-0.00484	0.00476	0.00495
195	H18	PZ	0.00000	0.00177	0.00000	0.00000	0.00000
196	C9	S	0.06629	0.00000	0.01687	-0.01121	-0.00426
197	C9	S	-0.04674	0.00000	-0.00452	0.02809	0.00447
198	C9	PX	0.06224	0.00000	0.05777	-0.02749	-0.01684
199	C9	PY	0.00726	0.00000	-0.11001	-0.09268	-0.05151
200	C9	PZ	0.00000	-0.00915	0.00000	0.00000	0.00000
201	C9	S	-1.23005	0.00000	-0.41039	-0.02981	-0.01542
202	C9	PX	0.43694	0.00000	0.17282	-0.24373	-0.34350
203	C9	PY	0.33875	0.00000	-0.16857	-0.31072	-0.13551
204	C9	PZ	0.00000	-0.03840	0.00000	0.00000	0.00000
205	C9	DXX	0.00452	0.00000	0.00826	-0.00103	-0.00335
206	C9	DYY	-0.00827	0.00000	-0.01684	-0.01076	-0.00509
207	C9	DZZ	0.00036	0.00000	0.00607	0.00946	0.01096
208	C9	DXY	0.01557	0.00000	0.00384	-0.00547	0.00396
209	C9	DXZ	0.00000	0.00978	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	-0.00135	0.00000	0.00000	0.00000
211	H3	S	-0.05470	0.00000	-0.05837	-0.01757	-0.01443
212	H3	S	0.26943	0.00000	0.49475	0.33937	0.12080
213	H3	PX	0.00488	0.00000	-0.00053	-0.00232	0.00082
214	H3	PY	0.00038	0.00000	-0.00109	-0.00185	0.00060
215	H3	PZ	0.00000	-0.00128	0.00000	0.00000	0.00000
216	H5	S	-0.00018	-0.02425	0.02426	0.03103	0.03121
217	H5	S	0.42355	-0.04936	-0.00432	0.04669	0.15230

218	H5	PX	-0.00119	-0.00174	0.00017	-0.00175	-0.00341
219	H5	PY	0.00677	-0.00140	0.00451	0.00206	0.00376
220	H5	PZ	0.00032	0.00117	0.00030	-0.00016	-0.00210
221	H7	S	-0.00018	0.02425	0.02426	0.03103	0.03121
222	H7	S	0.42355	0.04936	-0.00432	0.04669	0.15230
223	H7	PX	-0.00119	0.00174	0.00017	-0.00175	-0.00341
224	H7	PY	0.00677	0.00140	0.00451	0.00206	0.00376
225	H7	PZ	-0.00032	0.00117	-0.00030	0.00016	0.00210

M0:	61	62	63	64	65
Eigenvalues:	0.47510	0.48296	0.52777	0.54410	0.58615
(ev):	12.92810	13.14198	14.36134	14.80580	15.94991

			A	A	A	A	A
1	H1	S	-0.01773	0.08117	-0.00474	0.04481	0.03253
2	H1	S	-0.07907	-0.68322	0.24568	-0.87928	-0.16288
3	H1	PX	0.00150	0.00787	0.00168	0.00657	0.00202
4	H1	PY	-0.00904	0.00954	-0.00871	0.00529	0.00188
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.05204	-0.03251	0.01795	0.07163	0.01020
7	C1	S	0.10016	0.06327	-0.02989	-0.07724	-0.10584
8	C1	PX	-0.07915	-0.01594	0.03310	0.11134	0.10067
9	C1	PY	-0.07970	0.06482	-0.07929	0.14171	-0.12170
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.22583	0.48532	-0.09553	-1.94114	0.58689
12	C1	PX	0.48549	0.42346	0.19227	1.38850	0.55527
13	C1	PY	-1.79880	0.61493	-1.10533	1.07466	-1.36977
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.01855	0.02825	0.00166	0.00854	-0.00577
16	C1	DYY	-0.02328	-0.01246	-0.00047	0.00096	-0.01453
17	C1	DZZ	0.00364	-0.00204	0.00031	-0.01194	0.00437
18	C1	DXY	-0.01003	0.03256	-0.02318	0.01222	0.01576
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.03934	-0.00378	0.00249	0.05760	-0.02396
22	C2	S	0.02976	0.03759	-0.00712	-0.06923	0.11587
23	C2	PX	0.06595	0.00599	0.06534	-0.11388	0.13754
24	C2	PY	-0.06045	-0.03453	-0.10230	-0.15126	-0.07928
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	1.40739	0.09357	-0.34674	-2.02289	-0.66521
27	C2	PX	0.56950	-0.45794	0.72472	-0.85806	0.41589
28	C2	PY	-0.34751	0.62066	-1.49704	-1.62005	-1.03943
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.01296	0.03857	-0.02451	0.00299	0.00291
31	C2	DYY	-0.01229	-0.01333	0.02460	-0.00642	0.01105
32	C2	DZZ	0.00210	-0.00445	-0.00088	-0.00659	0.00232
33	C2	DXY	0.02635	0.00236	0.00021	0.01397	-0.00255
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.09614	0.00694	-0.04060	-0.05095	0.00223
37	C3	S	-0.11078	0.02914	0.06789	0.03005	0.11898
38	C3	PX	-0.01848	-0.00388	0.03603	-0.00903	-0.26456
39	C3	PY	-0.13630	-0.04907	-0.17090	0.08226	-0.03397
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

41	C3	S	-2.02561	-0.35604	0.48163	1.59967	-0.96161
42	C3	PX	-0.52808	-0.32397	0.26707	0.09379	-1.65224
43	C3	PY	-0.94777	0.10141	-1.37569	1.06263	-0.79829
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00649	0.00591	0.00326	0.02069	0.00917
46	C3	DYY	0.00721	0.02196	-0.00411	-0.01899	0.02476
47	C3	DZZ	-0.01290	-0.00845	0.00264	0.00443	-0.00265
48	C3	DXY	0.01516	-0.02840	0.02581	-0.01510	0.00023
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.04553	0.05688	-0.04880	-0.00162	-0.09495
52	C4	S	-0.04705	-0.05954	0.05256	-0.00283	-0.10834
53	C4	PX	0.09696	-0.10546	0.05535	0.02322	-0.03016
54	C4	PY	-0.14437	-0.06721	-0.08143	-0.09447	0.20541
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.24763	-0.96676	1.56054	0.80795	3.08555
57	C4	PX	1.37729	-0.40272	0.16708	-0.02434	-0.01136
58	C4	PY	-0.91973	-1.10263	-0.26926	-1.45530	0.83883
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.02005	0.00059	-0.01027	0.01216	-0.03458
61	C4	DYY	0.02712	0.01235	0.00698	-0.00129	-0.00986
62	C4	DZZ	-0.01104	-0.01578	0.00626	-0.01108	0.02124
63	C4	DXY	-0.02201	-0.01073	0.01206	0.03468	-0.00029
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.01911	0.01967	-0.01635	-0.04706	0.02919
67	C5	S	-0.01412	0.00173	0.04316	0.05981	-0.11302
68	C5	PX	-0.03766	0.01068	-0.06133	0.04961	-0.17684
69	C5	PY	0.02570	0.11736	-0.12399	-0.05096	-0.04245
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.89835	-0.62503	0.89532	1.68451	0.31788
72	C5	PX	0.38251	-0.17501	-0.87524	-0.75173	-0.98379
73	C5	PY	1.02999	0.75608	-0.82989	-1.52085	-0.78148
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.00080	0.00878	0.01060	0.02569	-0.01536
76	C5	DYY	0.01995	0.01108	-0.00681	-0.00993	-0.00546
77	C5	DZZ	-0.00813	-0.00533	0.00454	0.00163	-0.00107
78	C5	DXY	-0.02686	-0.01916	-0.01165	-0.02682	-0.00404
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.02002	0.02239	0.00467	0.02341	0.10547
82	C6	S	0.01502	0.04382	0.02275	-0.02782	0.09962
83	C6	PX	0.25979	-0.07575	0.07362	-0.00992	-0.01172
84	C6	PY	-0.05808	0.08923	-0.07377	0.04598	0.04203
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.81762	-1.23951	-1.19529	-0.65108	-3.76111
87	C6	PX	0.63036	-0.31984	0.65913	-0.04450	-0.35397
88	C6	PY	-0.32187	1.78064	-0.49941	0.91225	1.02233
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.00683	-0.00154	0.02346	0.00612	0.04088
91	C6	DYY	0.01192	0.01326	-0.03976	-0.00892	0.01920
92	C6	DZZ	-0.00054	-0.01071	0.00126	-0.00414	-0.02311
93	C6	DXY	-0.02335	0.00082	-0.01049	0.02067	0.00076
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000

95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.01125	-0.02178	0.02257	0.03784	-0.03270
97	C7	S	0.04720	0.09531	-0.03054	-0.08724	0.10138
98	C7	PX	-0.01806	-0.06477	0.02921	0.07127	-0.05166
99	C7	PY	-0.00005	0.12170	-0.15330	0.08486	0.00081
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.26216	0.45077	-0.54215	-0.60806	0.57534
102	C7	PX	0.83536	-1.09257	0.03986	0.41070	0.17598
103	C7	PY	0.75655	0.39575	-1.01105	0.20403	0.91674
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.01185	0.00980	-0.00647	-0.02618	0.04544
106	C7	DYY	-0.00423	0.01103	0.00940	0.01661	-0.01266
107	C7	DZZ	-0.00197	-0.00047	-0.00363	-0.00591	-0.00580
108	C7	DXY	0.00330	0.00132	-0.03163	0.01658	-0.00189
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.01467	-0.03332	0.00637	-0.03129	0.04862
112	O1	S	0.04246	0.01967	0.03830	0.07527	-0.03978
113	O1	PX	-0.04343	-0.02748	-0.04231	-0.10796	0.05831
114	O1	PY	-0.18720	-0.13956	-0.01204	-0.05225	0.17749
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.18677	0.73843	-0.33207	0.42023	-1.02738
117	O1	PX	-0.39897	-0.08056	-0.15564	-0.31107	0.15489
118	O1	PY	-0.57329	-0.59439	0.00022	-0.49095	0.79043
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00265	-0.01222	-0.00441	-0.03151	0.00161
121	O1	DYY	-0.00409	-0.00424	0.01465	0.02509	0.01014
122	O1	DZZ	0.00663	-0.02027	0.02368	0.00830	0.03507
123	O1	DXY	0.00061	0.00552	-0.01023	-0.02932	0.00352
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.09377	0.04560	0.04104	0.06678	0.01637
127	H4	S	-0.53728	-0.49752	-0.06686	0.10485	-0.17318
128	H4	PX	-0.00185	-0.00518	-0.00606	-0.01290	-0.00155
129	H4	PY	0.00988	0.00366	0.00120	-0.00484	0.00031
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01475	-0.10286	-0.01821	-0.02094	-0.07347
132	N1	S	0.00189	0.07644	-0.00343	-0.02184	0.06399
133	N1	PX	0.00418	-0.01055	0.12268	0.04550	0.00111
134	N1	PY	-0.01105	0.04241	-0.15597	0.02021	0.09403
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.24538	2.95948	0.68862	0.95415	2.32000
137	N1	PX	-0.08617	0.79739	0.35084	0.09185	0.37483
138	N1	PY	-0.26076	0.91515	0.12906	0.26577	0.88851
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.01252	-0.00417	-0.00193	0.00617	0.02221
141	N1	DYY	-0.00919	0.00705	0.01144	-0.00851	0.00382
142	N1	DZZ	-0.00746	-0.04170	-0.01442	-0.01968	-0.04726
143	N1	DXY	0.02107	0.00383	0.00127	-0.01608	-0.00300
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.06036	0.08245	-0.05009	0.02392	-0.03419
147	H6	S	0.04501	-0.20473	0.28476	-0.72222	0.18775
148	H6	PX	-0.00109	-0.01195	0.00665	-0.00109	0.00096

149	H6	PY	-0.01214	0.00675	-0.00553	-0.00438	-0.00004
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.04062	-0.01025	0.01150	-0.01740	0.03269
152	C8	S	-0.07440	0.09966	-0.01382	0.06253	0.14759
153	C8	PX	0.10261	0.09616	0.00415	0.02044	-0.05769
154	C8	PY	0.04595	-0.11718	-0.23509	0.18176	0.05187
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.64914	0.61965	1.33618	-0.94051	-0.97053
157	C8	PX	0.51967	1.16203	0.62629	0.34893	0.59215
158	C8	PY	1.17588	-1.90945	-2.55456	1.59541	0.38489
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.00230	-0.00226	0.02834	0.00967	0.00479
161	C8	DYY	0.01651	0.02475	0.01049	-0.03782	0.05032
162	C8	DZZ	-0.00821	-0.00618	-0.01401	0.01060	-0.00741
163	C8	DXY	0.00268	-0.00694	-0.00906	-0.00510	-0.00108
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.01358	-0.00025	-0.02129	-0.06346	0.05972
167	H8	S	-0.60637	0.76086	-0.00929	-0.12312	-0.28567
168	H8	PX	0.00437	-0.00308	-0.00263	-0.00330	0.00844
169	H8	PY	0.00316	-0.00161	-0.01983	0.00634	-0.00122
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.02620	0.03057	0.03852	-0.02054	-0.01809
172	C10	S	0.01744	0.08944	0.05217	-0.08434	0.12118
173	C10	PX	-0.01972	-0.04576	-0.05031	-0.04050	-0.00908
174	C10	PY	0.05236	0.07755	-0.00535	-0.10739	0.14191
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.97343	-2.03963	-2.37983	1.53269	0.21178
177	C10	PX	-0.68963	-0.06424	0.43201	-0.63449	-0.39663
178	C10	PY	0.85568	-1.46746	-2.13990	1.22162	0.59968
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00850	-0.01320	-0.02036	-0.00076	0.02065
181	C10	DYY	-0.00542	0.01529	0.00874	0.00988	-0.00186
182	C10	DZZ	-0.00343	0.00837	0.00586	-0.01084	0.00182
183	C10	DXY	0.00687	0.01541	0.01151	0.02494	0.00813
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.03144	-0.08488	-0.12873	-0.01860	0.04020
187	H16	S	0.53310	0.18387	-0.32839	0.44565	0.39406
188	H16	PX	-0.00147	-0.00235	-0.00207	-0.00051	0.00330
189	H16	PY	0.00446	0.00299	0.00065	0.00958	0.00705
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.01991	0.01856	-0.01808	0.11727	0.05559
192	H18	S	-0.13416	-0.26931	-0.42409	-0.14583	0.18722
193	H18	PX	-0.00425	0.00396	0.00718	0.00109	-0.00356
194	H18	PY	0.00150	-0.01252	-0.00840	-0.00553	-0.00586
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.00668	-0.00359	-0.00696	0.00029	0.00156
197	C9	S	0.03558	0.00617	-0.01155	-0.10849	-0.01571
198	C9	PX	-0.01194	-0.06174	0.07507	0.10599	0.09745
199	C9	PY	-0.12711	-0.00245	-0.04630	0.08182	-0.04781
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.09365	0.01643	0.17949	0.43624	-0.13494
202	C9	PX	-0.67083	-0.33838	-0.26582	-0.55480	0.30369

203	C9	PY	-0.12770	-0.04943	-0.16055	-0.12606	-0.02117
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00239	-0.00590	0.00514	-0.00255	0.01364
206	C9	DYY	-0.00294	0.00018	-0.01107	0.00291	-0.02674
207	C9	DZZ	0.02363	0.00705	0.00870	-0.00051	-0.00168
208	C9	DXY	0.00886	0.00231	0.00023	0.00065	0.00373
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.02758	0.01061	-0.02617	0.02779	-0.08731
212	H3	S	0.13379	-0.02145	0.12081	-0.14805	0.19663
213	H3	PX	0.00096	0.00193	-0.00071	0.00486	-0.00263
214	H3	PY	0.00539	0.00021	0.00073	0.00278	-0.00388
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.06696	0.01545	0.04034	0.03421	0.00744
217	H5	S	0.20436	0.20742	-0.03824	0.09237	-0.15246
218	H5	PX	-0.00484	-0.00305	0.00003	-0.00025	0.00175
219	H5	PY	0.00481	0.00251	0.00344	0.00142	0.00596
220	H5	PZ	-0.00295	-0.00352	0.00100	-0.00204	0.00450
221	H7	S	0.06696	0.01545	0.04034	0.03421	0.00744
222	H7	S	0.20436	0.20742	-0.03824	0.09237	-0.15246
223	H7	PX	-0.00484	-0.00305	0.00003	-0.00025	0.00175
224	H7	PY	0.00481	0.00251	0.00344	0.00142	0.00596
225	H7	PZ	0.00295	0.00352	-0.00100	0.00204	-0.00450

M0:	66	67	68	69	70
Eigenvalues:	0.62933	0.66412	0.69372	0.70634	0.72492
(ev):	17.12506	18.07154	18.87710	19.22061	19.72606

		A	A	A	A	A	
1	H1	S	-0.02214	-0.07197	0.03058	0.02816	0.00000
2	H1	S	0.05250	-0.00408	0.23581	-0.00180	0.00000
3	H1	PX	-0.00445	-0.00779	-0.00221	-0.01168	0.00000
4	H1	PY	-0.00326	0.01164	-0.00888	-0.00437	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.00499
6	C1	S	0.03655	-0.03055	0.00658	-0.02875	0.00000
7	C1	S	-0.08000	-0.10018	-0.15554	-0.35936	0.00000
8	C1	PX	0.09606	0.03557	0.17119	0.09098	0.00000
9	C1	PY	-0.04194	-0.24639	-0.19094	0.14172	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.39285
11	C1	S	-1.57939	0.97626	0.16734	0.99055	0.00000
12	C1	PX	0.79963	-0.82898	-0.83062	-0.13301	0.00000
13	C1	PY	-1.52800	1.48799	0.87577	-1.11391	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.22592
15	C1	DXX	-0.01367	-0.02354	0.00257	-0.02060	0.00000
16	C1	DYY	0.00703	-0.01193	-0.02371	-0.08736	0.00000
17	C1	DZZ	-0.00730	0.00724	-0.00246	0.01033	0.00000
18	C1	DXY	-0.00222	0.00382	-0.01766	0.01736	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.02037
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00087
21	C2	S	0.05155	0.00570	-0.04356	0.00031	0.00000
22	C2	S	-0.05986	-0.13560	-0.07273	-0.39537	0.00000
23	C2	PX	-0.09690	-0.00643	0.02584	-0.22485	0.00000
24	C2	PY	-0.06147	-0.23413	-0.09724	0.06433	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.27615

26	C2	S	-1.09914	-0.77693	0.78526	0.68042	0.00000
27	C2	PX	-1.42402	0.35524	0.44102	0.33207	0.00000
28	C2	PY	0.49070	-1.24798	-1.11538	0.94469	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.22033
30	C2	DXX	0.03067	-0.02730	0.03461	-0.05723	0.00000
31	C2	DYY	-0.00775	-0.03370	-0.06489	-0.02206	0.00000
32	C2	DZZ	-0.01130	0.01242	0.00784	-0.00320	0.00000
33	C2	DXY	0.02065	0.00031	0.01001	-0.00264	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	-0.01075
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01175
36	C3	S	0.02226	0.06136	0.03554	-0.01333	0.00000
37	C3	S	-0.00940	-0.08697	-0.11687	-0.39652	0.00000
38	C3	PX	-0.02852	0.13058	0.29684	-0.04529	0.00000
39	C3	PY	0.06318	0.07251	-0.05399	-0.18580	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.22618
41	C3	S	-1.97308	-1.76512	-0.04394	0.34096	0.00000
42	C3	PX	-0.21480	0.09130	2.22315	-1.34958	0.00000
43	C3	PY	0.26489	1.89734	0.14592	-0.48129	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.11839
45	C3	DXX	-0.02034	-0.02330	0.00175	-0.04372	0.00000
46	C3	DYY	-0.01716	0.02846	0.01091	-0.07882	0.00000
47	C3	DZZ	0.00792	-0.01495	-0.01773	0.00983	0.00000
48	C3	DXY	0.00339	0.02002	-0.01651	-0.05335	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00616
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00257
51	C4	S	0.01064	0.01230	-0.04342	0.01066	0.00000
52	C4	S	-0.13799	-0.26770	-0.13339	-0.57257	0.00000
53	C4	PX	0.25538	-0.13119	-0.02023	0.04503	0.00000
54	C4	PY	0.00477	0.06809	0.06079	0.00210	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.41199
56	C4	S	0.52568	-0.03650	0.47506	0.62108	0.00000
57	C4	PX	2.41324	-1.52799	-1.07419	0.62250	0.00000
58	C4	PY	-0.15601	1.15105	-0.06069	0.88991	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.43417
60	C4	DXX	-0.00784	-0.03772	-0.05903	-0.10070	0.00000
61	C4	DYY	-0.00096	0.00369	-0.01822	0.01006	0.00000
62	C4	DZZ	-0.00708	0.00115	0.02011	-0.00551	0.00000
63	C4	DXY	0.03845	0.03989	0.02946	-0.00950	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00242
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00718
66	C5	S	-0.05598	-0.02694	0.03542	-0.01582	0.00000
67	C5	S	-0.00002	-0.11995	-0.26084	-0.35636	0.00000
68	C5	PX	0.13229	0.00892	-0.12102	-0.17820	0.00000
69	C5	PY	0.05106	0.06618	0.18002	0.00906	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.30558
71	C5	S	1.81306	0.70773	-0.01676	0.09647	0.00000
72	C5	PX	1.40973	-0.95829	-1.02646	0.79472	0.00000
73	C5	PY	0.21460	-1.88406	-0.58568	0.47903	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.14726
75	C5	DXX	-0.00087	-0.01195	-0.01327	-0.05744	0.00000
76	C5	DYY	-0.01680	-0.04494	-0.00834	-0.06544	0.00000
77	C5	DZZ	0.01168	0.01265	-0.01610	0.01240	0.00000
78	C5	DXY	-0.03489	-0.01494	-0.04329	-0.00335	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00456

80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.01064
81	C6	S	-0.03653	-0.03283	0.01811	-0.00832	0.00000
82	C6	S	0.10496	-0.08631	-0.16880	-0.38049	0.00000
83	C6	PX	-0.13689	0.12932	0.23478	-0.16669	0.00000
84	C6	PY	-0.07563	-0.11427	0.05924	-0.08941	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	-0.29158
86	C6	S	0.92531	1.54867	-0.28528	0.50854	0.00000
87	C6	PX	-0.38031	1.08897	2.47459	-1.23598	0.00000
88	C6	PY	1.50929	-1.45598	1.01888	-1.08391	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.19210
90	C6	DXX	0.00660	-0.02098	-0.05345	-0.07946	0.00000
91	C6	DYY	0.00880	0.00861	0.03081	-0.03861	0.00000
92	C6	DZZ	0.00285	0.00973	-0.01247	0.00887	0.00000
93	C6	DXY	0.01770	-0.04577	-0.01593	0.03688	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00318
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00259
96	C7	S	-0.08098	-0.02843	0.01688	-0.00638	0.00000
97	C7	S	0.03392	0.18669	-0.07987	-0.18399	0.00000
98	C7	PX	-0.17825	-0.04943	0.06137	-0.03114	0.00000
99	C7	PY	-0.28287	-0.01273	0.22012	0.12138	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.17807
101	C7	S	2.42396	1.07181	-0.15627	0.19260	0.00000
102	C7	PX	-1.65369	-1.17378	0.00619	0.39456	0.00000
103	C7	PY	-0.18954	1.16211	-2.02885	0.53314	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.14268
105	C7	DXX	-0.00594	0.03333	-0.00720	-0.06447	0.00000
106	C7	DYY	0.00557	0.01380	-0.01127	-0.00654	0.00000
107	C7	DZZ	0.01011	0.00703	-0.00043	0.01090	0.00000
108	C7	DXY	-0.00809	0.00469	0.00240	-0.01603	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.01387
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00847
111	O1	S	0.00035	0.00743	0.00282	0.01571	0.00000
112	O1	S	0.05550	0.09873	0.01678	0.01763	0.00000
113	O1	PX	0.01815	-0.03638	-0.02659	0.09615	0.00000
114	O1	PY	0.01303	0.01645	0.04922	-0.07680	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	-0.13988
116	O1	S	-0.36978	-0.67935	-0.12198	-0.64793	0.00000
117	O1	PX	-0.36442	0.17322	0.09971	0.04986	0.00000
118	O1	PY	0.01300	0.35598	0.10212	0.31482	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	-0.19079
120	O1	DXX	-0.02116	0.01907	-0.01436	0.02425	0.00000
121	O1	DYY	0.00209	0.01886	0.02380	-0.05204	0.00000
122	O1	DZZ	0.03612	0.05265	0.01877	0.04502	0.00000
123	O1	DXY	-0.04706	-0.02459	-0.01460	-0.01036	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00899
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.02841
126	H4	S	0.02488	-0.01376	0.15678	-0.08690	0.00000
127	H4	S	0.13576	0.20434	-0.39925	0.01694	0.00000
128	H4	PX	-0.00151	0.00100	-0.00317	0.01977	0.00000
129	H4	PY	-0.00169	-0.01227	0.00336	-0.00776	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.00546
131	N1	S	0.00037	-0.00751	0.01717	0.00856	0.00000
132	N1	S	-0.01053	0.02781	-0.01378	0.03161	0.00000
133	N1	PX	-0.07537	0.15298	-0.16694	0.11491	0.00000

134	N1	PY	0.07414	-0.13387	0.22944	-0.06660	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.03543
136	N1	S	0.65280	-0.39675	-0.67569	-0.53338	0.00000
137	N1	PX	0.22740	0.41545	-1.46898	0.48381	0.00000
138	N1	PY	0.41532	-1.13591	1.23094	-0.69583	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00351
140	N1	DXX	-0.01076	-0.01901	-0.02025	0.01571	0.00000
141	N1	DYY	0.04433	-0.01309	-0.01710	-0.00450	0.00000
142	N1	DZZ	-0.01398	0.01130	0.02366	0.03036	0.00000
143	N1	DXY	-0.01530	0.03447	0.03130	-0.02522	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00634
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.02011
146	H6	S	0.15257	-0.03793	0.08113	-0.04443	0.00000
147	H6	S	-0.60046	0.02456	-0.23432	0.20497	0.00000
148	H6	PX	-0.01503	0.00972	-0.00346	0.01852	0.00000
149	H6	PY	0.00050	0.00359	0.00859	0.00093	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	-0.00289
151	C8	S	0.04083	0.05874	-0.04585	0.00097	0.00000
152	C8	S	0.00181	0.00842	-0.21833	-0.10959	0.00000
153	C8	PX	-0.16341	0.31643	-0.11036	-0.05228	0.00000
154	C8	PY	-0.11161	-0.09029	0.00942	-0.03201	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.10566
156	C8	S	-1.10207	-0.69664	1.26873	0.17717	0.00000
157	C8	PX	-0.98769	1.12815	-2.50200	1.01674	0.00000
158	C8	PY	-1.50762	-0.48600	-0.26252	-0.14141	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.03593
160	C8	DXX	-0.00384	0.01772	-0.05363	0.00350	0.00000
161	C8	DYY	0.01558	0.04752	-0.02548	-0.04971	0.00000
162	C8	DZZ	-0.01133	-0.02715	0.02500	0.00347	0.00000
163	C8	DXY	0.05242	-0.01123	-0.03516	-0.00576	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00635
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00346
166	H8	S	-0.07205	0.06647	0.03516	-0.15878	0.00000
167	H8	S	0.69414	0.60993	-0.08608	-0.14436	0.00000
168	H8	PX	-0.00559	0.00214	0.00129	-0.00885	0.00000
169	H8	PY	-0.00811	0.01047	-0.00283	-0.00413	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	-0.00181
171	C10	S	-0.00273	-0.00509	0.00237	0.00374	0.00000
172	C10	S	0.04547	0.17485	-0.17768	-0.07142	0.00000
173	C10	PX	0.10144	0.04493	-0.09694	-0.05289	0.00000
174	C10	PY	0.03960	0.18831	-0.07058	-0.10797	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	-0.11684
176	C10	S	-0.65557	-0.53620	0.14951	-0.17203	0.00000
177	C10	PX	0.68870	-0.59696	1.17864	-0.14487	0.00000
178	C10	PY	-0.17063	-0.53273	-0.13276	-0.11814	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.11198
180	C10	DXX	0.02773	0.01325	-0.04470	-0.01408	0.00000
181	C10	DYY	-0.02183	0.01269	-0.02594	0.00920	0.00000
182	C10	DZZ	-0.00170	0.00363	0.01386	-0.00427	0.00000
183	C10	DXY	-0.05939	0.01035	-0.01548	0.02653	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00302
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	-0.00918
186	H16	S	0.15829	0.01980	-0.08961	-0.10939	0.00000
187	H16	S	-0.59553	0.38825	-0.67956	0.11663	0.00000

188	H16	PX	0.00278	-0.00496	0.00202	-0.00126	0.00000
189	H16	PY	-0.01224	-0.00336	-0.00985	0.01239	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.00109
191	H18	S	-0.15292	-0.03680	-0.09506	0.10254	0.00000
192	H18	S	0.53293	-0.39746	0.38803	-0.21731	0.00000
193	H18	PX	-0.00288	-0.01181	0.01311	0.00578	0.00000
194	H18	PY	0.01580	-0.00276	0.01319	-0.00409	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	-0.00191
196	C9	S	0.01261	0.00283	-0.00050	0.00303	0.00000
197	C9	S	-0.13042	-0.08604	-0.04005	0.01314	0.00000
198	C9	PX	0.25695	0.05664	0.06748	0.09728	0.00000
199	C9	PY	0.04496	0.21855	0.09266	-0.08915	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	-0.38886
201	C9	S	0.32476	0.14383	0.07442	-0.10641	0.00000
202	C9	PX	-0.44834	0.18276	0.00504	-0.01005	0.00000
203	C9	PY	0.08864	-0.28389	-0.20948	0.28886	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	1.03858
205	C9	DXX	0.00789	-0.01342	0.00167	-0.00501	0.00000
206	C9	DYY	0.00117	0.03289	0.00637	0.00875	0.00000
207	C9	DZZ	-0.00274	-0.03287	-0.01374	0.00322	0.00000
208	C9	DXY	0.02187	-0.00638	-0.00907	0.03039	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	-0.03675
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.03229
211	H3	S	-0.01668	0.14942	0.05198	-0.04958	0.00000
212	H3	S	-0.18083	-0.07693	0.04829	-0.11050	0.00000
213	H3	PX	0.00844	0.00414	-0.00012	0.00635	0.00000
214	H3	PY	0.00756	-0.00473	-0.00342	0.00914	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.01690
216	H5	S	0.04061	-0.07852	-0.01623	-0.00513	0.26634
217	H5	S	0.01372	-0.11491	-0.06462	0.03506	0.28097
218	H5	PX	-0.00073	0.00428	0.00346	-0.00686	-0.00126
219	H5	PY	0.00601	-0.01022	-0.00381	0.00692	0.00358
220	H5	PZ	0.00290	0.00534	0.00467	0.00492	0.01944
221	H7	S	0.04061	-0.07852	-0.01623	-0.00513	-0.26634
222	H7	S	0.01372	-0.11491	-0.06462	0.03506	-0.28097
223	H7	PX	-0.00073	0.00428	0.00346	-0.00686	0.00126
224	H7	PY	0.00601	-0.01022	-0.00381	0.00692	-0.00358
225	H7	PZ	-0.00290	-0.00534	-0.00467	-0.00492	0.01944

M0:	71	72	73	74	75
Eigenvalues:	0.74659	0.74936	0.75623	0.77139	0.78976
(ev):	20.31564	20.39120	20.57810	20.99055	21.49039

		A	A	A	A	A	
1	H1	S	0.00000	0.01786	0.04667	0.00000	-0.33877
2	H1	S	0.00000	0.25864	0.15780	0.00000	-0.38812
3	H1	PX	0.00000	0.01043	0.00589	0.00000	-0.01791
4	H1	PY	0.00000	0.00294	0.00165	0.00000	0.00102
5	H1	PZ	-0.00619	0.00000	0.00000	-0.00128	0.00000
6	C1	S	0.00000	0.00295	-0.00666	0.00000	-0.04424
7	C1	S	0.00000	0.18971	0.22697	0.00000	-0.21474
8	C1	PX	0.00000	-0.08825	0.01120	0.00000	-0.08771
9	C1	PY	0.00000	-0.14588	-0.34666	0.00000	-0.13472
10	C1	PZ	-0.13790	0.00000	0.00000	-0.02067	0.00000

11	C1	S	0.00000	-0.18013	-0.66310	0.00000	0.58356
12	C1	PX	0.00000	0.25814	-0.01426	0.00000	0.53620
13	C1	PY	0.00000	-0.97803	-0.16037	0.00000	-0.33202
14	C1	PZ	0.15321	0.00000	0.00000	-0.00236	0.00000
15	C1	DXX	0.00000	0.01825	0.04551	0.00000	-0.07313
16	C1	DYY	0.00000	0.03195	-0.00609	0.00000	-0.07239
17	C1	DZZ	0.00000	0.00304	0.01334	0.00000	0.03701
18	C1	DXY	0.00000	0.00163	-0.01295	0.00000	-0.02663
19	C1	DXZ	-0.00189	0.00000	0.00000	0.00180	0.00000
20	C1	DYZ	-0.00764	0.00000	0.00000	-0.00743	0.00000
21	C2	S	0.00000	-0.03906	0.06265	0.00000	0.00416
22	C2	S	0.00000	-0.13306	0.00410	0.00000	0.14159
23	C2	PX	0.00000	0.10459	-0.25475	0.00000	0.11007
24	C2	PY	0.00000	-0.23276	0.30301	0.00000	-0.14977
25	C2	PZ	-0.26567	0.00000	0.00000	-0.36375	0.00000
26	C2	S	0.00000	1.01820	-0.42117	0.00000	-0.10384
27	C2	PX	0.00000	0.06812	-0.25035	0.00000	-0.08450
28	C2	PY	0.00000	2.22504	-0.70717	0.00000	0.29131
29	C2	PZ	0.18913	0.00000	0.00000	0.33126	0.00000
30	C2	DXX	0.00000	-0.05115	0.05102	0.00000	0.01539
31	C2	DYY	0.00000	-0.03044	0.05394	0.00000	0.05213
32	C2	DZZ	0.00000	0.02321	-0.05306	0.00000	-0.01351
33	C2	DXY	0.00000	-0.01454	-0.01605	0.00000	-0.00792
34	C2	DXZ	-0.01662	0.00000	0.00000	-0.01358	0.00000
35	C2	DYZ	-0.01218	0.00000	0.00000	-0.02867	0.00000
36	C3	S	0.00000	-0.01941	0.07731	0.00000	0.00138
37	C3	S	0.00000	0.17429	0.22161	0.00000	-0.15355
38	C3	PX	0.00000	-0.03611	0.17400	0.00000	-0.26829
39	C3	PY	0.00000	-0.06865	-0.12336	0.00000	-0.23862
40	C3	PZ	-0.26519	0.00000	0.00000	-0.02789	0.00000
41	C3	S	0.00000	1.50361	-1.29506	0.00000	0.25350
42	C3	PX	0.00000	-0.97332	-0.15550	0.00000	-0.03327
43	C3	PY	0.00000	-1.65632	0.65957	0.00000	-0.42889
44	C3	PZ	0.14269	0.00000	0.00000	0.06319	0.00000
45	C3	DXX	0.00000	0.00466	0.08622	0.00000	-0.02192
46	C3	DYY	0.00000	0.06131	0.07520	0.00000	0.00199
47	C3	DZZ	0.00000	-0.00113	-0.05252	0.00000	-0.00482
48	C3	DXY	0.00000	0.01593	0.00006	0.00000	0.05169
49	C3	DXZ	-0.00580	0.00000	0.00000	0.01678	0.00000
50	C3	DYZ	0.02275	0.00000	0.00000	-0.01582	0.00000
51	C4	S	0.00000	0.03318	-0.00644	0.00000	0.02109
52	C4	S	0.00000	-0.11281	-0.16887	0.00000	-0.45775
53	C4	PX	0.00000	0.16508	0.00585	0.00000	-0.16318
54	C4	PY	0.00000	-0.08252	-0.12508	0.00000	-0.28989
55	C4	PZ	-0.00708	0.00000	0.00000	-0.21618	0.00000
56	C4	S	0.00000	0.33029	0.27333	0.00000	0.98382
57	C4	PX	0.00000	0.80911	0.61746	0.00000	0.40337
58	C4	PY	0.00000	-0.19591	0.52436	0.00000	0.08768
59	C4	PZ	-0.11190	0.00000	0.00000	0.15656	0.00000
60	C4	DXX	0.00000	0.04429	-0.06945	0.00000	-0.02809
61	C4	DYY	0.00000	0.00771	0.01824	0.00000	0.01041
62	C4	DZZ	0.00000	-0.02975	0.00185	0.00000	-0.02739
63	C4	DXY	0.00000	0.04418	0.02322	0.00000	0.00091
64	C4	DXZ	-0.01448	0.00000	0.00000	0.00587	0.00000

65	C4	DYZ	0.00626	0.00000	0.00000	-0.00011	0.00000
66	C5	S	0.00000	-0.02105	-0.01475	0.00000	-0.00715
67	C5	S	0.00000	-0.00781	0.20775	0.00000	0.07749
68	C5	PX	0.00000	0.35951	-0.15337	0.00000	0.08008
69	C5	PY	0.00000	0.25831	-0.22839	0.00000	-0.07583
70	C5	PZ	-0.27032	0.00000	0.00000	-0.39111	0.00000
71	C5	S	0.00000	-1.24815	0.70698	0.00000	-0.12047
72	C5	PX	0.00000	0.38958	0.63800	0.00000	-0.18167
73	C5	PY	0.00000	1.00719	-0.09551	0.00000	0.27317
74	C5	PZ	0.25202	0.00000	0.00000	0.32177	0.00000
75	C5	DXX	0.00000	-0.04017	0.03173	0.00000	0.01751
76	C5	DYY	0.00000	-0.04493	0.01267	0.00000	-0.02845
77	C5	DZZ	0.00000	0.03737	0.00331	0.00000	0.01220
78	C5	DXY	0.00000	0.00702	0.01479	0.00000	-0.00973
79	C5	DXZ	0.00728	0.00000	0.00000	-0.00680	0.00000
80	C5	DYZ	0.01995	0.00000	0.00000	0.02882	0.00000
81	C6	S	0.00000	0.02909	-0.07405	0.00000	0.02788
82	C6	S	0.00000	-0.11572	0.37076	0.00000	0.29849
83	C6	PX	0.00000	-0.06517	0.04683	0.00000	-0.03619
84	C6	PY	0.00000	0.03806	0.30733	0.00000	0.09183
85	C6	PZ	-0.28922	0.00000	0.00000	-0.04337	0.00000
86	C6	S	0.00000	-0.03697	-0.07768	0.00000	-1.23083
87	C6	PX	0.00000	-1.69422	0.31665	0.00000	-0.22166
88	C6	PY	0.00000	-0.63205	0.10215	0.00000	0.55391
89	C6	PZ	0.21552	0.00000	0.00000	-0.03109	0.00000
90	C6	DXX	0.00000	0.02883	0.00062	0.00000	0.09978
91	C6	DYY	0.00000	-0.01194	-0.01906	0.00000	-0.00828
92	C6	DZZ	0.00000	-0.01264	0.04237	0.00000	-0.01246
93	C6	DXY	0.00000	-0.03877	0.03541	0.00000	-0.00772
94	C6	DXZ	0.00153	0.00000	0.00000	-0.00610	0.00000
95	C6	DYZ	0.00090	0.00000	0.00000	-0.01170	0.00000
96	C7	S	0.00000	0.05252	-0.00042	0.00000	-0.00480
97	C7	S	0.00000	0.03147	0.25086	0.00000	-0.27617
98	C7	PX	0.00000	0.10139	-0.03520	0.00000	0.01647
99	C7	PY	0.00000	0.15158	0.36029	0.00000	-0.12944
100	C7	PZ	-0.31421	0.00000	0.00000	0.46153	0.00000
101	C7	S	0.00000	-1.89340	0.57830	0.00000	0.23888
102	C7	PX	0.00000	1.61096	-0.39612	0.00000	0.30806
103	C7	PY	0.00000	-0.05182	-0.08851	0.00000	0.03717
104	C7	PZ	0.26234	0.00000	0.00000	-0.38629	0.00000
105	C7	DXX	0.00000	0.06418	0.04741	0.00000	-0.01315
106	C7	DYY	0.00000	-0.02643	0.04027	0.00000	-0.04424
107	C7	DZZ	0.00000	-0.02317	-0.01778	0.00000	-0.00934
108	C7	DXY	0.00000	-0.01101	0.01148	0.00000	-0.01733
109	C7	DXZ	0.02040	0.00000	0.00000	-0.01090	0.00000
110	C7	DYZ	-0.01302	0.00000	0.00000	0.00037	0.00000
111	O1	S	0.00000	-0.01422	0.00294	0.00000	-0.01105
112	O1	S	0.00000	0.11774	0.00883	0.00000	0.07925
113	O1	PX	0.00000	0.15663	0.11156	0.00000	-0.08539
114	O1	PY	0.00000	-0.02240	-0.01012	0.00000	-0.08217
115	O1	PZ	0.10989	0.00000	0.00000	0.01526	0.00000
116	O1	S	0.00000	-0.38667	-0.41096	0.00000	-0.12953
117	O1	PX	0.00000	-0.17666	-0.08784	0.00000	-0.03609
118	O1	PY	0.00000	-0.09418	0.19575	0.00000	0.09936

119	O1	PZ	0.17474	0.00000	0.00000	0.03723	0.00000
120	O1	DXX	0.00000	-0.03103	-0.01722	0.00000	0.06269
121	O1	DYY	0.00000	-0.00555	-0.04652	0.00000	-0.05735
122	O1	DZZ	0.00000	0.05339	0.02973	0.00000	0.03499
123	O1	DXY	0.00000	-0.07272	-0.03263	0.00000	0.00006
124	O1	DXZ	0.01078	0.00000	0.00000	-0.00032	0.00000
125	O1	DYZ	-0.01093	0.00000	0.00000	0.00823	0.00000
126	H4	S	0.00000	-0.17371	0.01827	0.00000	-0.07669
127	H4	S	0.00000	-0.04965	0.29580	0.00000	-0.15551
128	H4	PX	0.00000	0.01262	0.01047	0.00000	-0.00451
129	H4	PY	0.00000	-0.01004	0.00841	0.00000	-0.00030
130	H4	PZ	-0.00373	0.00000	0.00000	-0.00125	0.00000
131	N1	S	0.00000	0.00707	-0.00164	0.00000	-0.00874
132	N1	S	0.00000	0.01531	-0.09166	0.00000	0.02701
133	N1	PX	0.00000	-0.10136	-0.01403	0.00000	-0.15133
134	N1	PY	0.00000	-0.04224	-0.13857	0.00000	-0.01193
135	N1	PZ	-0.08089	0.00000	0.00000	0.08546	0.00000
136	N1	S	0.00000	-0.76198	0.52654	0.00000	0.57432
137	N1	PX	0.00000	0.06385	0.12382	0.00000	-0.01809
138	N1	PY	0.00000	-0.31884	0.30071	0.00000	0.57721
139	N1	PZ	0.00180	0.00000	0.00000	0.02094	0.00000
140	N1	DXX	0.00000	0.02142	0.00522	0.00000	0.03358
141	N1	DYY	0.00000	-0.02578	-0.00933	0.00000	0.02857
142	N1	DZZ	0.00000	0.01694	-0.02578	0.00000	-0.01779
143	N1	DXY	0.00000	0.01225	-0.02550	0.00000	-0.01648
144	N1	DXZ	-0.00808	0.00000	0.00000	-0.00045	0.00000
145	N1	DYZ	-0.01897	0.00000	0.00000	0.00181	0.00000
146	H6	S	0.00000	-0.17789	0.17405	0.00000	-0.01821
147	H6	S	0.00000	0.31468	-0.27155	0.00000	0.08003
148	H6	PX	0.00000	0.01253	-0.01309	0.00000	-0.00636
149	H6	PY	0.00000	0.01767	-0.00534	0.00000	0.00360
150	H6	PZ	-0.00108	0.00000	0.00000	-0.00212	0.00000
151	C8	S	0.00000	-0.02783	-0.01809	0.00000	-0.01677
152	C8	S	0.00000	0.04108	0.18952	0.00000	-0.04256
153	C8	PX	0.00000	0.02424	-0.05352	0.00000	-0.21254
154	C8	PY	0.00000	0.02849	0.10280	0.00000	-0.01250
155	C8	PZ	-0.20251	0.00000	0.00000	0.32522	0.00000
156	C8	S	0.00000	0.68604	-0.50138	0.00000	0.23690
157	C8	PX	0.00000	0.30456	0.12555	0.00000	-0.09083
158	C8	PY	0.00000	1.41085	-0.36785	0.00000	0.09925
159	C8	PZ	0.10206	0.00000	0.00000	-0.22853	0.00000
160	C8	DXX	0.00000	-0.02451	0.00652	0.00000	-0.01733
161	C8	DYY	0.00000	0.01935	-0.01194	0.00000	-0.00877
162	C8	DZZ	0.00000	0.01163	0.01788	0.00000	0.00752
163	C8	DXY	0.00000	-0.03008	-0.00836	0.00000	0.01759
164	C8	DXZ	-0.00820	0.00000	0.00000	0.01648	0.00000
165	C8	DYZ	0.01074	0.00000	0.00000	-0.02827	0.00000
166	H8	S	0.00000	0.22018	0.05915	0.00000	-0.08471
167	H8	S	0.00000	-0.88019	0.11050	0.00000	-0.30648
168	H8	PX	0.00000	0.01775	0.00969	0.00000	-0.00155
169	H8	PY	0.00000	-0.00400	0.00009	0.00000	-0.00174
170	H8	PZ	-0.00336	0.00000	0.00000	0.00920	0.00000
171	C10	S	0.00000	0.00318	0.00366	0.00000	0.00044
172	C10	S	0.00000	0.01084	-0.02804	0.00000	-0.06510

173	C10	PX	0.00000	-0.06136	-0.04517	0.00000	-0.04914
174	C10	PY	0.00000	0.06382	-0.09214	0.00000	-0.05434
175	C10	PZ	-0.28450	0.00000	0.00000	0.64844	0.00000
176	C10	S	0.00000	0.69607	-0.13941	0.00000	0.08103
177	C10	PX	0.00000	-0.20092	0.10698	0.00000	0.22343
178	C10	PY	0.00000	0.21825	0.13750	0.00000	0.20121
179	C10	PZ	0.26010	0.00000	0.00000	-0.58269	0.00000
180	C10	DXX	0.00000	-0.00751	-0.00641	0.00000	-0.00382
181	C10	DYY	0.00000	0.01633	0.00914	0.00000	-0.00854
182	C10	DZZ	0.00000	0.00244	-0.00517	0.00000	-0.00061
183	C10	DXY	0.00000	0.02767	0.02619	0.00000	-0.00579
184	C10	DXZ	0.00630	0.00000	0.00000	-0.01044	0.00000
185	C10	DYZ	-0.01699	0.00000	0.00000	0.02751	0.00000
186	H16	S	0.00000	-0.07778	-0.05736	0.00000	-0.01368
187	H16	S	0.00000	0.19577	0.03101	0.00000	-0.11026
188	H16	PX	0.00000	0.00461	0.00108	0.00000	0.00528
189	H16	PY	0.00000	0.00410	0.00813	0.00000	0.00409
190	H16	PZ	-0.00341	0.00000	0.00000	0.00925	0.00000
191	H18	S	0.00000	0.08509	0.11536	0.00000	0.03244
192	H18	S	0.00000	-0.12631	0.02167	0.00000	0.20076
193	H18	PX	0.00000	-0.00009	0.00518	0.00000	0.00710
194	H18	PY	0.00000	-0.01243	-0.00665	0.00000	-0.00141
195	H18	PZ	-0.00512	0.00000	0.00000	0.01215	0.00000
196	C9	S	0.00000	0.01713	0.01140	0.00000	0.00643
197	C9	S	0.00000	-0.21008	-0.09373	0.00000	0.04466
198	C9	PX	0.00000	0.44790	0.16778	0.00000	-0.19420
199	C9	PY	0.00000	0.13925	0.09299	0.00000	0.18039
200	C9	PZ	0.51230	0.00000	0.00000	0.16317	0.00000
201	C9	S	0.00000	0.35114	0.11523	0.00000	-0.13970
202	C9	PX	0.00000	-0.69038	-0.09987	0.00000	0.41417
203	C9	PY	0.00000	-0.07685	-0.00533	0.00000	-0.39658
204	C9	PZ	-1.21351	0.00000	0.00000	-0.38146	0.00000
205	C9	DXX	0.00000	0.02163	0.00539	0.00000	-0.03861
206	C9	DYY	0.00000	-0.01038	0.02469	0.00000	0.10200
207	C9	DZZ	0.00000	-0.01177	-0.02300	0.00000	-0.04292
208	C9	DXY	0.00000	0.04128	0.02606	0.00000	-0.00153
209	C9	DXZ	0.03546	0.00000	0.00000	0.01087	0.00000
210	C9	DYZ	-0.04599	0.00000	0.00000	-0.01677	0.00000
211	H3	S	0.00000	-0.01034	0.06264	0.00000	0.33631
212	H3	S	0.00000	-0.10329	-0.13773	0.00000	-0.07031
213	H3	PX	0.00000	0.01506	0.00940	0.00000	0.00911
214	H3	PY	0.00000	0.00465	0.00455	0.00000	0.00486
215	H3	PZ	-0.02192	0.00000	0.00000	-0.00833	0.00000
216	H5	S	-0.29670	0.05861	-0.03654	-0.09153	-0.16146
217	H5	S	-0.25033	0.04521	-0.00697	-0.06997	0.02982
218	H5	PX	0.00946	0.00260	0.00059	0.00418	-0.00024
219	H5	PY	0.00277	0.01319	-0.00128	0.00239	-0.02371
220	H5	PZ	-0.02735	0.00731	0.00747	-0.00903	0.00242
221	H7	S	0.29670	0.05861	-0.03654	0.09153	-0.16146
222	H7	S	0.25033	0.04521	-0.00697	0.06997	0.02982
223	H7	PX	-0.00946	0.00260	0.00059	-0.00418	-0.00024
224	H7	PY	-0.00277	0.01319	-0.00128	-0.00239	-0.02371
225	H7	PZ	-0.02735	-0.00731	-0.00747	-0.00903	-0.00242

MO:	76	77	78	79	80
Eigenvalues:	0.79398	0.81386	0.81512	0.81972	0.84843
(ev):	21.60542	22.14624	22.18057	22.30575	23.08688

		A	A	A	A	A	
1	H1	S	0.02840	0.00000	-0.02220	0.13827	0.00000
2	H1	S	0.03542	0.00000	-0.08125	-0.11507	0.00000
3	H1	PX	0.00215	0.00000	-0.00685	0.00359	0.00000
4	H1	PY	0.00859	0.00000	0.01078	0.00794	0.00000
5	H1	PZ	0.00000	-0.00455	0.00000	0.00000	-0.00116
6	C1	S	-0.02650	0.00000	0.00384	0.03057	0.00000
7	C1	S	0.00182	0.00000	-0.34518	-0.17788	0.00000
8	C1	PX	-0.08284	0.00000	0.05447	0.12238	0.00000
9	C1	PY	0.00609	0.00000	0.11568	0.11422	0.00000
10	C1	PZ	0.00000	-0.59400	0.00000	0.00000	-0.30439
11	C1	S	0.71472	0.00000	0.62580	0.25262	0.00000
12	C1	PX	-0.39540	0.00000	-0.21370	-0.08153	0.00000
13	C1	PY	0.31985	0.00000	0.20750	-0.10674	0.00000
14	C1	PZ	0.00000	0.60741	0.00000	0.00000	0.29751
15	C1	DXX	-0.00109	0.00000	-0.02891	0.03974	0.00000
16	C1	DYY	-0.01808	0.00000	-0.03533	-0.01918	0.00000
17	C1	DZZ	0.00980	0.00000	-0.01037	-0.02617	0.00000
18	C1	DXY	0.04578	0.00000	0.00179	-0.00900	0.00000
19	C1	DXZ	0.00000	0.02903	0.00000	0.00000	0.02749
20	C1	DYZ	0.00000	0.00749	0.00000	0.00000	-0.01865
21	C2	S	0.00246	0.00000	-0.02105	-0.01981	0.00000
22	C2	S	0.42459	0.00000	0.29734	0.06648	0.00000
23	C2	PX	0.13939	0.00000	-0.03542	0.03984	0.00000
24	C2	PY	-0.05631	0.00000	0.30941	-0.10373	0.00000
25	C2	PZ	0.00000	0.39949	0.00000	0.00000	0.34998
26	C2	S	-0.73535	0.00000	0.55690	0.35392	0.00000
27	C2	PX	0.13231	0.00000	0.51129	0.51342	0.00000
28	C2	PY	-0.38125	0.00000	0.53304	0.32520	0.00000
29	C2	PZ	0.00000	-0.36451	0.00000	0.00000	-0.34422
30	C2	DXX	0.04130	0.00000	0.04651	-0.02133	0.00000
31	C2	DYY	0.05534	0.00000	0.00926	0.03181	0.00000
32	C2	DZZ	0.00293	0.00000	0.00456	0.00804	0.00000
33	C2	DXY	-0.00193	0.00000	-0.02521	0.00105	0.00000
34	C2	DXZ	0.00000	0.02436	0.00000	0.00000	0.02197
35	C2	DYZ	0.00000	0.02176	0.00000	0.00000	-0.02819
36	C3	S	0.01658	0.00000	-0.05583	-0.06316	0.00000
37	C3	S	0.02811	0.00000	-0.30291	0.37524	0.00000
38	C3	PX	-0.27998	0.00000	0.13563	0.09471	0.00000
39	C3	PY	0.06304	0.00000	0.04101	-0.16229	0.00000
40	C3	PZ	0.00000	-0.28737	0.00000	0.00000	0.21913
41	C3	S	-1.35894	0.00000	1.60593	0.69218	0.00000
42	C3	PX	-0.19306	0.00000	0.11486	-0.13526	0.00000
43	C3	PY	0.68377	0.00000	-0.66720	-0.32876	0.00000
44	C3	PZ	0.00000	0.15150	0.00000	0.00000	-0.18422
45	C3	DXX	-0.02329	0.00000	-0.06502	0.03381	0.00000
46	C3	DYY	0.00913	0.00000	-0.07191	-0.01933	0.00000
47	C3	DZZ	0.01050	0.00000	0.03372	0.02682	0.00000
48	C3	DXY	-0.03146	0.00000	0.01258	0.02477	0.00000
49	C3	DXZ	0.00000	-0.00260	0.00000	0.00000	-0.00812

50	C3	DYZ	0.00000	-0.00154	0.00000	0.00000	-0.01821
51	C4	S	0.00632	0.00000	-0.01025	-0.01935	0.00000
52	C4	S	0.03072	0.00000	0.12745	-0.30071	0.00000
53	C4	PX	-0.23354	0.00000	-0.35787	-0.00115	0.00000
54	C4	PY	0.05978	0.00000	-0.24421	-0.37485	0.00000
55	C4	PZ	0.00000	-0.02103	0.00000	0.00000	-0.42796
56	C4	S	-0.16443	0.00000	-0.52527	0.66870	0.00000
57	C4	PX	-0.56683	0.00000	0.00133	-0.22838	0.00000
58	C4	PY	0.56211	0.00000	-0.19709	0.40413	0.00000
59	C4	PZ	0.00000	0.00723	0.00000	0.00000	0.44037
60	C4	DXX	0.01552	0.00000	-0.01237	-0.09334	0.00000
61	C4	DYY	0.01088	0.00000	0.01284	0.02129	0.00000
62	C4	DZZ	0.00014	0.00000	0.01580	0.00653	0.00000
63	C4	DXY	-0.00045	0.00000	0.01163	0.01076	0.00000
64	C4	DXZ	0.00000	-0.03801	0.00000	0.00000	-0.00303
65	C4	DYZ	0.00000	0.02438	0.00000	0.00000	0.02415
66	C5	S	0.02072	0.00000	0.08017	0.01417	0.00000
67	C5	S	0.27094	0.00000	0.23584	-0.22059	0.00000
68	C5	PX	-0.03198	0.00000	-0.17934	-0.21673	0.00000
69	C5	PY	-0.02721	0.00000	0.05375	-0.06915	0.00000
70	C5	PZ	0.00000	0.26688	0.00000	0.00000	-0.33736
71	C5	S	-0.36082	0.00000	-1.49611	-0.31082	0.00000
72	C5	PX	-0.32577	0.00000	0.13141	-0.07889	0.00000
73	C5	PY	-0.52719	0.00000	0.73648	0.34140	0.00000
74	C5	PZ	0.00000	-0.27442	0.00000	0.00000	0.32998
75	C5	DXX	0.04238	0.00000	0.09981	-0.01100	0.00000
76	C5	DYY	0.04448	0.00000	0.08961	-0.04735	0.00000
77	C5	DZZ	-0.01265	0.00000	-0.06081	-0.00580	0.00000
78	C5	DXY	0.00318	0.00000	0.00220	-0.02829	0.00000
79	C5	DXZ	0.00000	0.01324	0.00000	0.00000	-0.02112
80	C5	DYZ	0.00000	-0.03595	0.00000	0.00000	-0.01259
81	C6	S	0.02314	0.00000	-0.00331	0.02492	0.00000
82	C6	S	0.24805	0.00000	-0.27694	0.23650	0.00000
83	C6	PX	-0.13659	0.00000	-0.14130	-0.05060	0.00000
84	C6	PY	-0.17443	0.00000	0.06973	-0.27843	0.00000
85	C6	PZ	0.00000	0.07776	0.00000	0.00000	0.48543
86	C6	S	-0.09771	0.00000	0.18065	-0.68935	0.00000
87	C6	PX	0.41986	0.00000	-0.19137	-0.16602	0.00000
88	C6	PY	-0.21704	0.00000	-0.36112	-0.13320	0.00000
89	C6	PZ	0.00000	-0.07347	0.00000	0.00000	-0.47453
90	C6	DXX	0.05608	0.00000	-0.06802	0.05182	0.00000
91	C6	DYY	0.03906	0.00000	-0.02251	0.01894	0.00000
92	C6	DZZ	-0.01501	0.00000	0.00820	-0.01274	0.00000
93	C6	DXY	-0.00642	0.00000	-0.00707	0.00341	0.00000
94	C6	DXZ	0.00000	-0.01643	0.00000	0.00000	-0.00734
95	C6	DYZ	0.00000	-0.00284	0.00000	0.00000	0.01865
96	C7	S	-0.03668	0.00000	0.02300	0.08130	0.00000
97	C7	S	-0.29411	0.00000	-0.05353	0.19937	0.00000
98	C7	PX	0.04490	0.00000	0.02113	0.10928	0.00000
99	C7	PY	0.21340	0.00000	-0.27114	-0.10568	0.00000
100	C7	PZ	0.00000	-0.40536	0.00000	0.00000	0.21539
101	C7	S	1.40513	0.00000	-1.10053	-1.31108	0.00000
102	C7	PX	-0.69500	0.00000	0.64875	0.46094	0.00000
103	C7	PY	0.71217	0.00000	-0.23841	0.00825	0.00000

104	C7	PZ	0.00000	0.48071	0.00000	0.00000	-0.14824
105	C7	DXX	-0.08594	0.00000	0.00757	0.07973	0.00000
106	C7	DYY	-0.03001	0.00000	-0.01342	0.10492	0.00000
107	C7	DZZ	0.01954	0.00000	0.00338	-0.05519	0.00000
108	C7	DXY	0.01884	0.00000	-0.01828	0.00312	0.00000
109	C7	DXZ	0.00000	0.02906	0.00000	0.00000	-0.00720
110	C7	DYZ	0.00000	-0.00059	0.00000	0.00000	0.00013
111	O1	S	0.00032	0.00000	-0.02172	-0.00459	0.00000
112	O1	S	0.08432	0.00000	0.13436	0.02993	0.00000
113	O1	PX	0.16872	0.00000	0.18121	0.04093	0.00000
114	O1	PY	0.04880	0.00000	0.02651	-0.11391	0.00000
115	O1	PZ	0.00000	-0.01266	0.00000	0.00000	-0.08163
116	O1	S	-0.53726	0.00000	-0.14228	-0.27372	0.00000
117	O1	PX	0.02396	0.00000	-0.10484	0.06555	0.00000
118	O1	PY	0.08550	0.00000	-0.22172	0.05775	0.00000
119	O1	PZ	0.00000	0.03108	0.00000	0.00000	0.03991
120	O1	DXX	-0.03552	0.00000	-0.02867	0.02386	0.00000
121	O1	DYY	0.01809	0.00000	0.00275	-0.08048	0.00000
122	O1	DZZ	0.04770	0.00000	0.05414	0.04070	0.00000
123	O1	DXY	-0.03289	0.00000	-0.03882	-0.00906	0.00000
124	O1	DXZ	0.00000	0.01784	0.00000	0.00000	0.00520
125	O1	DYZ	0.00000	-0.00539	0.00000	0.00000	0.01154
126	H4	S	0.08880	0.00000	0.28539	0.01787	0.00000
127	H4	S	0.12619	0.00000	-0.15453	-0.28611	0.00000
128	H4	PX	-0.00310	0.00000	-0.00473	0.00609	0.00000
129	H4	PY	0.00465	0.00000	0.01932	0.00220	0.00000
130	H4	PZ	0.00000	-0.00595	0.00000	0.00000	-0.00393
131	N1	S	0.00403	0.00000	-0.00089	0.01267	0.00000
132	N1	S	0.00089	0.00000	0.03261	-0.04696	0.00000
133	N1	PX	0.04230	0.00000	0.02997	-0.04100	0.00000
134	N1	PY	0.06357	0.00000	-0.03564	0.12805	0.00000
135	N1	PZ	0.00000	0.13439	0.00000	0.00000	0.13369
136	N1	S	-0.04827	0.00000	-0.42442	0.05288	0.00000
137	N1	PX	0.08685	0.00000	-0.11865	0.13840	0.00000
138	N1	PY	-0.29893	0.00000	-0.12868	-0.30033	0.00000
139	N1	PZ	0.00000	-0.05387	0.00000	0.00000	0.00262
140	N1	DXX	-0.04190	0.00000	0.00918	-0.03036	0.00000
141	N1	DYY	0.02296	0.00000	-0.02264	0.03528	0.00000
142	N1	DZZ	0.00879	0.00000	0.01982	-0.03166	0.00000
143	N1	DXY	0.01165	0.00000	0.00641	0.00030	0.00000
144	N1	DXZ	0.00000	0.01634	0.00000	0.00000	0.01984
145	N1	DYZ	0.00000	0.01159	0.00000	0.00000	0.01629
146	H6	S	0.06823	0.00000	0.05642	-0.00999	0.00000
147	H6	S	0.21149	0.00000	0.35246	0.39355	0.00000
148	H6	PX	-0.00771	0.00000	-0.00156	0.00657	0.00000
149	H6	PY	-0.00392	0.00000	0.00327	0.00160	0.00000
150	H6	PZ	0.00000	0.00017	0.00000	0.00000	0.00312
151	C8	S	-0.02972	0.00000	0.03303	-0.04821	0.00000
152	C8	S	-0.53701	0.00000	0.17198	0.26498	0.00000
153	C8	PX	0.16477	0.00000	-0.02077	0.32616	0.00000
154	C8	PY	0.00445	0.00000	-0.06717	0.17482	0.00000
155	C8	PZ	0.00000	0.16225	0.00000	0.00000	0.19660
156	C8	S	0.94269	0.00000	-0.25310	0.15199	0.00000
157	C8	PX	0.34532	0.00000	-0.08399	0.17230	0.00000

158	C8	PY	-0.74691	0.00000	0.69385	0.04875	0.00000
159	C8	PZ	0.00000	-0.22681	0.00000	0.00000	-0.24304
160	C8	DXX	-0.04784	0.00000	0.02403	0.03091	0.00000
161	C8	DYY	-0.10876	0.00000	0.06038	-0.02279	0.00000
162	C8	DZZ	0.01333	0.00000	-0.01894	0.02440	0.00000
163	C8	DXY	-0.00756	0.00000	-0.00644	0.02540	0.00000
164	C8	DXZ	0.00000	-0.01152	0.00000	0.00000	-0.00740
165	C8	DYZ	0.00000	-0.04423	0.00000	0.00000	0.03261
166	H8	S	-0.21038	0.00000	0.09179	0.26167	0.00000
167	H8	S	0.33755	0.00000	-0.26704	-0.14738	0.00000
168	H8	PX	-0.01975	0.00000	0.00440	0.02166	0.00000
169	H8	PY	0.02075	0.00000	-0.00997	-0.00232	0.00000
170	H8	PZ	0.00000	0.00015	0.00000	0.00000	0.00374
171	C10	S	-0.00619	0.00000	0.00100	0.02000	0.00000
172	C10	S	-0.42047	0.00000	0.31220	-0.09482	0.00000
173	C10	PX	0.07998	0.00000	-0.04695	0.24388	0.00000
174	C10	PY	-0.22428	0.00000	0.20974	-0.21459	0.00000
175	C10	PZ	0.00000	0.47762	0.00000	0.00000	-0.48884
176	C10	S	-0.07050	0.00000	0.05089	-0.04912	0.00000
177	C10	PX	-0.16073	0.00000	-0.02351	-0.75725	0.00000
178	C10	PY	-0.33241	0.00000	0.09056	0.10536	0.00000
179	C10	PZ	0.00000	-0.44474	0.00000	0.00000	0.55813
180	C10	DXX	-0.08093	0.00000	0.05101	0.01308	0.00000
181	C10	DYY	-0.03804	0.00000	0.02949	0.00741	0.00000
182	C10	DZZ	0.00863	0.00000	-0.00089	-0.02073	0.00000
183	C10	DXY	0.00554	0.00000	0.00192	-0.02203	0.00000
184	C10	DXZ	0.00000	0.00189	0.00000	0.00000	-0.00215
185	C10	DYZ	0.00000	0.02291	0.00000	0.00000	0.00048
186	H16	S	-0.14138	0.00000	0.07748	0.21110	0.00000
187	H16	S	0.04524	0.00000	0.05448	0.30130	0.00000
188	H16	PX	-0.02136	0.00000	0.01201	-0.01609	0.00000
189	H16	PY	0.00307	0.00000	-0.00183	-0.01452	0.00000
190	H16	PZ	0.00000	0.00802	0.00000	0.00000	-0.00808
191	H18	S	-0.13001	0.00000	0.06995	-0.07815	0.00000
192	H18	S	-0.29837	0.00000	0.07772	-0.27716	0.00000
193	H18	PX	0.00794	0.00000	-0.00868	-0.01278	0.00000
194	H18	PY	0.01142	0.00000	-0.00638	0.00370	0.00000
195	H18	PZ	0.00000	0.00459	0.00000	0.00000	-0.00745
196	C9	S	0.01318	0.00000	0.02188	-0.00078	0.00000
197	C9	S	-0.16643	0.00000	-0.17775	0.00659	0.00000
198	C9	PX	0.37650	0.00000	0.37873	0.02036	0.00000
199	C9	PY	0.08221	0.00000	0.18471	-0.03736	0.00000
200	C9	PZ	0.00000	0.16172	0.00000	0.00000	0.19759
201	C9	S	0.20466	0.00000	0.21412	-0.04040	0.00000
202	C9	PX	-0.44843	0.00000	-0.53530	-0.00958	0.00000
203	C9	PY	0.02303	0.00000	-0.18449	0.13576	0.00000
204	C9	PZ	0.00000	-0.23287	0.00000	0.00000	-0.35931
205	C9	DXX	0.03182	0.00000	0.03011	-0.01955	0.00000
206	C9	DYY	-0.02583	0.00000	0.00970	0.02208	0.00000
207	C9	DZZ	-0.01142	0.00000	-0.02658	-0.00268	0.00000
208	C9	DXY	0.03203	0.00000	0.04092	0.02738	0.00000
209	C9	DXZ	0.00000	-0.00913	0.00000	0.00000	0.00036
210	C9	DYZ	0.00000	-0.01194	0.00000	0.00000	-0.02089
211	H3	S	-0.07516	0.00000	0.06196	0.03393	0.00000

212	H3	S	-0.03451	0.00000	-0.05247	-0.12164	0.00000
213	H3	PX	0.01072	0.00000	0.01877	0.00924	0.00000
214	H3	PY	0.00188	0.00000	0.00526	0.00823	0.00000
215	H3	PZ	0.00000	-0.00242	0.00000	0.00000	-0.00863
216	H5	S	0.04797	-0.01364	0.01401	-0.03885	-0.04682
217	H5	S	0.00210	-0.01284	0.07023	0.06829	-0.03726
218	H5	PX	0.00286	0.01153	0.00400	-0.00730	0.01377
219	H5	PY	0.01145	0.00574	0.00542	0.00322	0.00876
220	H5	PZ	0.00877	-0.01142	0.00855	0.00201	-0.01339
221	H7	S	0.04797	0.01364	0.01401	-0.03885	0.04682
222	H7	S	0.00210	0.01284	0.07023	0.06829	0.03726
223	H7	PX	0.00286	-0.01153	0.00400	-0.00730	-0.01377
224	H7	PY	0.01145	-0.00574	0.00542	0.00322	-0.00876
225	H7	PZ	-0.00877	-0.01142	-0.00855	-0.00201	-0.01339

MO:	81	82	83	84	85
Eigenvalues:	0.85238	0.87614	0.87640	0.89436	0.91131
(ev):	23.19457	23.84103	23.84796	24.33683	24.79810

		A	A	A	A	A	
1	H1	S	0.09784	0.00000	-0.23481	0.00000	0.18368
2	H1	S	0.08025	0.00000	0.11908	0.00000	0.10641
3	H1	PX	0.00870	0.00000	-0.01304	0.00000	0.00979
4	H1	PY	0.01464	0.00000	-0.00181	0.00000	0.00124
5	H1	PZ	0.00000	0.00007	0.00000	-0.00276	0.00000
6	C1	S	0.01561	0.00000	-0.06156	0.00000	0.02476
7	C1	S	0.22409	0.00000	-0.06639	0.00000	0.16070
8	C1	PX	-0.13001	0.00000	-0.14963	0.00000	0.07363
9	C1	PY	0.23045	0.00000	-0.00669	0.00000	-0.09446
10	C1	PZ	0.00000	-0.10311	0.00000	0.47764	0.00000
11	C1	S	0.43231	0.00000	0.66852	0.00000	-0.21869
12	C1	PX	-0.61504	0.00000	-0.16032	0.00000	-0.40983
13	C1	PY	0.98470	0.00000	0.12024	0.00000	0.51449
14	C1	PZ	0.00000	-0.02551	0.00000	-0.69219	0.00000
15	C1	DXX	0.06674	0.00000	-0.08132	0.00000	0.06294
16	C1	DYY	0.03590	0.00000	-0.05118	0.00000	0.03670
17	C1	DZZ	-0.02139	0.00000	0.04968	0.00000	-0.01946
18	C1	DXY	0.00259	0.00000	0.01293	0.00000	-0.00017
19	C1	DXZ	0.00000	0.01191	0.00000	-0.01370	0.00000
20	C1	DYZ	0.00000	0.00720	0.00000	-0.00937	0.00000
21	C2	S	-0.03424	0.00000	-0.04866	0.00000	0.02237
22	C2	S	-0.11525	0.00000	-0.18517	0.00000	0.21413
23	C2	PX	0.06323	0.00000	0.01389	0.00000	0.08727
24	C2	PY	0.05394	0.00000	0.20276	0.00000	-0.25221
25	C2	PZ	0.00000	0.23750	0.00000	0.60821	0.00000
26	C2	S	-0.36495	0.00000	0.74084	0.00000	-0.88094
27	C2	PX	0.10714	0.00000	0.30583	0.00000	-0.17778
28	C2	PY	-1.74042	0.00000	-0.25637	0.00000	0.03092
29	C2	PZ	0.00000	-0.33700	0.00000	-0.89955	0.00000
30	C2	DXX	-0.06255	0.00000	-0.05028	0.00000	0.03773
31	C2	DYY	-0.04614	0.00000	-0.08882	0.00000	0.05088
32	C2	DZZ	0.02972	0.00000	0.03540	0.00000	-0.00785
33	C2	DXY	-0.02834	0.00000	0.01260	0.00000	0.01848
34	C2	DXZ	0.00000	0.03018	0.00000	0.00901	0.00000

35	C2	DYZ	0.00000	0.03606	0.00000	-0.01199	0.00000
36	C3	S	0.01964	0.00000	0.03054	0.00000	0.00526
37	C3	S	0.10749	0.00000	0.00850	0.00000	-0.13551
38	C3	PX	0.05601	0.00000	-0.05994	0.00000	0.00775
39	C3	PY	0.24774	0.00000	-0.27177	0.00000	0.20699
40	C3	PZ	0.00000	-0.10660	0.00000	-0.11645	0.00000
41	C3	S	-1.34345	0.00000	-0.09195	0.00000	-0.41714
42	C3	PX	0.80748	0.00000	0.31858	0.00000	0.26676
43	C3	PY	1.42970	0.00000	-0.11758	0.00000	0.55602
44	C3	PZ	0.00000	0.09814	0.00000	0.21658	0.00000
45	C3	DXX	0.07716	0.00000	0.03420	0.00000	-0.03557
46	C3	DYY	-0.02359	0.00000	0.01215	0.00000	-0.01130
47	C3	DZZ	-0.01561	0.00000	-0.02342	0.00000	0.01180
48	C3	DXY	0.00103	0.00000	0.00237	0.00000	0.00498
49	C3	DXZ	0.00000	0.01682	0.00000	-0.01210	0.00000
50	C3	DYZ	0.00000	-0.04407	0.00000	0.02090	0.00000
51	C4	S	0.02413	0.00000	0.02051	0.00000	-0.01158
52	C4	S	-0.15859	0.00000	0.07739	0.00000	-0.01085
53	C4	PX	-0.05495	0.00000	-0.20238	0.00000	0.12753
54	C4	PY	-0.44171	0.00000	0.36953	0.00000	-0.09656
55	C4	PZ	0.00000	-0.39994	0.00000	-0.26554	0.00000
56	C4	S	0.01235	0.00000	-0.34414	0.00000	-0.08849
57	C4	PX	-1.69996	0.00000	-0.25646	0.00000	-0.55625
58	C4	PY	1.57922	0.00000	-0.55078	0.00000	0.57315
59	C4	PZ	0.00000	0.67617	0.00000	0.34279	0.00000
60	C4	DXX	-0.00865	0.00000	0.06538	0.00000	-0.04269
61	C4	DYY	0.04377	0.00000	-0.02465	0.00000	0.02143
62	C4	DZZ	-0.02732	0.00000	-0.00763	0.00000	0.01071
63	C4	DXY	-0.01661	0.00000	-0.03058	0.00000	0.02222
64	C4	DXZ	0.00000	-0.01784	0.00000	0.03734	0.00000
65	C4	DYZ	0.00000	-0.01236	0.00000	-0.01208	0.00000
66	C5	S	0.00043	0.00000	0.03335	0.00000	-0.01857
67	C5	S	-0.22116	0.00000	-0.00719	0.00000	0.01489
68	C5	PX	-0.03823	0.00000	0.17434	0.00000	-0.09375
69	C5	PY	0.07424	0.00000	0.18762	0.00000	-0.11255
70	C5	PZ	0.00000	0.46553	0.00000	-0.50393	0.00000
71	C5	S	0.80954	0.00000	-0.50311	0.00000	0.17208
72	C5	PX	-0.95662	0.00000	-0.52267	0.00000	-0.01635
73	C5	PY	-1.53713	0.00000	0.10884	0.00000	-0.42465
74	C5	PZ	0.00000	-0.65053	0.00000	0.70076	0.00000
75	C5	DXX	-0.03980	0.00000	-0.01059	0.00000	-0.00305
76	C5	DYY	-0.01855	0.00000	0.06933	0.00000	-0.03776
77	C5	DZZ	0.00464	0.00000	-0.01489	0.00000	0.01454
78	C5	DXY	0.05185	0.00000	0.02387	0.00000	-0.03634
79	C5	DXZ	0.00000	0.01951	0.00000	-0.02823	0.00000
80	C5	DYZ	0.00000	-0.04022	0.00000	-0.02646	0.00000
81	C6	S	0.01053	0.00000	-0.00790	0.00000	-0.00063
82	C6	S	0.13540	0.00000	0.06339	0.00000	-0.00196
83	C6	PX	0.43682	0.00000	0.30853	0.00000	-0.05325
84	C6	PY	0.15271	0.00000	-0.20912	0.00000	-0.04044
85	C6	PZ	0.00000	-0.48219	0.00000	-0.09535	0.00000
86	C6	S	-0.70020	0.00000	-0.25069	0.00000	0.56499
87	C6	PX	1.23486	0.00000	-0.09528	0.00000	0.25634
88	C6	PY	0.34160	0.00000	0.16275	0.00000	0.07300

89	C6	PZ	0.00000	0.71731	0.00000	0.25094	0.00000
90	C6	DXX	-0.00502	0.00000	0.00448	0.00000	0.00576
91	C6	DYY	0.03737	0.00000	-0.01294	0.00000	-0.01980
92	C6	DZZ	-0.00286	0.00000	0.00556	0.00000	0.00661
93	C6	DXY	0.00041	0.00000	0.03309	0.00000	-0.02660
94	C6	DXZ	0.00000	-0.01070	0.00000	-0.00117	0.00000
95	C6	DYZ	0.00000	0.02370	0.00000	0.00975	0.00000
96	C7	S	-0.06178	0.00000	0.00764	0.00000	-0.03640
97	C7	S	-0.02343	0.00000	0.18641	0.00000	-0.36076
98	C7	PX	-0.04706	0.00000	-0.04896	0.00000	0.19145
99	C7	PY	-0.13242	0.00000	0.02304	0.00000	0.13235
100	C7	PZ	0.00000	0.60355	0.00000	-0.15546	0.00000
101	C7	S	1.82572	0.00000	-0.48436	0.00000	1.04408
102	C7	PX	-1.49090	0.00000	0.08057	0.00000	-0.95128
103	C7	PY	-0.03240	0.00000	-0.08161	0.00000	-0.04938
104	C7	PZ	0.00000	-0.85059	0.00000	-0.00833	0.00000
105	C7	DXX	-0.08790	0.00000	-0.00842	0.00000	-0.09595
106	C7	DYY	0.01833	0.00000	0.05876	0.00000	-0.05765
107	C7	DZZ	0.03232	0.00000	-0.00773	0.00000	0.03787
108	C7	DXY	0.01353	0.00000	0.00184	0.00000	0.00132
109	C7	DXZ	0.00000	-0.03506	0.00000	0.00570	0.00000
110	C7	DYZ	0.00000	-0.00181	0.00000	-0.00027	0.00000
111	O1	S	-0.00717	0.00000	-0.00169	0.00000	0.00676
112	O1	S	0.09103	0.00000	0.08217	0.00000	-0.05542
113	O1	PX	0.16988	0.00000	0.06838	0.00000	-0.02046
114	O1	PY	-0.12904	0.00000	0.10628	0.00000	-0.04851
115	O1	PZ	0.00000	0.01604	0.00000	-0.05199	0.00000
116	O1	S	-0.78626	0.00000	0.05441	0.00000	-0.14466
117	O1	PX	0.15651	0.00000	-0.04200	0.00000	0.11565
118	O1	PY	0.11852	0.00000	-0.09659	0.00000	0.14831
119	O1	PZ	0.00000	-0.06869	0.00000	-0.00518	0.00000
120	O1	DXX	0.01259	0.00000	-0.01748	0.00000	-0.00636
121	O1	DYY	-0.09578	0.00000	0.10010	0.00000	-0.04003
122	O1	DZZ	0.06589	0.00000	0.00535	0.00000	-0.00060
123	O1	DXY	-0.02507	0.00000	0.00564	0.00000	-0.00553
124	O1	DXZ	0.00000	0.01944	0.00000	-0.03078	0.00000
125	O1	DYZ	0.00000	0.02337	0.00000	0.00992	0.00000
126	H4	S	-0.21659	0.00000	0.07321	0.00000	-0.00380
127	H4	S	0.17630	0.00000	-0.13389	0.00000	0.04255
128	H4	PX	0.02334	0.00000	-0.00536	0.00000	-0.00168
129	H4	PY	-0.00680	0.00000	0.00999	0.00000	-0.00630
130	H4	PZ	0.00000	-0.00780	0.00000	-0.00252	0.00000
131	N1	S	-0.01260	0.00000	0.01581	0.00000	0.00699
132	N1	S	0.02038	0.00000	-0.06815	0.00000	0.00989
133	N1	PX	0.11042	0.00000	-0.05303	0.00000	-0.17831
134	N1	PY	0.10199	0.00000	0.04603	0.00000	-0.06151
135	N1	PZ	0.00000	-0.15115	0.00000	0.06565	0.00000
136	N1	S	0.55006	0.00000	0.40273	0.00000	-0.32647
137	N1	PX	-0.37202	0.00000	0.18751	0.00000	-0.04333
138	N1	PY	0.58911	0.00000	-0.04819	0.00000	-0.01638
139	N1	PZ	0.00000	-0.06299	0.00000	-0.22620	0.00000
140	N1	DXX	0.02146	0.00000	0.00995	0.00000	-0.01106
141	N1	DYY	-0.02181	0.00000	0.03966	0.00000	0.01327
142	N1	DZZ	-0.01889	0.00000	-0.04135	0.00000	0.02923

143	N1	DXY	0.00811	0.00000	-0.04159	0.00000	0.00867
144	N1	DXZ	0.00000	-0.02133	0.00000	-0.00054	0.00000
145	N1	DYZ	0.00000	-0.03640	0.00000	0.00054	0.00000
146	H6	S	-0.24512	0.00000	-0.16397	0.00000	0.14713
147	H6	S	-0.11608	0.00000	0.02561	0.00000	0.01340
148	H6	PX	0.01858	0.00000	0.00783	0.00000	-0.00672
149	H6	PY	0.00091	0.00000	0.00411	0.00000	-0.00853
150	H6	PZ	0.00000	-0.00967	0.00000	0.00170	0.00000
151	C8	S	0.02882	0.00000	-0.04853	0.00000	-0.04591
152	C8	S	0.00749	0.00000	0.43293	0.00000	0.09510
153	C8	PX	-0.20835	0.00000	-0.08793	0.00000	0.02292
154	C8	PY	-0.03254	0.00000	-0.11832	0.00000	-0.46663
155	C8	PZ	0.00000	-0.27001	0.00000	-0.44768	0.00000
156	C8	S	-0.55725	0.00000	-0.20012	0.00000	-0.06071
157	C8	PX	-0.54332	0.00000	0.39702	0.00000	-0.34087
158	C8	PY	-1.02123	0.00000	-0.33149	0.00000	0.05370
159	C8	PZ	0.00000	0.48300	0.00000	0.66663	0.00000
160	C8	DXX	0.02431	0.00000	0.05669	0.00000	-0.01864
161	C8	DYY	0.01403	0.00000	-0.04488	0.00000	-0.09506
162	C8	DZZ	-0.01649	0.00000	0.02926	0.00000	0.04281
163	C8	DXY	0.00963	0.00000	0.06314	0.00000	0.01108
164	C8	DXZ	0.00000	0.01257	0.00000	-0.00449	0.00000
165	C8	DYZ	0.00000	0.03293	0.00000	-0.01304	0.00000
166	H8	S	-0.29557	0.00000	-0.10073	0.00000	-0.11294
167	H8	S	0.85416	0.00000	0.12151	0.00000	0.48349
168	H8	PX	-0.02851	0.00000	-0.00394	0.00000	-0.02843
169	H8	PY	-0.00299	0.00000	0.00201	0.00000	0.01026
170	H8	PZ	0.00000	-0.00648	0.00000	-0.00451	0.00000
171	C10	S	-0.00860	0.00000	0.05513	0.00000	0.07885
172	C10	S	0.07080	0.00000	0.11322	0.00000	0.45964
173	C10	PX	-0.07025	0.00000	0.11399	0.00000	-0.02502
174	C10	PY	0.01753	0.00000	-0.39407	0.00000	-0.29143
175	C10	PZ	0.00000	-0.01667	0.00000	0.33851	0.00000
176	C10	S	-0.53161	0.00000	-0.92507	0.00000	-1.40023
177	C10	PX	0.52250	0.00000	-0.20005	0.00000	0.31852
178	C10	PY	-0.09412	0.00000	0.25380	0.00000	0.33500
179	C10	PZ	0.00000	-0.06091	0.00000	-0.51099	0.00000
180	C10	DXX	0.01349	0.00000	0.07318	0.00000	0.11999
181	C10	DYY	-0.02294	0.00000	0.07700	0.00000	0.16867
182	C10	DZZ	0.00682	0.00000	-0.05733	0.00000	-0.07052
183	C10	DXY	-0.03341	0.00000	-0.03045	0.00000	-0.00694
184	C10	DXZ	0.00000	-0.00664	0.00000	0.00720	0.00000
185	C10	DYZ	0.00000	-0.02679	0.00000	-0.01586	0.00000
186	H16	S	0.03736	0.00000	0.29469	0.00000	0.36124
187	H16	S	-0.31175	0.00000	0.05732	0.00000	-0.01681
188	H16	PX	0.00651	0.00000	0.00361	0.00000	0.02126
189	H16	PY	-0.00413	0.00000	-0.00812	0.00000	-0.01239
190	H16	PZ	0.00000	-0.00059	0.00000	0.00549	0.00000
191	H18	S	-0.06046	0.00000	0.19439	0.00000	0.43865
192	H18	S	0.33605	0.00000	0.09860	0.00000	0.31388
193	H18	PX	0.00753	0.00000	0.00132	0.00000	-0.00204
194	H18	PY	0.01369	0.00000	-0.00916	0.00000	-0.01708
195	H18	PZ	0.00000	0.00601	0.00000	0.00421	0.00000
196	C9	S	0.00492	0.00000	0.01228	0.00000	-0.00963

197	C9	S	-0.09949	0.00000	-0.02118	0.00000	-0.01051
198	C9	PX	0.22409	0.00000	0.15919	0.00000	-0.03529
199	C9	PY	-0.01130	0.00000	0.13336	0.00000	-0.06838
200	C9	PZ	0.00000	0.14791	0.00000	-0.08375	0.00000
201	C9	S	0.10245	0.00000	-0.03912	0.00000	0.05151
202	C9	PX	-0.27470	0.00000	-0.22414	0.00000	0.09281
203	C9	PY	0.21273	0.00000	-0.30930	0.00000	0.18107
204	C9	PZ	0.00000	-0.29104	0.00000	0.05261	0.00000
205	C9	DXX	-0.00263	0.00000	0.04381	0.00000	-0.01621
206	C9	DYY	0.00222	0.00000	-0.01622	0.00000	-0.01238
207	C9	DZZ	-0.00663	0.00000	-0.00647	0.00000	0.00646
208	C9	DXY	0.05010	0.00000	-0.00966	0.00000	0.00022
209	C9	DXZ	0.00000	-0.00775	0.00000	0.02976	0.00000
210	C9	DYZ	0.00000	-0.02486	0.00000	-0.00303	0.00000
211	H3	S	-0.02165	0.00000	0.00156	0.00000	-0.06189
212	H3	S	-0.17468	0.00000	0.20443	0.00000	-0.07219
213	H3	PX	0.01547	0.00000	-0.00217	0.00000	-0.00244
214	H3	PY	0.01011	0.00000	-0.00809	0.00000	-0.00044
215	H3	PZ	0.00000	-0.01020	0.00000	-0.00603	0.00000
216	H5	S	-0.01015	-0.03438	0.05344	-0.06594	-0.01105
217	H5	S	0.06683	-0.05369	-0.02044	0.04675	-0.02836
218	H5	PX	-0.00534	0.01039	0.01084	-0.01001	-0.00413
219	H5	PY	0.00989	0.00781	-0.00110	-0.00142	0.00333
220	H5	PZ	0.00605	-0.01059	0.00420	0.00844	-0.00014
221	H7	S	-0.01015	0.03438	0.05344	0.06594	-0.01105
222	H7	S	0.06683	0.05369	-0.02044	-0.04675	-0.02836
223	H7	PX	-0.00534	-0.01039	0.01084	0.01001	-0.00413
224	H7	PY	0.00989	-0.00781	-0.00110	0.00142	0.00333
225	H7	PZ	-0.00605	-0.01059	-0.00420	0.00844	0.00014

MO:	86	87	88	89	90
Eigenvalues:	0.92840	0.96524	0.97925	0.98288	0.99443
(ev):	25.26314	26.26542	26.64664	26.74547	27.05974

		A	A	A	A	A	
1	H1	S	-0.22739	0.00000	-0.08795	0.00000	0.01319
2	H1	S	0.66028	0.00000	0.28861	0.00000	0.27057
3	H1	PX	-0.01928	0.00000	0.00135	0.00000	0.00319
4	H1	PY	0.00009	0.00000	-0.01430	0.00000	0.01922
5	H1	PZ	0.00000	-0.00060	0.00000	-0.02139	0.00000
6	C1	S	-0.06019	0.00000	-0.00180	0.00000	-0.00057
7	C1	S	-0.07939	0.00000	-0.10237	0.00000	-0.05336
8	C1	PX	-0.25856	0.00000	0.00946	0.00000	-0.05233
9	C1	PY	0.32233	0.00000	-0.11620	0.00000	-0.01527
10	C1	PZ	0.00000	-0.15672	0.00000	0.46187	0.00000
11	C1	S	0.70415	0.00000	-1.10229	0.00000	0.14230
12	C1	PX	-0.84845	0.00000	0.33114	0.00000	-0.33809
13	C1	PY	0.86298	0.00000	-0.65986	0.00000	0.27074
14	C1	PZ	0.00000	0.22774	0.00000	-0.95542	0.00000
15	C1	DXX	-0.12183	0.00000	-0.03698	0.00000	-0.02373
16	C1	DYY	-0.05436	0.00000	-0.03478	0.00000	0.01358
17	C1	DZZ	0.08502	0.00000	0.00783	0.00000	0.00287
18	C1	DXY	0.00584	0.00000	0.01709	0.00000	0.03253
19	C1	DXZ	0.00000	-0.01644	0.00000	-0.02301	0.00000

20	C1	DYZ	0.00000	0.02710	0.00000	-0.02791	0.00000
21	C2	S	0.05445	0.00000	-0.01156	0.00000	-0.02222
22	C2	S	0.08319	0.00000	0.07179	0.00000	-0.12196
23	C2	PX	-0.03129	0.00000	0.06610	0.00000	0.03511
24	C2	PY	-0.23285	0.00000	0.08509	0.00000	-0.02970
25	C2	PZ	0.00000	0.29503	0.00000	0.06911	0.00000
26	C2	S	-0.58379	0.00000	-0.33960	0.00000	0.18629
27	C2	PX	0.34225	0.00000	-0.68502	0.00000	0.29006
28	C2	PY	-1.50115	0.00000	0.46260	0.00000	-0.12505
29	C2	PZ	0.00000	-0.59174	0.00000	-0.05907	0.00000
30	C2	DXX	0.09618	0.00000	0.01214	0.00000	-0.05094
31	C2	DYY	0.06226	0.00000	-0.05582	0.00000	-0.01831
32	C2	DZZ	-0.06793	0.00000	0.01615	0.00000	0.02551
33	C2	DXY	0.00868	0.00000	-0.01874	0.00000	0.02665
34	C2	DXZ	0.00000	0.01525	0.00000	0.02282	0.00000
35	C2	DYZ	0.00000	-0.00253	0.00000	0.00610	0.00000
36	C3	S	-0.01582	0.00000	0.00863	0.00000	0.00126
37	C3	S	-0.19146	0.00000	0.17739	0.00000	-0.10964
38	C3	PX	0.24530	0.00000	-0.04789	0.00000	0.15762
39	C3	PY	-0.22289	0.00000	-0.05450	0.00000	0.21939
40	C3	PZ	0.00000	-0.65606	0.00000	-0.32864	0.00000
41	C3	S	0.09985	0.00000	-0.33674	0.00000	-0.25453
42	C3	PX	0.99313	0.00000	-0.52446	0.00000	0.08703
43	C3	PY	1.03287	0.00000	0.32220	0.00000	-0.20462
44	C3	PZ	0.00000	0.98464	0.00000	0.55541	0.00000
45	C3	DXX	-0.03010	0.00000	0.01574	0.00000	-0.01374
46	C3	DYY	-0.06806	0.00000	0.02953	0.00000	0.00150
47	C3	DZZ	0.01526	0.00000	-0.00399	0.00000	-0.00064
48	C3	DXY	0.00308	0.00000	-0.02449	0.00000	0.04554
49	C3	DXZ	0.00000	0.02360	0.00000	0.00930	0.00000
50	C3	DYZ	0.00000	-0.02928	0.00000	0.06100	0.00000
51	C4	S	0.03968	0.00000	-0.00085	0.00000	-0.00046
52	C4	S	-0.42280	0.00000	-0.10270	0.00000	-0.12075
53	C4	PX	-0.09967	0.00000	-0.24993	0.00000	-0.22286
54	C4	PY	0.30436	0.00000	-0.18184	0.00000	-0.02685
55	C4	PZ	0.00000	0.57123	0.00000	-0.35352	0.00000
56	C4	S	0.24497	0.00000	0.16905	0.00000	0.04372
57	C4	PX	-1.61764	0.00000	2.18827	0.00000	0.17054
58	C4	PY	0.66486	0.00000	0.40570	0.00000	0.25751
59	C4	PZ	0.00000	-1.05073	0.00000	0.83654	0.00000
60	C4	DXX	0.02670	0.00000	0.02731	0.00000	-0.00776
61	C4	DYY	-0.00806	0.00000	-0.01026	0.00000	0.01808
62	C4	DZZ	-0.04244	0.00000	-0.01901	0.00000	-0.00926
63	C4	DXY	-0.05513	0.00000	-0.00604	0.00000	-0.00057
64	C4	DXZ	0.00000	-0.00308	0.00000	-0.00181	0.00000
65	C4	DYZ	0.00000	0.00274	0.00000	-0.03244	0.00000
66	C5	S	-0.04468	0.00000	0.00929	0.00000	0.02025
67	C5	S	0.20510	0.00000	0.22005	0.00000	0.01768
68	C5	PX	0.09496	0.00000	0.13582	0.00000	0.07697
69	C5	PY	-0.18193	0.00000	0.28917	0.00000	-0.03707
70	C5	PZ	0.00000	-0.34308	0.00000	0.18726	0.00000
71	C5	S	0.30636	0.00000	0.63749	0.00000	-0.00097
72	C5	PX	-1.20725	0.00000	1.06499	0.00000	-0.33890
73	C5	PY	-1.33336	0.00000	-0.23281	0.00000	0.08220

74	C5	PZ	0.00000	0.80194	0.00000	-0.42748	0.00000
75	C5	DXX	-0.02576	0.00000	0.08261	0.00000	0.03927
76	C5	DYY	-0.03889	0.00000	0.05840	0.00000	0.01858
77	C5	DZZ	0.05420	0.00000	-0.03352	0.00000	-0.01455
78	C5	DXY	0.01276	0.00000	0.01603	0.00000	-0.03728
79	C5	DXZ	0.00000	0.00210	0.00000	0.01801	0.00000
80	C5	DYZ	0.00000	-0.01292	0.00000	-0.01392	0.00000
81	C6	S	0.00153	0.00000	0.02067	0.00000	-0.05143
82	C6	S	0.25154	0.00000	-0.18898	0.00000	0.08236
83	C6	PX	-0.09277	0.00000	0.02622	0.00000	0.13379
84	C6	PY	0.29305	0.00000	0.15482	0.00000	-0.39844
85	C6	PZ	0.00000	-0.05743	0.00000	-0.24174	0.00000
86	C6	S	-0.49502	0.00000	0.74267	0.00000	-0.17584
87	C6	PX	1.81713	0.00000	-0.61606	0.00000	0.03615
88	C6	PY	-0.46637	0.00000	-0.20521	0.00000	0.44290
89	C6	PZ	0.00000	0.03948	0.00000	0.25618	0.00000
90	C6	DXX	0.01698	0.00000	-0.03489	0.00000	0.02796
91	C6	DYY	0.05590	0.00000	0.06795	0.00000	-0.14939
92	C6	DZZ	0.00450	0.00000	-0.02703	0.00000	0.05653
93	C6	DXY	-0.01589	0.00000	-0.00790	0.00000	-0.00547
94	C6	DXZ	0.00000	-0.02291	0.00000	-0.02952	0.00000
95	C6	DYZ	0.00000	0.01448	0.00000	-0.00149	0.00000
96	C7	S	0.03062	0.00000	-0.00724	0.00000	-0.00276
97	C7	S	-0.02730	0.00000	0.13868	0.00000	-0.03185
98	C7	PX	0.11182	0.00000	-0.05371	0.00000	0.16538
99	C7	PY	-0.07571	0.00000	0.11411	0.00000	-0.00520
100	C7	PZ	0.00000	0.45724	0.00000	-0.17679	0.00000
101	C7	S	0.48636	0.00000	0.23891	0.00000	0.14995
102	C7	PX	-0.49509	0.00000	0.06416	0.00000	-0.79854
103	C7	PY	-0.81085	0.00000	0.02140	0.00000	0.25584
104	C7	PZ	0.00000	-0.78415	0.00000	0.38328	0.00000
105	C7	DXX	0.03612	0.00000	-0.00905	0.00000	0.03184
106	C7	DYY	0.04948	0.00000	0.02094	0.00000	-0.01289
107	C7	DZZ	-0.03690	0.00000	0.00678	0.00000	-0.00672
108	C7	DXY	-0.01621	0.00000	-0.01986	0.00000	0.03674
109	C7	DXZ	0.00000	-0.00995	0.00000	0.01139	0.00000
110	C7	DYZ	0.00000	-0.01842	0.00000	-0.02856	0.00000
111	O1	S	0.00894	0.00000	0.00058	0.00000	0.00404
112	O1	S	0.01789	0.00000	-0.17890	0.00000	-0.09474
113	O1	PX	0.06824	0.00000	-0.27921	0.00000	-0.08834
114	O1	PY	-0.08245	0.00000	-0.02057	0.00000	-0.04542
115	O1	PZ	0.00000	0.08761	0.00000	0.01137	0.00000
116	O1	S	-0.36982	0.00000	0.21415	0.00000	0.03654
117	O1	PX	0.22220	0.00000	-0.08799	0.00000	0.06574
118	O1	PY	0.15115	0.00000	-0.15725	0.00000	-0.02579
119	O1	PZ	0.00000	0.03685	0.00000	-0.13447	0.00000
120	O1	DXX	0.00140	0.00000	0.01741	0.00000	-0.00606
121	O1	DYY	0.00212	0.00000	-0.11471	0.00000	-0.05759
122	O1	DZZ	0.01727	0.00000	-0.04325	0.00000	-0.01168
123	O1	DXY	0.01307	0.00000	-0.02009	0.00000	0.00139
124	O1	DXZ	0.00000	-0.02201	0.00000	-0.02728	0.00000
125	O1	DYZ	0.00000	-0.02331	0.00000	0.01362	0.00000
126	H4	S	-0.22350	0.00000	0.13963	0.00000	0.17361
127	H4	S	0.23587	0.00000	0.41663	0.00000	-0.31007

128	H4	PX	-0.00223	0.00000	-0.00424	0.00000	-0.02445
129	H4	PY	-0.01488	0.00000	-0.00969	0.00000	0.01085
130	H4	PZ	0.00000	0.00416	0.00000	-0.01005	0.00000
131	N1	S	-0.00401	0.00000	-0.01076	0.00000	0.02509
132	N1	S	0.04179	0.00000	-0.00154	0.00000	-0.04174
133	N1	PX	0.00605	0.00000	0.23705	0.00000	-0.52713
134	N1	PY	0.07243	0.00000	0.16293	0.00000	-0.35099
135	N1	PZ	0.00000	0.03789	0.00000	0.14075	0.00000
136	N1	S	-0.37754	0.00000	-0.53573	0.00000	0.91469
137	N1	PX	-0.56519	0.00000	-0.21224	0.00000	0.82705
138	N1	PY	0.35273	0.00000	-0.20536	0.00000	0.11667
139	N1	PZ	0.00000	-0.03380	0.00000	0.03233	0.00000
140	N1	DXX	0.00986	0.00000	-0.04723	0.00000	0.08964
141	N1	DYY	-0.03924	0.00000	-0.08362	0.00000	0.15134
142	N1	DZZ	0.01075	0.00000	0.03039	0.00000	-0.04902
143	N1	DXY	0.02064	0.00000	0.01038	0.00000	-0.02072
144	N1	DXZ	0.00000	0.02497	0.00000	0.03435	0.00000
145	N1	DYZ	0.00000	-0.01414	0.00000	-0.01616	0.00000
146	H6	S	0.24167	0.00000	-0.07412	0.00000	-0.02869
147	H6	S	-0.22961	0.00000	-0.22849	0.00000	0.19131
148	H6	PX	-0.01792	0.00000	-0.00119	0.00000	0.00098
149	H6	PY	-0.00930	0.00000	0.00590	0.00000	-0.00339
150	H6	PZ	0.00000	-0.00855	0.00000	-0.00622	0.00000
151	C8	S	0.01030	0.00000	-0.00277	0.00000	-0.00701
152	C8	S	0.16149	0.00000	-0.13576	0.00000	0.24649
153	C8	PX	0.08873	0.00000	0.14909	0.00000	-0.31373
154	C8	PY	0.10064	0.00000	-0.16715	0.00000	0.27296
155	C8	PZ	0.00000	0.12806	0.00000	0.72622	0.00000
156	C8	S	-0.35120	0.00000	0.37545	0.00000	-1.07949
157	C8	PX	-1.02773	0.00000	-0.33543	0.00000	0.90358
158	C8	PY	-0.55340	0.00000	0.42030	0.00000	-0.89606
159	C8	PZ	0.00000	-0.09818	0.00000	-1.27280	0.00000
160	C8	DXX	0.01000	0.00000	0.02415	0.00000	-0.06812
161	C8	DYY	0.03283	0.00000	-0.03588	0.00000	0.04277
162	C8	DZZ	0.00230	0.00000	-0.00695	0.00000	0.02738
163	C8	DXY	-0.03100	0.00000	-0.02628	0.00000	0.05697
164	C8	DXZ	0.00000	-0.01367	0.00000	-0.01873	0.00000
165	C8	DYZ	0.00000	0.04628	0.00000	0.03309	0.00000
166	H8	S	0.13098	0.00000	-0.00663	0.00000	0.03386
167	H8	S	0.06326	0.00000	-0.02369	0.00000	0.36900
168	H8	PX	0.00491	0.00000	-0.00011	0.00000	-0.01372
169	H8	PY	-0.01404	0.00000	-0.00314	0.00000	0.00639
170	H8	PZ	0.00000	-0.00923	0.00000	0.01094	0.00000
171	C10	S	-0.00015	0.00000	0.01482	0.00000	-0.02336
172	C10	S	0.15640	0.00000	0.03953	0.00000	-0.15118
173	C10	PX	-0.08370	0.00000	0.00808	0.00000	-0.04121
174	C10	PY	0.05822	0.00000	-0.08002	0.00000	0.09289
175	C10	PZ	0.00000	-0.18885	0.00000	-0.26368	0.00000
176	C10	S	-0.38094	0.00000	0.02799	0.00000	0.00759
177	C10	PX	0.47880	0.00000	0.03097	0.00000	0.02850
178	C10	PY	-0.05516	0.00000	0.09845	0.00000	-0.11322
179	C10	PZ	0.00000	0.27487	0.00000	0.64716	0.00000
180	C10	DXX	0.02142	0.00000	0.00682	0.00000	-0.01809
181	C10	DYY	-0.00313	0.00000	0.03757	0.00000	-0.06296

182	C10	DZZ	0.00489	0.00000	-0.01541	0.00000	0.02370
183	C10	DXY	-0.00588	0.00000	-0.00204	0.00000	0.00431
184	C10	DXZ	0.00000	-0.01134	0.00000	0.00449	0.00000
185	C10	DYZ	0.00000	-0.01745	0.00000	0.00594	0.00000
186	H16	S	0.06160	0.00000	0.04543	0.00000	-0.11075
187	H16	S	-0.21335	0.00000	0.01788	0.00000	-0.07932
188	H16	PX	0.00837	0.00000	-0.00060	0.00000	0.00480
189	H16	PY	-0.01045	0.00000	-0.01035	0.00000	0.02196
190	H16	PZ	0.00000	-0.00077	0.00000	0.00816	0.00000
191	H18	S	-0.01020	0.00000	0.04418	0.00000	-0.03795
192	H18	S	0.22168	0.00000	-0.00319	0.00000	0.03310
193	H18	PX	-0.00048	0.00000	0.00039	0.00000	0.00272
194	H18	PY	0.01279	0.00000	0.00140	0.00000	-0.00552
195	H18	PZ	0.00000	0.00649	0.00000	0.00355	0.00000
196	C9	S	-0.01667	0.00000	-0.04403	0.00000	-0.03362
197	C9	S	0.07124	0.00000	-0.11890	0.00000	-0.07189
198	C9	PX	0.18050	0.00000	-0.02766	0.00000	0.07048
199	C9	PY	-0.20128	0.00000	-0.60655	0.00000	-0.30858
200	C9	PZ	0.00000	-0.14874	0.00000	-0.17265	0.00000
201	C9	S	0.01042	0.00000	0.85278	0.00000	0.51585
202	C9	PX	-0.23178	0.00000	-0.03914	0.00000	-0.10921
203	C9	PY	0.58116	0.00000	1.66054	0.00000	0.91428
204	C9	PZ	0.00000	0.32304	0.00000	0.19766	0.00000
205	C9	DXX	0.01338	0.00000	-0.11671	0.00000	-0.04676
206	C9	DYY	-0.04070	0.00000	0.07667	0.00000	-0.00633
207	C9	DZZ	0.01510	0.00000	-0.04431	0.00000	-0.01481
208	C9	DXY	0.01926	0.00000	0.03792	0.00000	0.03050
209	C9	DXZ	0.00000	0.00711	0.00000	0.05762	0.00000
210	C9	DYZ	0.00000	0.03534	0.00000	-0.02829	0.00000
211	H3	S	-0.25672	0.00000	-0.10202	0.00000	-0.21540
212	H3	S	-0.15471	0.00000	-1.27083	0.00000	-0.57564
213	H3	PX	-0.00150	0.00000	0.02033	0.00000	0.00999
214	H3	PY	0.00351	0.00000	0.06183	0.00000	0.01947
215	H3	PZ	0.00000	0.01590	0.00000	-0.01793	0.00000
216	H5	S	0.00874	0.02411	-0.26379	-0.15642	-0.13565
217	H5	S	0.02044	0.07300	0.17017	0.22212	0.05723
218	H5	PX	-0.00858	-0.01544	-0.04466	-0.02015	-0.02384
219	H5	PY	0.01640	-0.01355	0.00540	0.00499	0.01525
220	H5	PZ	0.01613	0.01128	0.02346	0.01714	0.01656
221	H7	S	0.00874	-0.02411	-0.26379	0.15642	-0.13565
222	H7	S	0.02044	-0.07300	0.17017	-0.22212	0.05723
223	H7	PX	-0.00858	0.01544	-0.04466	0.02015	-0.02384
224	H7	PY	0.01640	0.01355	0.00540	-0.00499	0.01525
225	H7	PZ	-0.01613	0.01128	-0.02346	0.01714	-0.01656

MO:	91	92	93	94	95
Eigenvalues:	1.03696	1.05039	1.05945	1.08470	1.09571
(ev):	28.21712	28.58250	28.82904	29.51622	29.81568

		A	A	A	A	A	
1	H1	S	0.00000	-0.03631	-0.15787	-0.24662	0.05396
2	H1	S	0.00000	-0.18511	0.99060	1.69870	-0.46265
3	H1	PX	0.00000	0.00583	-0.05003	-0.09496	0.02362
4	H1	PY	0.00000	0.00476	-0.03914	-0.04044	-0.00215

5	H1	PZ	-0.02666	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	-0.00128	-0.02001	-0.02458	0.01016
7	C1	S	0.00000	0.12555	0.20064	0.28612	-0.04367
8	C1	PX	0.00000	-0.12678	0.31169	0.55259	-0.14050
9	C1	PY	0.00000	0.01865	0.04827	0.28326	-0.05161
10	C1	PZ	0.12260	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-0.13628	-0.37854	-0.24934	-0.95596
12	C1	PX	0.00000	0.36586	-1.12336	-2.05295	0.87377
13	C1	PY	0.00000	0.08707	-0.29613	-1.01430	0.48399
14	C1	PZ	-0.70709	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.01169	-0.04465	-0.08361	0.00533
16	C1	DYY	0.00000	-0.00295	0.01047	0.06174	-0.00869
17	C1	DZZ	0.00000	0.00592	0.05267	0.04646	-0.00736
18	C1	DXY	0.00000	-0.00881	-0.06935	-0.04084	0.01642
19	C1	DXZ	-0.01467	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.01162	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.00532	0.00078	-0.01145	0.02793
22	C2	S	0.00000	-0.25025	-0.10659	0.14916	-0.41492
23	C2	PX	0.00000	0.10230	0.05869	-0.26949	0.57143
24	C2	PY	0.00000	0.05687	0.11160	-0.12437	0.19551
25	C2	PZ	-0.34990	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-0.35057	0.04718	0.32318	0.91828
27	C2	PX	0.00000	-0.55561	-0.28901	1.28879	-2.08669
28	C2	PY	0.00000	-0.42664	-0.23626	0.58434	-0.54618
29	C2	PZ	1.03970	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	-0.01552	0.01682	-0.04066	0.07138
31	C2	DYY	0.00000	-0.02843	-0.02017	0.05691	-0.04275
32	C2	DZZ	0.00000	0.00337	-0.01192	0.01716	-0.05721
33	C2	DXY	0.00000	0.01592	0.00812	0.00467	0.07006
34	C2	DXZ	-0.01632	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02082	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	0.00077	-0.01559	0.00988	-0.00206
37	C3	S	0.00000	0.06431	-0.19429	0.21427	0.09247
38	C3	PX	0.00000	0.06778	-0.03138	-0.21534	0.00341
39	C3	PY	0.00000	-0.13295	-0.09612	0.12525	0.07870
40	C3	PZ	-0.55244	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	-0.23682	-1.02897	-1.11290	-0.09854
42	C3	PX	0.00000	-0.45898	0.44022	1.04085	0.35349
43	C3	PY	0.00000	0.59842	0.56292	-0.68465	0.33064
44	C3	PZ	1.42463	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	-0.00435	-0.00628	0.04126	-0.01991
46	C3	DYY	0.00000	0.00039	-0.10795	-0.03508	0.03570
47	C3	DZZ	0.00000	0.01075	0.03117	0.00802	0.00634
48	C3	DXY	0.00000	0.03313	0.03595	-0.02265	0.00239
49	C3	DXZ	-0.01113	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	-0.00228	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.00982	0.00137	-0.00570	-0.03230
52	C4	S	0.00000	0.14070	0.05695	-0.04576	-0.00212
53	C4	PX	0.00000	-0.06726	0.08550	-0.06239	-0.03773
54	C4	PY	0.00000	-0.03284	-0.03421	-0.01374	0.09524
55	C4	PZ	-0.24153	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-0.10206	-0.22687	-0.10039	-0.55333
57	C4	PX	0.00000	-0.02167	-0.17409	0.19109	0.66243
58	C4	PY	0.00000	0.41599	0.46689	0.34399	-1.50605

59	C4	PZ	0.75603	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	0.01456	0.01540	0.02035	-0.03016
61	C4	DYY	0.00000	0.03085	-0.01206	-0.04563	-0.11498
62	C4	DZZ	0.00000	-0.00533	0.00606	0.00856	0.03968
63	C4	DXY	0.00000	-0.02447	0.02419	0.04012	-0.06221
64	C4	DXZ	-0.00939	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.02157	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.00395	0.01022	0.01747	-0.00484
67	C5	S	0.00000	0.08271	0.03889	-0.09143	-0.60564
68	C5	PX	0.00000	-0.11692	0.15902	0.24441	0.03173
69	C5	PY	0.00000	-0.00030	-0.02739	-0.24496	-0.34615
70	C5	PZ	0.28413	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	0.33898	0.13620	-0.21827	1.91362
72	C5	PX	0.00000	0.25490	-0.32178	-0.83575	0.31499
73	C5	PY	0.00000	-0.53402	0.01922	1.05320	1.09794
74	C5	PZ	-0.82824	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.00910	0.01528	0.04339	-0.06258
76	C5	DYY	0.00000	0.01089	0.02702	-0.02812	0.01455
77	C5	DZZ	0.00000	0.00798	-0.01086	-0.02255	-0.03272
78	C5	DXY	0.00000	0.02302	-0.02535	-0.05637	-0.03494
79	C5	DXZ	0.00850	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.00531	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	-0.00145	0.00849	-0.00332	-0.01131
82	C6	S	0.00000	-0.51445	-0.12791	-0.13738	0.01389
83	C6	PX	0.00000	0.12802	0.03015	-0.01099	-0.06690
84	C6	PY	0.00000	0.32950	0.18391	-0.00062	-0.07714
85	C6	PZ	0.61103	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	-0.40963	0.03941	0.66179	0.52865
87	C6	PX	0.00000	-0.49228	-0.03284	0.29020	0.40371
88	C6	PY	0.00000	0.47921	0.34456	-0.33203	1.19635
89	C6	PZ	-1.45643	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	-0.07163	-0.00733	0.01753	0.00777
91	C6	DYY	0.00000	-0.08556	-0.00911	-0.02179	0.00964
92	C6	DZZ	0.00000	0.01326	-0.00382	-0.00748	-0.00035
93	C6	DXY	0.00000	0.04219	0.02026	0.04583	-0.03169
94	C6	DXZ	0.02212	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.03439	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	0.01274	-0.03250	-0.00345	-0.00045
97	C7	S	0.00000	-0.01508	0.17870	0.26854	-0.06528
98	C7	PX	0.00000	-0.08260	0.73399	0.04456	0.00203
99	C7	PY	0.00000	-0.18322	0.02451	0.11007	0.01669
100	C7	PZ	0.16376	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.00000	1.10378	0.11877	-0.16220	0.24397
102	C7	PX	0.00000	-0.30898	-3.10671	-0.34940	-0.07334
103	C7	PY	0.00000	0.31428	0.06300	-0.63836	-0.18943
104	C7	PZ	-0.71505	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.03544	-0.06211	0.00245	-0.00053
106	C7	DYY	0.00000	0.03177	0.04087	0.04434	-0.00892
107	C7	DZZ	0.00000	-0.01744	0.05805	0.00770	-0.00380
108	C7	DXY	0.00000	-0.02436	-0.01239	0.04876	0.00348
109	C7	DXZ	0.01713	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	-0.00476	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	0.00353	0.00103	0.00106	-0.01010
112	O1	S	0.00000	-0.00739	0.03450	0.09153	0.14602

113	O1	PX	0.00000	0.05402	0.00064	-0.00665	0.02284
114	O1	PY	0.00000	-0.00856	-0.00443	0.02611	0.33820
115	O1	PZ	0.05845	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	-0.17232	-0.18604	-0.25715	0.45353
117	O1	PX	0.00000	-0.02427	0.05826	0.07036	-0.05283
118	O1	PY	0.00000	0.12283	0.08360	0.01320	-0.79896
119	O1	PZ	-0.18666	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.00775	0.01303	0.03607	0.06983
121	O1	DYY	0.00000	-0.01199	0.00309	0.01809	0.08832
122	O1	DZZ	0.00000	0.00131	0.01074	0.03348	0.02293
123	O1	DXY	0.00000	0.00550	-0.00517	0.01055	0.00777
124	O1	DXZ	-0.01964	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00163	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	-0.06353	0.05412	0.18933	0.01884
127	H4	S	0.00000	0.33268	-0.25393	-0.94894	-0.76371
128	H4	PX	0.00000	0.00485	-0.01243	-0.04372	-0.04017
129	H4	PY	0.00000	-0.01919	0.01665	0.04080	0.03091
130	H4	PZ	-0.01797	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	-0.06139	-0.01427	-0.00338	0.00197
132	N1	S	0.00000	0.20014	0.00156	0.06143	-0.07354
133	N1	PX	0.00000	-0.31201	-0.01927	0.03029	0.09529
134	N1	PY	0.00000	-0.17821	0.02157	-0.04711	-0.08478
135	N1	PZ	0.15801	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	0.26729	1.13423	-0.84569	0.37370
137	N1	PX	0.00000	0.89785	0.38862	-0.14733	-0.32382
138	N1	PY	0.00000	1.23290	0.31677	0.08477	0.33164
139	N1	PZ	-0.05732	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.05617	0.03979	-0.02669	-0.02835
141	N1	DYY	0.00000	0.01344	-0.02460	-0.01630	0.00675
142	N1	DZZ	0.00000	0.14508	0.00343	0.04399	-0.01890
143	N1	DXY	0.00000	-0.01980	-0.01701	0.02206	0.00533
144	N1	DXZ	0.01472	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.03651	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00000	0.00307	-0.01421	-0.11910	0.25773
147	H6	S	0.00000	-0.36641	-0.27609	0.94293	-1.74895
148	H6	PX	0.00000	-0.01099	-0.01355	0.04506	-0.10102
149	H6	PY	0.00000	-0.03275	-0.00063	0.01719	-0.02803
150	H6	PZ	0.02315	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.01741	-0.00655	0.00975	0.00239
152	C8	S	0.00000	-0.61982	-0.05829	0.01649	-0.04311
153	C8	PX	0.00000	0.41679	-0.06480	0.22705	0.07429
154	C8	PY	0.00000	-0.08129	0.09239	0.10183	-0.04054
155	C8	PZ	-0.39775	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	0.82808	-0.89763	-0.02811	0.04669
157	C8	PX	0.00000	-0.82734	1.00103	-1.31261	-0.58011
158	C8	PY	0.00000	-0.93337	-1.52459	-0.78680	0.33858
159	C8	PZ	0.84236	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.05058	-0.01243	0.00327	0.01097
161	C8	DYY	0.00000	-0.11508	-0.07989	0.01489	0.00053
162	C8	DZZ	0.00000	0.01426	0.03002	-0.00670	-0.00780
163	C8	DXY	0.00000	0.06506	-0.07396	0.02839	-0.01177
164	C8	DXZ	-0.01327	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	-0.00430	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	0.14150	-0.11305	-0.07125	0.02550

167	H8	S	0.00000	-0.03840	2.01648	0.28866	-0.03398
168	H8	PX	0.00000	0.02297	-0.10216	-0.01605	0.00340
169	H8	PY	0.00000	0.00128	-0.00089	0.02127	0.00316
170	H8	PZ	-0.01513	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	0.01214	-0.00780	0.00094	-0.00108
172	C10	S	0.00000	-0.31063	0.06965	0.07535	0.02058
173	C10	PX	0.00000	-0.03724	0.57430	-0.58020	-0.09354
174	C10	PY	0.00000	-0.08205	0.07567	-0.08537	0.00643
175	C10	PZ	0.04703	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	-0.41712	-1.11317	-0.45587	0.27666
177	C10	PX	0.00000	0.40253	-1.63362	1.94013	0.33411
178	C10	PY	0.00000	0.02398	-0.56424	0.16725	0.17763
179	C10	PZ	-0.27803	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	0.01870	-0.03795	0.03882	-0.00232
181	C10	DYY	0.00000	-0.03435	0.01310	-0.03512	0.00807
182	C10	DZZ	0.00000	-0.00664	0.03087	0.00388	-0.00128
183	C10	DXY	0.00000	-0.01927	0.07426	-0.06973	-0.00275
184	C10	DXZ	-0.01220	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	-0.00561	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.25316	-0.13287	0.15370	0.00266
187	H16	S	0.00000	-0.32481	1.12618	-1.15014	-0.16444
188	H16	PX	0.00000	0.02252	-0.06796	0.06196	0.00869
189	H16	PY	0.00000	-0.01067	0.03120	-0.02695	-0.00740
190	H16	PZ	-0.00925	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	0.01201	0.07663	-0.12122	-0.00549
192	H18	S	0.00000	0.25150	-0.89571	1.09647	0.17847
193	H18	PX	0.00000	-0.02242	-0.04171	0.04027	0.00722
194	H18	PY	0.00000	0.02029	-0.03224	0.05666	0.00444
195	H18	PZ	-0.00128	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.00333	0.00963	0.01478	0.03405
197	C9	S	0.00000	-0.02887	0.14752	0.27062	0.14285
198	C9	PX	0.00000	0.00873	0.05535	0.11913	0.28249
199	C9	PY	0.00000	0.04174	-0.03653	-0.07906	-0.30126
200	C9	PZ	-0.21984	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	0.00383	-0.41942	-0.71182	-0.40406
202	C9	PX	0.00000	0.04803	-0.07737	-0.21799	-0.75477
203	C9	PY	0.00000	-0.08407	-0.00970	0.05053	0.62353
204	C9	PZ	0.34077	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	0.00842	0.00900	0.01505	0.00726
206	C9	DYY	0.00000	0.00102	0.03709	0.05100	0.13463
207	C9	DZZ	0.00000	-0.00880	-0.01012	-0.01185	-0.05328
208	C9	DXY	0.00000	0.00105	-0.01823	-0.01545	0.02061
209	C9	DXZ	0.07300	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	-0.03997	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.01570	0.14102	0.19946	0.40569
212	H3	S	0.00000	0.03447	-0.02227	-0.04524	-0.71288
213	H3	PX	0.00000	-0.00060	-0.00655	-0.00402	0.02257
214	H3	PY	0.00000	-0.00291	0.01040	0.01852	0.08000
215	H3	PZ	-0.02139	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.19797	-0.00566	0.00141	-0.00477	-0.03266
217	H5	S	0.36973	-0.02492	0.11218	0.23761	0.56014
218	H5	PX	-0.02508	0.00381	0.00374	0.00196	-0.01597
219	H5	PY	0.00906	-0.00353	-0.01003	-0.00827	-0.00741
220	H5	PZ	0.02066	0.00100	0.01157	0.01812	0.01825

221	H7	S	0.19797	-0.00566	0.00141	-0.00477	-0.03266
222	H7	S	-0.36973	-0.02492	0.11218	0.23761	0.56014
223	H7	PX	0.02508	0.00381	0.00374	0.00196	-0.01597
224	H7	PY	-0.00906	-0.00353	-0.01003	-0.00827	-0.00741
225	H7	PZ	0.02066	-0.00100	-0.01157	-0.01812	-0.01825

MO:		96	97	98	99	100
Eigenvalues:		1.10661	1.10759	1.11104	1.12374	1.12979
(ev):		30.11254	30.13895	30.23296	30.57848	30.74320

		A	A	A	A	A	
1	H1	S	0.00000	-0.12310	0.02617	-0.08109	0.00000
2	H1	S	0.00000	0.48044	-0.04944	1.10620	0.00000
3	H1	PX	0.00000	-0.03682	-0.00091	-0.06812	0.00000
4	H1	PY	0.00000	0.01376	0.01604	-0.02380	0.00000
5	H1	PZ	-0.00294	0.00000	0.00000	0.00000	0.00691
6	C1	S	0.00000	-0.00688	-0.00136	0.00052	0.00000
7	C1	S	0.00000	0.18057	-0.08169	0.83559	0.00000
8	C1	PX	0.00000	0.11062	0.01919	0.24713	0.00000
9	C1	PY	0.00000	0.09633	-0.10158	0.32793	0.00000
10	C1	PZ	0.26121	0.00000	0.00000	0.00000	-0.16921
11	C1	S	0.00000	0.14131	-0.03635	-0.76144	0.00000
12	C1	PX	0.00000	-0.39458	-0.04108	-1.15092	0.00000
13	C1	PY	0.00000	-0.36692	0.07331	-0.88008	0.00000
14	C1	PZ	-0.60198	0.00000	0.00000	0.00000	0.50524
15	C1	DXX	0.00000	-0.05470	-0.00448	0.01079	0.00000
16	C1	DYY	0.00000	0.07652	-0.00759	0.07349	0.00000
17	C1	DZZ	0.00000	0.00829	0.00496	0.04204	0.00000
18	C1	DXY	0.00000	-0.00110	-0.00019	-0.02287	0.00000
19	C1	DXZ	-0.02607	0.00000	0.00000	0.00000	-0.00789
20	C1	DYZ	0.01079	0.00000	0.00000	0.00000	0.00745
21	C2	S	0.00000	-0.00367	0.00936	-0.00087	0.00000
22	C2	S	0.00000	0.00427	-0.23269	-0.37780	0.00000
23	C2	PX	0.00000	-0.23634	0.43430	0.27037	0.00000
24	C2	PY	0.00000	0.03148	0.22316	0.19806	0.00000
25	C2	PZ	-0.08248	0.00000	0.00000	0.00000	-0.03746
26	C2	S	0.00000	0.42342	0.21412	0.10231	0.00000
27	C2	PX	0.00000	1.45364	-1.57363	-0.41177	0.00000
28	C2	PY	0.00000	-0.20443	-0.31815	-2.15579	0.00000
29	C2	PZ	0.19596	0.00000	0.00000	0.00000	-0.23564
30	C2	DXX	0.00000	0.03515	0.07615	0.07596	0.00000
31	C2	DYY	0.00000	0.00039	-0.05886	-0.10486	0.00000
32	C2	DZZ	0.00000	-0.00907	-0.04459	-0.03773	0.00000
33	C2	DXY	0.00000	0.01954	0.05636	0.01331	0.00000
34	C2	DXZ	-0.00378	0.00000	0.00000	0.00000	0.01890
35	C2	DYZ	0.01694	0.00000	0.00000	0.00000	0.02131
36	C3	S	0.00000	0.01331	-0.00525	-0.00724	0.00000
37	C3	S	0.00000	0.26712	0.09902	0.01158	0.00000
38	C3	PX	0.00000	0.12081	-0.04166	0.08093	0.00000
39	C3	PY	0.00000	0.14603	-0.13078	-0.07326	0.00000
40	C3	PZ	-0.22691	0.00000	0.00000	0.00000	0.28134
41	C3	S	0.00000	0.20817	-1.13588	-1.73929	0.00000
42	C3	PX	0.00000	-0.45432	0.09280	-0.05805	0.00000
43	C3	PY	0.00000	-1.10329	0.65167	0.54324	0.00000

44	C3	PZ	0.55827	0.00000	0.00000	0.00000	-0.77311
45	C3	DXX	0.00000	0.01882	-0.02461	-0.06886	0.00000
46	C3	DYY	0.00000	0.05903	-0.01857	-0.01261	0.00000
47	C3	DZZ	0.00000	-0.00896	0.01873	0.02304	0.00000
48	C3	DXY	0.00000	0.00980	0.03922	0.00555	0.00000
49	C3	DXZ	-0.01640	0.00000	0.00000	0.00000	-0.02958
50	C3	DYZ	0.00395	0.00000	0.00000	0.00000	0.00369
51	C4	S	0.00000	-0.00434	0.00518	0.00888	0.00000
52	C4	S	0.00000	-0.28591	-0.26529	-0.13134	0.00000
53	C4	PX	0.00000	-0.09314	0.05617	-0.02509	0.00000
54	C4	PY	0.00000	-0.03449	-0.13379	-0.06985	0.00000
55	C4	PZ	-0.03548	0.00000	0.00000	0.00000	0.09916
56	C4	S	0.00000	1.20742	0.77795	1.62247	0.00000
57	C4	PX	0.00000	-0.33350	-0.25338	-0.87793	0.00000
58	C4	PY	0.00000	-0.23271	0.19370	1.93784	0.00000
59	C4	PZ	0.24800	0.00000	0.00000	0.00000	-0.29024
60	C4	DXX	0.00000	-0.00468	-0.03120	0.05925	0.00000
61	C4	DYY	0.00000	-0.01145	0.06622	0.04234	0.00000
62	C4	DZZ	0.00000	-0.01424	-0.01968	-0.05136	0.00000
63	C4	DXY	0.00000	0.02392	0.04915	-0.02492	0.00000
64	C4	DXZ	0.01505	0.00000	0.00000	0.00000	0.00082
65	C4	DYZ	-0.04071	0.00000	0.00000	0.00000	0.00493
66	C5	S	0.00000	0.01821	0.02677	0.01295	0.00000
67	C5	S	0.00000	-0.44611	-0.09187	0.36228	0.00000
68	C5	PX	0.00000	0.41630	0.30704	-0.03581	0.00000
69	C5	PY	0.00000	-0.33856	-0.09491	0.35723	0.00000
70	C5	PZ	0.05867	0.00000	0.00000	0.00000	0.01515
71	C5	S	0.00000	0.41183	0.33283	0.06862	0.00000
72	C5	PX	0.00000	-1.85431	-0.51560	-0.61322	0.00000
73	C5	PY	0.00000	0.94078	0.12176	-2.55360	0.00000
74	C5	PZ	-0.20466	0.00000	0.00000	0.00000	0.09982
75	C5	DXX	0.00000	0.01083	0.01935	0.01205	0.00000
76	C5	DYY	0.00000	-0.01670	0.07655	0.06477	0.00000
77	C5	DZZ	0.00000	-0.04878	-0.06202	0.00834	0.00000
78	C5	DXY	0.00000	-0.09138	-0.12005	0.01054	0.00000
79	C5	DXZ	0.01055	0.00000	0.00000	0.00000	0.01517
80	C5	DYZ	-0.00657	0.00000	0.00000	0.00000	-0.01928
81	C6	S	0.00000	-0.00580	-0.00824	-0.00384	0.00000
82	C6	S	0.00000	0.06274	-0.07998	-0.03556	0.00000
83	C6	PX	0.00000	0.01521	-0.02924	-0.26281	0.00000
84	C6	PY	0.00000	0.13068	-0.05521	-0.19904	0.00000
85	C6	PZ	0.00165	0.00000	0.00000	0.00000	-0.34314
86	C6	S	0.00000	-1.33537	0.62073	0.02159	0.00000
87	C6	PX	0.00000	0.08634	0.10393	1.92689	0.00000
88	C6	PY	0.00000	-0.28912	1.05211	-0.30993	0.00000
89	C6	PZ	-0.05813	0.00000	0.00000	0.00000	1.08485
90	C6	DXX	0.00000	-0.03009	0.01508	-0.04735	0.00000
91	C6	DYY	0.00000	-0.00611	-0.01441	0.02500	0.00000
92	C6	DZZ	0.00000	0.01325	-0.00704	0.00962	0.00000
93	C6	DXY	0.00000	0.02705	-0.03213	0.00798	0.00000
94	C6	DXZ	0.02269	0.00000	0.00000	0.00000	0.02420
95	C6	DYZ	-0.03587	0.00000	0.00000	0.00000	-0.06000
96	C7	S	0.00000	0.00596	-0.00362	0.01124	0.00000
97	C7	S	0.00000	-0.17344	0.07891	-0.29183	0.00000

98	C7	PX	0.00000	-0.50565	0.20985	-0.23492	0.00000
99	C7	PY	0.00000	-0.11700	-0.08792	-0.00217	0.00000
100	C7	PZ	0.02435	0.00000	0.00000	0.00000	0.04102
101	C7	S	0.00000	-1.00091	0.62783	1.19777	0.00000
102	C7	PX	0.00000	2.39636	-1.03053	0.48004	0.00000
103	C7	PY	0.00000	0.48318	0.34285	0.44170	0.00000
104	C7	PZ	-0.23068	0.00000	0.00000	0.00000	-0.02069
105	C7	DXX	0.00000	0.02130	-0.01657	0.05903	0.00000
106	C7	DYY	0.00000	-0.08268	0.05736	-0.03969	0.00000
107	C7	DZZ	0.00000	-0.00001	-0.00380	-0.03997	0.00000
108	C7	DXY	0.00000	-0.04523	-0.01474	-0.03086	0.00000
109	C7	DXZ	-0.00879	0.00000	0.00000	0.00000	-0.01799
110	C7	DYZ	-0.01491	0.00000	0.00000	0.00000	-0.04032
111	O1	S	0.00000	0.00064	0.00010	0.01148	0.00000
112	O1	S	0.00000	0.02287	-0.15680	-0.05236	0.00000
113	O1	PX	0.00000	-0.03241	0.00498	0.02490	0.00000
114	O1	PY	0.00000	-0.03556	-0.24423	-0.12963	0.00000
115	O1	PZ	-0.09121	0.00000	0.00000	0.00000	0.13667
116	O1	S	0.00000	-0.10509	0.06502	-0.91737	0.00000
117	O1	PX	0.00000	0.10794	-0.02441	0.14578	0.00000
118	O1	PY	0.00000	0.03113	0.38263	0.73669	0.00000
119	O1	PZ	0.13415	0.00000	0.00000	0.00000	-0.14026
120	O1	DXX	0.00000	0.00473	-0.07386	-0.03915	0.00000
121	O1	DYY	0.00000	-0.01534	-0.08508	-0.08923	0.00000
122	O1	DZZ	0.00000	0.03261	-0.01705	0.03496	0.00000
123	O1	DXY	0.00000	0.02911	0.01296	0.00575	0.00000
124	O1	DXZ	0.08596	0.00000	0.00000	0.00000	-0.02087
125	O1	DYZ	0.04799	0.00000	0.00000	0.00000	-0.01454
126	H4	S	0.00000	0.29226	0.31306	-0.01356	0.00000
127	H4	S	0.00000	-1.56954	-0.79139	0.88323	0.00000
128	H4	PX	0.00000	-0.07144	-0.03879	0.01422	0.00000
129	H4	PY	0.00000	0.06728	0.04574	-0.04316	0.00000
130	H4	PZ	-0.00797	0.00000	0.00000	0.00000	-0.00452
131	N1	S	0.00000	-0.00885	-0.00187	0.01754	0.00000
132	N1	S	0.00000	-0.04551	-0.06977	0.05095	0.00000
133	N1	PX	0.00000	0.00077	0.20621	-0.01683	0.00000
134	N1	PY	0.00000	0.03069	-0.08081	0.04653	0.00000
135	N1	PZ	0.39910	0.00000	0.00000	0.00000	0.85409
136	N1	S	0.00000	0.22344	0.32528	-0.06610	0.00000
137	N1	PX	0.00000	-0.05061	-0.37009	-0.20380	0.00000
138	N1	PY	0.00000	0.09484	0.39755	-0.37490	0.00000
139	N1	PZ	-0.53171	0.00000	0.00000	0.00000	-1.41006
140	N1	DXX	0.00000	-0.03827	-0.03035	0.03460	0.00000
141	N1	DYY	0.00000	-0.00471	-0.01251	0.05812	0.00000
142	N1	DZZ	0.00000	0.00841	-0.01260	-0.02607	0.00000
143	N1	DXY	0.00000	-0.03253	0.00618	-0.03514	0.00000
144	N1	DXZ	0.03315	0.00000	0.00000	0.00000	0.03053
145	N1	DYZ	0.01458	0.00000	0.00000	0.00000	0.02780
146	H6	S	0.00000	0.04588	0.17155	0.29442	0.00000
147	H6	S	0.00000	0.59361	-1.31207	-1.01172	0.00000
148	H6	PX	0.00000	0.01904	-0.07703	-0.06533	0.00000
149	H6	PY	0.00000	0.01743	0.00001	-0.02046	0.00000
150	H6	PZ	0.00492	0.00000	0.00000	0.00000	-0.01641
151	C8	S	0.00000	-0.00703	0.00239	0.00318	0.00000

152	C8	S	0.00000	-0.31267	-0.06004	0.17059	0.00000
153	C8	PX	0.00000	-0.14901	0.10459	-0.12418	0.00000
154	C8	PY	0.00000	-0.23060	0.01525	0.02715	0.00000
155	C8	PZ	-0.04838	0.00000	0.00000	0.00000	-0.16153
156	C8	S	0.00000	1.43045	0.05383	-0.08289	0.00000
157	C8	PX	0.00000	0.91244	-0.65861	0.46430	0.00000
158	C8	PY	0.00000	1.40360	-0.17447	-0.24691	0.00000
159	C8	PZ	0.23707	0.00000	0.00000	0.00000	0.59227
160	C8	DXX	0.00000	-0.00516	0.04171	0.00441	0.00000
161	C8	DYY	0.00000	-0.02207	-0.02293	0.02499	0.00000
162	C8	DZZ	0.00000	-0.01093	-0.01018	0.00246	0.00000
163	C8	DXY	0.00000	0.00975	-0.00426	0.00654	0.00000
164	C8	DXZ	-0.01329	0.00000	0.00000	0.00000	0.01639
165	C8	DYZ	0.02923	0.00000	0.00000	0.00000	0.04491
166	H8	S	0.00000	0.09932	-0.05044	0.17192	0.00000
167	H8	S	0.00000	-1.41085	0.61681	-0.75540	0.00000
168	H8	PX	0.00000	0.06508	-0.02869	0.04991	0.00000
169	H8	PY	0.00000	-0.01281	0.01306	0.00240	0.00000
170	H8	PZ	-0.01101	0.00000	0.00000	0.00000	-0.00538
171	C10	S	0.00000	0.01145	-0.00736	0.00385	0.00000
172	C10	S	0.00000	-0.16354	0.00065	-0.06058	0.00000
173	C10	PX	0.00000	0.49806	-0.30519	-0.00499	0.00000
174	C10	PY	0.00000	0.10267	-0.10071	-0.04762	0.00000
175	C10	PZ	-0.04429	0.00000	0.00000	0.00000	-0.04432
176	C10	S	0.00000	0.67639	-0.05208	-0.11576	0.00000
177	C10	PX	0.00000	-1.61045	0.96337	-0.03210	0.00000
178	C10	PY	0.00000	-0.16464	0.33807	-0.08762	0.00000
179	C10	PZ	0.00923	0.00000	0.00000	0.00000	-0.08386
180	C10	DXX	0.00000	-0.01163	-0.00840	-0.00096	0.00000
181	C10	DYY	0.00000	0.03615	-0.01842	0.00186	0.00000
182	C10	DZZ	0.00000	-0.02662	0.01607	-0.01443	0.00000
183	C10	DXY	0.00000	0.07423	-0.03469	0.01821	0.00000
184	C10	DXZ	0.01172	0.00000	0.00000	0.00000	0.04713
185	C10	DYZ	-0.00757	0.00000	0.00000	0.00000	0.00100
186	H16	S	0.00000	-0.05860	0.02185	-0.04270	0.00000
187	H16	S	0.00000	0.86784	-0.46282	0.03970	0.00000
188	H16	PX	0.00000	-0.04096	0.02717	0.00137	0.00000
189	H16	PY	0.00000	0.02645	-0.01580	0.00538	0.00000
190	H16	PZ	0.00337	0.00000	0.00000	0.00000	0.00890
191	H18	S	0.00000	0.22636	-0.08757	0.06514	0.00000
192	H18	S	0.00000	-1.05406	0.65494	-0.11473	0.00000
193	H18	PX	0.00000	-0.04747	0.02954	0.00289	0.00000
194	H18	PY	0.00000	-0.05997	0.03145	-0.00793	0.00000
195	H18	PZ	-0.00145	0.00000	0.00000	0.00000	-0.01404
196	C9	S	0.00000	-0.01379	-0.03222	0.00169	0.00000
197	C9	S	0.00000	0.14500	-0.11783	0.00645	0.00000
198	C9	PX	0.00000	0.03967	-0.24027	-0.01292	0.00000
199	C9	PY	0.00000	0.07162	0.36112	0.01730	0.00000
200	C9	PZ	0.65349	0.00000	0.00000	0.00000	-0.23725
201	C9	S	0.00000	-0.25677	0.41047	-0.25680	0.00000
202	C9	PX	0.00000	-0.03070	0.57413	0.30956	0.00000
203	C9	PY	0.00000	-0.08792	-0.60743	-0.29425	0.00000
204	C9	PZ	-1.24135	0.00000	0.00000	0.00000	0.51949
205	C9	DXX	0.00000	0.00856	0.00673	-0.00343	0.00000

206	C9	DYY	0.00000	-0.05052	-0.16258	0.03810	0.00000
207	C9	DZZ	0.00000	0.02434	0.07880	-0.04540	0.00000
208	C9	DXY	0.00000	0.01610	0.01285	-0.03949	0.00000
209	C9	DXZ	-0.22602	0.00000	0.00000	0.00000	0.07476
210	C9	DYZ	0.08996	0.00000	0.00000	0.00000	-0.02756
211	H3	S	0.00000	-0.19684	-0.54593	0.24388	0.00000
212	H3	S	0.00000	0.29124	0.83694	0.02800	0.00000
213	H3	PX	0.00000	0.00589	-0.00605	-0.01923	0.00000
214	H3	PY	0.00000	-0.02620	-0.08865	0.00281	0.00000
215	H3	PZ	0.04292	0.00000	0.00000	0.00000	-0.01032
216	H5	S	0.56050	-0.02906	0.05695	-0.06884	-0.18971
217	H5	S	-1.31884	0.01506	-0.53167	-0.02543	0.50794
218	H5	PX	0.07106	-0.00516	0.00812	0.01675	-0.02734
219	H5	PY	-0.03182	0.01417	0.01972	-0.02320	0.00940
220	H5	PZ	-0.05455	0.00487	-0.02594	0.01866	0.01875
221	H7	S	-0.56050	-0.02906	0.05695	-0.06884	0.18971
222	H7	S	1.31884	0.01506	-0.53167	-0.02543	-0.50794
223	H7	PX	-0.07106	-0.00516	0.00812	0.01675	0.02734
224	H7	PY	0.03182	0.01417	0.01972	-0.02320	-0.00940
225	H7	PZ	-0.05455	-0.00487	0.02594	-0.01866	0.01875

MO:	101	102	103	104	105
Eigenvalues:	1.14664	1.16819	1.17462	1.17763	1.18515
(ev):	31.20181	31.78807	31.96313	32.04497	32.24946

		A	A	A	A	A	
1	H1	S	-0.20003	-0.10678	-0.07597	-0.03766	0.20388
2	H1	S	0.71477	0.08673	-0.04791	-0.20105	-0.76487
3	H1	PX	-0.06381	-0.00576	-0.01092	0.00718	0.03012
4	H1	PY	0.00834	-0.01348	-0.00066	-0.00058	0.01067
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00517	-0.00421	0.00882	0.00360	0.00527
7	C1	S	0.23802	-0.16266	-0.11574	-0.02955	0.17839
8	C1	PX	0.31079	0.13350	0.09571	-0.09085	-0.10577
9	C1	PY	-0.02818	-0.13247	0.06422	0.09048	-0.26580
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-1.97572	0.36233	0.24354	0.23597	0.66077
12	C1	PX	-0.50863	-0.40600	0.15311	0.38846	0.13263
13	C1	PY	-0.07102	0.49643	-0.17097	-0.42434	1.72866
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.03522	-0.00371	-0.04389	-0.01244	0.10264
16	C1	DYY	0.02461	-0.03018	0.02760	0.01572	-0.01403
17	C1	DZZ	0.02002	-0.00103	0.00462	-0.00710	-0.03640
18	C1	DXY	-0.00780	-0.05125	-0.00122	0.01815	-0.03325
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.01003	-0.01340	-0.00048	0.00017	0.00660
22	C2	S	-0.40351	-0.43948	0.13696	-0.03262	0.24628
23	C2	PX	0.24318	0.06706	0.13840	0.05281	-0.25618
24	C2	PY	-0.41579	0.10610	0.05520	-0.04797	0.05644
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	2.13108	1.41619	-0.26466	-0.03010	-1.12690
27	C2	PX	-1.17262	-0.32245	-0.53244	0.07503	0.77765
28	C2	PY	2.69939	-0.38033	0.43029	0.11130	-0.72908

29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.04808	-0.05834	0.02595	0.00361	0.02626
31	C2	DYY	0.04337	-0.00939	-0.01056	-0.00443	-0.00198
32	C2	DZZ	-0.03181	-0.00858	0.00633	0.00256	0.00992
33	C2	DXY	0.03384	-0.01454	-0.00637	0.02619	-0.02312
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00746	-0.00663	0.00896	0.00932	-0.01646
37	C3	S	0.33260	-0.49182	0.38194	0.11574	-0.14504
38	C3	PX	-0.05598	-0.23292	0.00089	-0.07874	0.14432
39	C3	PY	-0.11090	0.09772	0.12692	0.14647	-0.30911
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-0.00417	1.91913	-0.95726	-0.16243	0.37743
42	C3	PX	0.08389	1.22261	-0.37803	0.00190	-0.42078
43	C3	PY	0.38254	-0.72858	0.05381	-0.44663	1.15124
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.03359	0.00696	0.04153	0.00810	-0.06133
46	C3	DYY	0.03777	-0.01560	0.02091	0.02493	-0.00837
47	C3	DZZ	-0.01213	-0.02157	0.00487	-0.00730	0.01960
48	C3	DXY	0.04566	-0.03620	0.00872	-0.03989	0.08011
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.01340	0.00639	-0.02221	-0.00987	0.01364
52	C4	S	0.55998	0.43003	-0.37387	-0.16071	0.33612
53	C4	PX	-0.36640	0.06716	0.08937	-0.04315	0.28486
54	C4	PY	0.10435	-0.08804	-0.04799	-0.08676	0.13624
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-3.31086	-1.67128	0.63601	0.85785	-0.60503
57	C4	PX	2.86900	0.06246	-0.27039	-0.02735	-2.05858
58	C4	PY	-0.99787	-0.39285	-0.03118	0.09385	0.11786
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.03837	0.00701	-0.03389	0.00735	-0.00176
61	C4	DYY	0.04362	0.03497	-0.10707	-0.03353	0.07447
62	C4	DZZ	0.02924	0.00960	0.03048	-0.00013	-0.01699
63	C4	DXY	0.01620	0.04213	-0.05009	-0.03124	0.02666
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02245	-0.00303	0.00132	0.00040	0.00022
67	C5	S	-0.08779	-0.01442	0.26844	0.12159	-0.16350
68	C5	PX	-0.53361	-0.00820	-0.24957	-0.04508	0.16941
69	C5	PY	-0.25572	-0.09504	0.31706	-0.01248	0.04165
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.12638	0.34511	-1.28885	-0.47871	0.03664
72	C5	PX	3.12324	0.24173	0.87239	-0.04849	-1.29526
73	C5	PY	2.38858	0.63313	-0.74333	-0.17157	-0.72941
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.07795	0.02342	-0.04619	-0.00166	-0.02823
76	C5	DYY	-0.11619	-0.01614	0.01927	-0.00204	0.01967
77	C5	DZZ	0.01540	0.00121	0.04160	0.01353	-0.01723
78	C5	DXY	0.00191	0.01464	0.03390	-0.00040	-0.01996
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01434	0.00688	0.00259	-0.00850	0.00502
82	C6	S	-0.19986	0.18584	0.03687	-0.37448	0.13800

83	C6	PX	0.13007	-0.00079	0.02739	-0.00194	-0.09570
84	C6	PY	0.05052	0.04822	-0.02766	0.07218	-0.03917
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	2.44592	-0.83770	0.79772	0.75735	-1.19029
87	C6	PX	-1.16233	0.39477	-0.46039	-0.04088	0.32666
88	C6	PY	-0.76368	0.65884	-0.56410	-0.29969	0.26450
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.04021	0.01217	0.01778	-0.04381	0.00422
91	C6	DYY	0.04488	0.02006	0.02550	-0.01239	-0.04127
92	C6	DZZ	-0.04330	-0.00252	-0.00851	0.00041	0.01380
93	C6	DXY	-0.01902	0.03373	-0.00708	0.03095	-0.02493
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00940	-0.01745	-0.00404	0.00425	0.01578
97	C7	S	0.22431	-0.62707	0.20511	0.20731	-0.03401
98	C7	PX	-0.04728	-0.15428	0.05009	-0.12853	0.09941
99	C7	PY	-0.22602	0.44943	-0.07338	0.08027	-0.44542
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.21570	1.28348	-0.28850	-0.45449	-0.13912
102	C7	PX	0.63799	0.22417	-0.26508	0.59969	-0.14113
103	C7	PY	0.87035	-2.26304	0.65825	-0.13855	1.46064
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00498	-0.00213	-0.00180	0.03879	-0.01930
106	C7	DYY	0.01714	-0.09689	0.01458	-0.00935	0.03687
107	C7	DZZ	0.00124	-0.00603	0.00961	-0.00068	-0.00515
108	C7	DXY	-0.04715	0.09715	-0.01574	0.02069	-0.06391
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.00805	-0.01061	-0.00213	0.00012	0.00301
112	O1	S	-0.16892	-0.17014	0.27850	0.08461	-0.19641
113	O1	PX	0.20919	0.04696	-0.22833	-0.07138	0.02161
114	O1	PY	-0.11630	-0.11409	0.11984	0.05714	-0.04909
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.98819	0.80080	-0.25642	-0.20035	0.41087
117	O1	PX	-0.58907	-0.10741	0.39592	0.14497	0.20031
118	O1	PY	-0.24601	-0.09421	-0.20476	-0.01953	0.18589
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.05067	-0.04089	0.10763	0.03338	-0.06025
121	O1	DYY	0.00201	-0.03771	0.08308	0.00317	-0.02923
122	O1	DZZ	-0.12072	-0.10013	0.08868	0.04461	-0.08757
123	O1	DXY	0.00029	-0.01674	0.04787	0.02606	-0.02959
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.08356	-0.06733	-0.09411	0.00378	0.03941
127	H4	S	0.28429	-0.17680	1.09115	0.16408	-0.36203
128	H4	PX	0.00739	0.00269	0.04635	-0.00265	-0.00521
129	H4	PY	-0.03811	0.00439	-0.03816	-0.01229	0.02089
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00694	-0.00940	0.01110	-0.00949	-0.00052
132	N1	S	-0.06107	0.10825	-0.07349	-0.00858	0.08266
133	N1	PX	-0.00161	-0.01208	-0.00775	-0.18097	0.15605
134	N1	PY	0.13209	0.03397	-0.04997	0.03489	-0.05709
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.77712	0.29957	-0.38373	-0.12056	0.15982

137	N1	PX	0.09621	0.02421	0.10865	0.42586	-0.42377
138	N1	PY	-0.88707	0.49606	-0.42717	-0.13631	0.34839
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00403	0.02726	-0.00965	-0.01500	0.00250
141	N1	DYY	-0.07636	0.03173	-0.02322	-0.02890	0.05091
142	N1	DZZ	0.00528	-0.01196	0.00131	0.04060	-0.00545
143	N1	DXY	-0.01663	0.03105	-0.00978	-0.01820	-0.01485
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.05383	-0.13782	0.07007	0.09683	-0.02689
147	H6	S	-0.45080	-0.39645	-0.22824	-0.00484	0.49298
148	H6	PX	-0.03034	-0.01162	-0.01878	-0.00721	0.03164
149	H6	PY	-0.02271	-0.01437	0.00146	-0.01346	0.02268
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.00600	0.01925	-0.00445	0.00047	-0.00974
152	C8	S	-0.04913	0.36273	-0.19416	0.18178	-0.16815
153	C8	PX	-0.26067	0.34130	-0.13295	0.01867	-0.05912
154	C8	PY	-0.12096	0.23742	-0.03568	-0.11802	-0.13126
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.40313	-1.38695	0.49358	-0.46983	0.87188
157	C8	PX	1.02411	-1.46553	0.55939	0.17345	0.27864
158	C8	PY	1.37325	-1.15792	0.11697	0.15788	0.84439
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00762	-0.02302	-0.01013	-0.02792	0.06430
161	C8	DYY	0.00616	0.06587	-0.01005	-0.00308	-0.05683
162	C8	DZZ	-0.01090	0.00481	-0.00527	0.01636	-0.00512
163	C8	DXY	0.02515	-0.06768	0.01432	0.02978	0.03386
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.09255	0.03154	-0.02469	0.01918	0.03142
167	H8	S	-0.09934	-0.59593	0.31407	-0.39009	0.20660
168	H8	PX	-0.00910	0.04253	-0.01394	0.00620	-0.00813
169	H8	PY	0.00406	-0.00823	0.00511	-0.00798	0.02037
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00556	0.00740	0.00715	-0.01893	-0.01301
172	C10	S	-0.05148	0.19632	-0.33812	0.99306	-0.03232
173	C10	PX	0.04867	0.07408	-0.05942	0.16977	-0.11219
174	C10	PY	-0.00343	0.18581	0.14558	-0.50497	-0.25379
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.80049	-0.42904	0.60750	-2.06809	0.18155
177	C10	PX	-0.42862	0.01508	0.11369	-0.31916	0.14401
178	C10	PY	0.27929	-0.54960	-0.27087	0.87379	0.74511
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.02112	0.05039	0.04248	-0.14717	-0.06652
181	C10	DYY	0.00741	0.00742	-0.03067	0.10789	-0.00411
182	C10	DZZ	0.00526	-0.02615	-0.03945	0.12961	0.04740
183	C10	DXY	-0.00121	0.00623	0.03136	-0.05484	-0.03679
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.12297	0.16498	0.09960	-0.54482	-0.10191
187	H16	S	0.25178	-0.17985	-0.37392	1.31945	0.19548
188	H16	PX	-0.00667	-0.00559	0.03711	-0.11270	-0.00428
189	H16	PY	0.01229	-0.02209	0.01251	0.00644	-0.00422
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

191	H18	S	0.02860	-0.08736	0.24363	-0.47483	-0.14578
192	H18	S	-0.15377	-0.21689	-0.39165	1.15214	0.57292
193	H18	PX	0.00672	-0.02756	-0.02522	0.09174	0.03810
194	H18	PY	-0.01658	0.01203	-0.02070	0.03124	0.01759
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.01236	-0.02849	0.00799	0.00547	-0.03432
197	C9	S	-0.06911	0.57228	1.25476	0.40205	0.51909
198	C9	PX	0.07609	0.16679	0.17055	0.03054	0.29920
199	C9	PY	-0.02740	0.10872	0.23477	0.13860	-0.05993
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.47601	-1.17172	-3.04260	-1.04100	-1.25220
202	C9	PX	-0.21715	-0.24607	-0.36210	-0.03775	-0.32452
203	C9	PY	0.24417	-0.17398	-0.32523	-0.24162	-0.06693
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.03379	0.04808	0.05331	0.01569	0.04232
206	C9	DYY	-0.00624	0.00176	-0.02027	-0.01486	0.07522
207	C9	DZZ	-0.04445	-0.04389	0.08540	0.03831	-0.14096
208	C9	DXY	0.02616	0.03219	0.05260	0.02504	-0.00925
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.18089	-0.27685	-0.30122	-0.10247	0.01494
212	H3	S	-0.20351	0.47793	1.15773	0.49988	0.08984
213	H3	PX	-0.00377	0.00831	0.04010	0.01852	-0.00587
214	H3	PY	-0.01167	-0.05317	-0.06557	-0.02706	-0.01898
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.11222	-0.27764	-0.07562	-0.00761	-0.43512
217	H5	S	0.02722	0.48511	0.75554	0.20346	0.76038
218	H5	PX	0.00496	-0.00882	-0.03493	-0.01149	-0.00289
219	H5	PY	0.00447	0.01474	0.03049	0.01029	-0.00099
220	H5	PZ	0.01744	0.04893	0.02318	0.00138	0.08127
221	H7	S	-0.11222	-0.27764	-0.07562	-0.00761	-0.43512
222	H7	S	0.02722	0.48511	0.75554	0.20346	0.76038
223	H7	PX	0.00496	-0.00882	-0.03493	-0.01149	-0.00289
224	H7	PY	0.00447	0.01474	0.03049	0.01029	-0.00099
225	H7	PZ	-0.01744	-0.04893	-0.02318	-0.00138	-0.08127

MO:	106	107	108	109	110
Eigenvalues:	1.21214	1.24414	1.26238	1.28992	1.31200
(ev):	32.98403	33.85491	34.35121	35.10064	35.70137

			A	A	A	A	A
1	H1	S	-0.21684	0.10511	0.14845	-0.02904	0.00000
2	H1	S	0.92582	0.69236	0.51114	0.70170	0.00000
3	H1	PX	-0.04564	-0.03309	-0.00218	-0.01319	0.00000
4	H1	PY	0.00637	0.00951	0.02277	-0.01011	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	-0.03548
6	C1	S	0.00014	-0.00323	-0.00353	-0.00175	0.00000
7	C1	S	0.14693	-0.13303	0.57927	0.17415	0.00000
8	C1	PX	0.24925	0.37690	-0.01844	0.21698	0.00000
9	C1	PY	-0.07951	-0.06265	-0.33775	-0.30189	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.01390
11	C1	S	-0.87398	0.36068	-0.44056	-0.30671	0.00000
12	C1	PX	-0.77387	-1.07033	-1.28753	-0.71555	0.00000
13	C1	PY	-0.03738	0.29432	1.66558	0.20174	0.00000

14	C1	PZ	0.00000	0.00000	0.00000	0.00000	-0.21785
15	C1	DXX	-0.05619	-0.04457	0.07925	-0.00427	0.00000
16	C1	DYY	0.05271	-0.01272	0.01317	0.02305	0.00000
17	C1	DZZ	0.02848	0.03999	0.01289	0.02255	0.00000
18	C1	DXY	-0.02345	-0.02680	0.01112	-0.06611	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.08396
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00360
21	C2	S	-0.02085	0.00693	0.00160	0.01114	0.00000
22	C2	S	-0.35139	0.31731	0.05248	0.02432	0.00000
23	C2	PX	-0.15789	0.26498	-0.10126	0.02719	0.00000
24	C2	PY	0.35363	-0.06370	0.06379	-0.12691	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.04122
26	C2	S	1.55560	-0.52828	-0.36334	0.09000	0.00000
27	C2	PX	0.35162	-1.36803	0.82629	-0.06519	0.00000
28	C2	PY	-1.81122	2.08660	-0.25918	0.45881	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	-0.01100
30	C2	DXX	-0.03936	0.03295	0.04439	0.00069	0.00000
31	C2	DYY	-0.03216	0.04995	-0.05189	0.02117	0.00000
32	C2	DZZ	0.02102	-0.03604	0.02401	-0.01806	0.00000
33	C2	DXY	-0.13341	0.03193	-0.00570	0.02561	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.03471
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00073
36	C3	S	-0.00013	-0.00937	-0.01052	-0.02177	0.00000
37	C3	S	0.15695	-0.16640	0.22837	-0.67691	0.00000
38	C3	PX	0.07443	0.23517	-0.28117	0.22769	0.00000
39	C3	PY	0.01834	-0.01184	-0.32622	-0.09252	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.06487
41	C3	S	-1.14572	2.07966	0.68063	1.10364	0.00000
42	C3	PX	0.34925	-1.28077	1.57095	-1.37294	0.00000
43	C3	PY	0.07034	-0.84208	0.54933	0.00485	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	-0.04037
45	C3	DXX	-0.00420	0.04583	-0.00273	-0.10594	0.00000
46	C3	DYY	0.00950	-0.02016	0.05300	-0.06192	0.00000
47	C3	DZZ	0.01496	-0.00625	0.00203	0.03893	0.00000
48	C3	DXY	0.06571	0.08598	0.03538	0.04433	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	-0.02804
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00753
51	C4	S	0.00976	-0.01933	-0.00720	-0.00344	0.00000
52	C4	S	0.12006	-0.44846	-0.18026	0.29140	0.00000
53	C4	PX	-0.19026	0.27922	-0.00718	-0.01154	0.00000
54	C4	PY	-0.02341	0.19748	0.06910	-0.24838	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	-0.16381
56	C4	S	-1.57462	0.23481	-0.74958	-1.50099	0.00000
57	C4	PX	1.35779	-0.83939	-1.27590	0.43759	0.00000
58	C4	PY	-0.10404	-0.41852	0.58809	0.32299	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.69294
60	C4	DXX	-0.01790	-0.06747	-0.07124	0.03832	0.00000
61	C4	DYY	-0.03703	-0.04126	-0.03021	-0.09389	0.00000
62	C4	DZZ	0.02894	0.02705	0.03266	0.02599	0.00000
63	C4	DXY	-0.00380	0.05902	-0.02974	0.03162	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00700
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	-0.06147
66	C5	S	-0.01406	0.02573	-0.01000	-0.00792	0.00000
67	C5	S	-0.53880	0.62714	-0.30958	0.18540	0.00000

68	C5	PX	-0.15006	-0.00840	-0.06003	0.08041	0.00000
69	C5	PY	0.22151	0.11783	0.15149	-0.23924	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.06600
71	C5	S	2.54324	-3.06001	0.05453	0.22546	0.00000
72	C5	PX	0.80489	0.56768	-0.09964	0.03376	0.00000
73	C5	PY	-0.18922	0.50219	-1.04922	0.87647	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	-0.07711
75	C5	DXX	-0.03524	0.00330	-0.06985	0.05628	0.00000
76	C5	DYY	-0.04361	0.07013	-0.01293	-0.01525	0.00000
77	C5	DZZ	0.01826	-0.00066	0.02794	-0.00231	0.00000
78	C5	DXY	0.10458	-0.06102	-0.01080	0.03842	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.05756
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	-0.05389
81	C6	S	0.02446	0.00443	-0.00344	0.00929	0.00000
82	C6	S	0.87775	0.27574	-0.39825	-0.24555	0.00000
83	C6	PX	-0.31966	0.49141	-0.17371	0.10802	0.00000
84	C6	PY	0.06245	0.07181	0.24238	0.08697	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.06706
86	C6	S	-3.18225	-0.44922	1.99264	0.27736	0.00000
87	C6	PX	1.91084	-3.11440	0.79990	-1.00934	0.00000
88	C6	PY	0.24671	0.28706	-1.69868	-0.57133	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	-0.16109
90	C6	DXX	0.06563	0.06516	0.01234	-0.10385	0.00000
91	C6	DYY	0.00035	-0.00958	0.01212	0.06077	0.00000
92	C6	DZZ	0.02516	-0.01305	-0.01937	0.00219	0.00000
93	C6	DXY	0.00626	-0.07061	0.05334	-0.02431	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00344
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.02578
96	C7	S	-0.00066	-0.01154	0.01902	-0.00120	0.00000
97	C7	S	-0.35655	-0.59170	-0.42509	-0.15167	0.00000
98	C7	PX	0.11873	-0.23889	0.11479	-0.06216	0.00000
99	C7	PY	-0.15885	-0.13028	-0.15763	-0.10909	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	-0.05110
101	C7	S	0.66998	0.80359	0.20595	0.29866	0.00000
102	C7	PX	-0.40449	1.17914	0.50624	-0.04455	0.00000
103	C7	PY	0.27831	0.34328	-0.29365	1.08222	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.12496
105	C7	DXX	0.00041	-0.04629	-0.06840	0.01228	0.00000
106	C7	DYY	-0.05436	-0.01509	0.02018	-0.00258	0.00000
107	C7	DZZ	0.00264	-0.01394	-0.02453	-0.00177	0.00000
108	C7	DXY	-0.03772	0.00323	0.01843	-0.01125	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.01754
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00090
111	O1	S	-0.00272	-0.00063	0.00932	-0.00154	0.00000
112	O1	S	0.18752	0.06420	0.17595	0.07162	0.00000
113	O1	PX	-0.08752	0.02307	-0.17924	-0.11557	0.00000
114	O1	PY	0.02853	-0.06486	0.09293	0.32979	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.89368
116	O1	S	-0.10384	0.03755	-0.55689	-0.06412	0.00000
117	O1	PX	-0.13813	0.08208	0.38265	0.04772	0.00000
118	O1	PY	-0.34777	0.03851	-0.09649	-0.71209	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	-1.30584
120	O1	DXX	0.05940	0.01518	0.02244	0.06313	0.00000
121	O1	DYY	0.08882	0.03872	0.07831	0.00208	0.00000

122	O1	DZZ	0.03487	0.00626	0.10047	0.04051	0.00000
123	O1	DXY	0.01417	-0.02438	0.02176	-0.00398	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.02743
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.01129
126	H4	S	-0.20388	0.08075	0.12908	-0.21431	0.00000
127	H4	S	0.37254	0.36507	0.31973	-0.23741	0.00000
128	H4	PX	0.02849	0.03560	0.00194	-0.00954	0.00000
129	H4	PY	-0.00097	-0.00161	0.00118	0.00052	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	-0.03337
131	N1	S	0.00462	0.00087	-0.00902	-0.00385	0.00000
132	N1	S	0.18821	-0.01975	-0.05145	0.27352	0.00000
133	N1	PX	0.10133	0.05949	-0.13284	0.02056	0.00000
134	N1	PY	-0.20812	-0.22705	0.14274	0.28361	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	-0.08362
136	N1	S	0.03652	-0.09087	-0.39746	0.01071	0.00000
137	N1	PX	-0.79117	0.28853	0.60960	0.50981	0.00000
138	N1	PY	0.95984	0.43751	-0.78939	-0.94533	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.18710
140	N1	DXX	0.01205	0.01095	0.02856	0.10460	0.00000
141	N1	DYY	0.11397	0.00096	-0.10642	0.02044	0.00000
142	N1	DZZ	-0.00600	-0.00726	0.02334	-0.00252	0.00000
143	N1	DXY	0.01198	0.02598	-0.05041	-0.02137	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00884
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01394
146	H6	S	-0.22127	-0.13569	0.23004	-0.04675	0.00000
147	H6	S	-0.10305	-0.36045	0.35207	0.02711	0.00000
148	H6	PX	0.00374	-0.01370	-0.00852	0.01046	0.00000
149	H6	PY	0.01106	0.01448	0.01363	-0.02725	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	-0.01043
151	C8	S	-0.00876	0.00163	0.01724	0.00824	0.00000
152	C8	S	-0.39288	0.03776	0.37415	0.52273	0.00000
153	C8	PX	0.11474	0.09484	0.00837	-0.08659	0.00000
154	C8	PY	-0.10454	0.01533	0.34543	-0.09524	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.02018
156	C8	S	1.31443	0.05389	-0.77535	-1.73110	0.00000
157	C8	PX	-0.78614	-0.24986	0.90102	1.32473	0.00000
158	C8	PY	-0.11046	0.74193	-1.01047	0.27627	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	-0.10435
160	C8	DXX	-0.00308	0.04237	0.00866	0.05745	0.00000
161	C8	DYY	-0.04885	0.00022	0.06034	-0.00940	0.00000
162	C8	DZZ	0.00690	-0.01054	-0.02498	0.01696	0.00000
163	C8	DXY	-0.02782	0.00635	-0.00176	0.04306	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00463
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	-0.01434
166	H8	S	0.16773	-0.02269	-0.43883	0.18006	0.00000
167	H8	S	-0.04077	-0.85450	-0.18300	-0.11173	0.00000
168	H8	PX	0.00572	0.04548	-0.02534	0.02336	0.00000
169	H8	PY	0.00538	0.00500	0.00723	0.03225	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.01428
171	C10	S	-0.00069	-0.01109	-0.00352	-0.00650	0.00000
172	C10	S	0.34930	0.13360	0.21959	-0.60561	0.00000
173	C10	PX	-0.06801	0.09289	0.00996	-0.05760	0.00000
174	C10	PY	-0.17295	-0.05461	0.19299	-0.24572	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.01152

176	C10	S	-1.19547	0.22603	-0.75172	1.48110	0.00000
177	C10	PX	0.36691	-0.42311	-0.52336	-0.35827	0.00000
178	C10	PY	0.29228	0.42100	-0.73235	0.52709	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00637
180	C10	DXX	-0.04040	-0.03413	0.08028	-0.04491	0.00000
181	C10	DYY	0.02166	0.00058	-0.04783	-0.00945	0.00000
182	C10	DZZ	0.05376	0.03714	-0.01048	-0.02583	0.00000
183	C10	DXY	-0.00660	-0.02546	-0.03952	-0.05106	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	-0.00562
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00161
186	H16	S	-0.04818	-0.04376	0.18791	0.02707	0.00000
187	H16	S	0.25763	0.41301	0.00957	-0.08654	0.00000
188	H16	PX	-0.01735	-0.02579	0.00351	0.01965	0.00000
189	H16	PY	-0.00792	-0.01187	-0.01270	-0.01068	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	-0.00139
191	H18	S	-0.09729	-0.19962	-0.19232	-0.13063	0.00000
192	H18	S	0.63962	0.18212	-0.28093	-0.10504	0.00000
193	H18	PX	0.03015	0.00378	-0.01844	0.01172	0.00000
194	H18	PY	0.02232	0.01301	0.02793	0.00491	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00115
196	C9	S	-0.00030	0.01094	-0.01323	0.00810	0.00000
197	C9	S	-0.25940	-0.00676	-0.24006	-0.00135	0.00000
198	C9	PX	-0.06453	-0.01280	0.05003	-0.03826	0.00000
199	C9	PY	-0.04055	-0.20053	-0.04761	0.07557	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.03576
201	C9	S	0.88392	0.07191	0.59488	0.15526	0.00000
202	C9	PX	-0.09423	-0.06363	-0.08421	-0.19331	0.00000
203	C9	PY	0.39010	0.29738	0.30830	0.21125	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.47754
205	C9	DXX	-0.03115	0.00638	-0.03902	-0.05157	0.00000
206	C9	DYY	-0.05500	0.01864	-0.04208	-0.04265	0.00000
207	C9	DZZ	0.06973	0.00588	0.02837	0.12195	0.00000
208	C9	DXY	0.01495	-0.03736	-0.01191	0.09204	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	-0.01271
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.13669
211	H3	S	-0.18435	0.16437	-0.10238	-0.19870	0.00000
212	H3	S	-0.23111	-0.32332	-0.22466	0.09266	0.00000
213	H3	PX	0.00897	-0.02624	0.00597	0.06077	0.00000
214	H3	PY	0.00694	0.03091	0.00976	0.00224	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.07959
216	H5	S	0.14212	0.11151	0.01905	0.13284	0.12674
217	H5	S	-0.31950	-0.02019	-0.15374	-0.13259	0.08823
218	H5	PX	-0.01206	0.00982	-0.01450	-0.03980	-0.02936
219	H5	PY	0.00926	-0.00147	0.00250	0.02351	-0.06824
220	H5	PZ	-0.03157	0.00016	-0.00870	-0.04583	0.00031
221	H7	S	0.14212	0.11151	0.01905	0.13284	-0.12674
222	H7	S	-0.31950	-0.02019	-0.15374	-0.13259	-0.08823
223	H7	PX	-0.01206	0.00982	-0.01450	-0.03980	0.02936
224	H7	PY	0.00926	-0.00147	0.00250	0.02351	0.06824
225	H7	PZ	0.03157	-0.00016	0.00870	0.04583	0.00031

MO:	111	112	113	114	115
Eigenvalues:	1.32518	1.38955	1.40283	1.43085	1.44189
(ev):	36.05988	37.81152	38.17308	38.93552	39.23593

		A	A	A	A	A	
1	H1	S	0.24323	-0.18973	-0.15681	0.39863	0.41746
2	H1	S	-0.31426	0.20582	-0.30281	0.28971	0.52346
3	H1	PX	0.03043	-0.02886	-0.00866	-0.00712	0.00789
4	H1	PY	0.00012	-0.02112	-0.00137	-0.02258	0.00920
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.00226	0.02531	0.01688	0.01250	0.01621
7	C1	S	0.37608	0.45633	0.30298	0.01441	0.49269
8	C1	PX	-0.31523	0.10331	-0.16626	0.22062	-0.08212
9	C1	PY	0.20206	0.09509	0.13929	0.19378	0.25830
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.97764	-2.56479	-1.60913	-2.67605	-1.76407
12	C1	PX	1.51170	0.44336	1.50669	0.44054	-0.88679
13	C1	PY	-3.94887	0.73740	-0.99287	-3.47423	-0.64809
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.04321	0.03832	-0.03234	0.05481	0.10750
16	C1	DYY	0.03874	0.01596	0.03994	-0.05737	-0.03212
17	C1	DZZ	-0.01780	-0.02297	0.01094	-0.00787	-0.01061
18	C1	DXY	0.11616	-0.03919	0.04169	0.12768	0.05879
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00416	0.02343	0.01165	0.00787	-0.01066
22	C2	S	-0.38503	0.59148	0.21648	0.63036	-0.28439
23	C2	PX	-0.15856	0.04926	-0.06282	0.29974	0.02257
24	C2	PY	-0.25834	-0.12448	0.02914	0.21034	-0.10859
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.64566	-2.24522	-1.23886	-0.16494	0.89136
27	C2	PX	-0.89269	-0.34595	-0.14029	-0.41590	-0.96315
28	C2	PY	2.09254	0.37308	1.12802	-0.90981	0.72873
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.09734	0.06048	0.04620	0.05965	-0.06467
31	C2	DYY	0.03500	0.04792	-0.02036	0.02190	0.02150
32	C2	DZZ	-0.00864	-0.03573	0.00570	0.00317	0.01106
33	C2	DXY	0.01216	0.05762	-0.00293	-0.06686	-0.03878
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00843	0.00276	-0.00511	-0.00622	-0.02441
37	C3	S	0.34117	-0.25382	-0.08341	-0.10878	-0.73411
38	C3	PX	0.39302	-0.09602	-0.11995	0.29704	-0.18955
39	C3	PY	-0.05948	-0.25964	0.32786	0.02348	-0.03781
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-2.11717	1.91337	1.69674	-0.86518	2.60288
42	C3	PX	-2.69227	1.11612	-0.28756	-1.78607	1.39338
43	C3	PY	-2.19785	1.23906	-1.29306	-1.21229	-0.51876
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.02060	0.00579	0.00047	-0.02281	0.00166
46	C3	DYY	-0.01637	0.03353	0.03122	-0.03278	-0.05025
47	C3	DZZ	0.01668	-0.05734	-0.00703	0.01494	-0.01015
48	C3	DXY	-0.00902	-0.00304	-0.00244	-0.06955	-0.00822
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00828	-0.00474	-0.00471	0.00804	0.00679
52	C4	S	-0.17955	0.16306	-0.24883	-0.02840	-0.14671

53	C4	PX	-0.43119	0.00737	-0.15378	-0.37145	-0.13771
54	C4	PY	0.15094	-0.08479	0.08048	0.14315	0.19012
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	1.62738	-0.28058	1.76256	1.01312	-0.71170
57	C4	PX	4.15538	-0.08707	1.48868	4.94507	1.11645
58	C4	PY	0.06531	-0.99243	-0.76069	-1.22448	0.39803
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.03552	0.08391	-0.03413	0.02010	-0.03066
61	C4	DYY	0.01799	-0.06916	0.04795	0.03397	0.00170
62	C4	DZZ	-0.04420	-0.04393	-0.00839	-0.01827	-0.00295
63	C4	DXY	-0.06181	-0.04635	-0.06761	0.00009	-0.06036
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.00170	0.00214	-0.01077	-0.03814	-0.00689
67	C5	S	0.25751	-0.19340	-0.37421	-0.62970	-0.04697
68	C5	PX	-0.06005	-0.09713	-0.17901	0.22268	-0.11751
69	C5	PY	-0.22758	0.04228	0.09477	0.03601	-0.07210
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.18830	0.48761	0.44628	4.74132	0.16194
72	C5	PX	2.16539	-0.43037	0.90094	0.61882	1.81747
73	C5	PY	1.59804	0.18840	0.27157	1.54207	0.19289
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.10789	-0.03357	-0.05696	-0.05394	-0.00621
76	C5	DYY	-0.02922	0.02669	-0.03635	-0.00980	-0.01157
77	C5	DZZ	-0.01558	-0.03596	0.03237	-0.00112	0.01858
78	C5	DXY	-0.03334	0.03949	-0.00109	0.13816	-0.03926
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.00035	-0.02231	0.00423	-0.00236	0.01779
82	C6	S	0.05511	-0.19606	-0.07892	0.00874	0.54520
83	C6	PX	0.05306	0.16798	0.06233	-0.08332	0.11214
84	C6	PY	-0.09501	-0.46294	0.09580	0.14460	0.22395
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.95290	0.15908	-0.19989	-0.89825	-0.93891
87	C6	PX	-2.08402	-0.24963	-1.84162	0.21772	-0.56176
88	C6	PY	1.42065	2.20170	0.41451	-1.03758	0.42661
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.01524	0.06493	0.00229	-0.04735	0.06447
91	C6	DYY	-0.04205	-0.13524	-0.03636	0.03031	0.02718
92	C6	DZZ	0.00517	0.00523	0.01387	0.01421	-0.01735
93	C6	DXY	-0.05356	-0.05620	-0.03953	-0.05661	0.00923
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.00840	-0.00034	-0.01532	0.01666	-0.00271
97	C7	S	-0.54378	0.12312	-0.05757	0.24504	0.16078
98	C7	PX	0.22628	-0.09855	0.10957	-0.06683	-0.03049
99	C7	PY	0.03857	0.16623	0.16741	0.02780	-0.15762
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	0.73761	0.04372	-0.93031	-0.52063	-0.24779
102	C7	PX	0.25722	0.41346	0.20207	1.19984	-0.42775
103	C7	PY	0.82272	-1.43309	-0.94841	0.56331	-1.70423
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.10499	-0.00547	-0.02805	-0.03168	0.05217
106	C7	DYY	0.02021	0.02112	-0.02540	0.08943	-0.00955

107	C7	DZZ	-0.00679	-0.00613	0.02636	-0.02722	0.00208
108	C7	DXY	-0.06936	-0.00056	0.04233	-0.00026	0.08102
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00936	-0.01011	0.00257	-0.00689	0.00796
112	O1	S	-0.13271	-0.14846	0.11623	-0.09084	-0.03382
113	O1	PX	-0.01542	-0.03818	-0.03358	-0.08543	-0.20422
114	O1	PY	0.17242	0.28150	-0.18753	-0.14049	0.16030
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	-0.06742	0.46115	-0.16238	0.56299	-0.25144
117	O1	PX	-0.28673	-0.18563	-0.02686	-0.47662	0.23509
118	O1	PY	0.21259	-0.86861	0.39587	0.26626	-0.04301
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.00532	-0.04312	0.00467	0.00704	-0.06193
121	O1	DYY	-0.07358	-0.05462	0.05149	0.01127	0.00927
122	O1	DZZ	-0.01254	-0.01140	0.02639	-0.09812	0.07172
123	O1	DXY	0.02760	0.00124	0.03308	-0.05112	0.02564
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.24532	-0.29586	0.03924	-0.47545	0.32724
127	H4	S	0.07100	-0.16563	0.19434	-0.65234	0.43555
128	H4	PX	-0.02593	0.00688	0.00500	0.00323	0.00089
129	H4	PY	0.00622	-0.02287	-0.00497	0.01825	0.03306
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00108	0.01638	-0.00129	-0.00857	-0.01034
132	N1	S	0.13323	-0.13317	0.12693	-0.15497	-0.22945
133	N1	PX	0.16654	0.19043	0.14532	-0.19196	-0.04724
134	N1	PY	-0.05851	-0.47065	-0.19863	-0.01248	0.06398
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.66026	-0.15586	-0.03572	0.45536	0.09086
137	N1	PX	-0.16932	-1.13382	0.01918	0.54388	-0.05230
138	N1	PY	0.36282	1.81563	0.12648	-0.27014	0.65464
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.07098	-0.06692	0.06500	-0.01372	-0.09706
141	N1	DYY	0.03875	0.07078	0.02835	-0.05620	-0.04289
142	N1	DZZ	-0.02865	-0.01287	-0.01312	0.00056	0.00120
143	N1	DXY	0.05557	0.02458	-0.01846	0.00337	0.00416
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.20019	0.22357	0.18740	-0.05120	-0.28056
147	H6	S	-0.03485	0.12300	0.21197	-0.20600	-0.31056
148	H6	PX	0.01991	0.00059	-0.00573	-0.01344	0.00432
149	H6	PY	0.01688	0.00984	0.02623	-0.02785	0.01954
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.01295	-0.00776	0.03698	0.00210	0.01444
152	C8	S	-0.22683	-0.19863	0.97491	0.08825	0.25837
153	C8	PX	-0.00373	0.14467	0.18258	-0.06063	0.27689
154	C8	PY	0.07710	0.04746	-0.47018	0.06600	-0.03778
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	1.15944	1.06689	-4.86905	0.30701	-1.55296
157	C8	PX	0.60537	-2.42147	-0.60283	1.16673	-2.57434
158	C8	PY	0.33020	0.96963	3.14729	-0.44958	-0.46389
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00042	0.05795	0.10979	-0.00720	0.00483

161	C8	DYY	-0.02017	-0.01737	-0.05661	0.03292	0.01504
162	C8	DZZ	0.00422	-0.01514	0.02788	-0.01747	0.00093
163	C8	DXY	-0.06930	-0.04073	-0.00054	0.04317	0.02431
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.10264	-0.09844	0.04286	-0.25029	0.12811
167	H8	S	-0.13271	-0.22347	-0.00192	-0.37853	0.14519
168	H8	PX	-0.01951	0.00241	-0.01309	-0.01801	0.00531
169	H8	PY	-0.02732	-0.02821	-0.00645	-0.00310	-0.01173
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.00112	-0.00484	-0.03301	0.00252	-0.00223
172	C10	S	0.22121	0.19612	-1.07890	-0.00060	-0.18095
173	C10	PX	-0.01205	0.10953	0.08257	0.05305	-0.01913
174	C10	PY	0.06332	0.13894	-0.17635	-0.02165	-0.02950
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-0.54625	0.41071	5.52727	-0.53744	0.79424
177	C10	PX	-0.72910	0.20724	-1.04782	-0.47740	1.59106
178	C10	PY	-0.23231	0.30781	2.01238	-0.36103	0.53351
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.03701	-0.02004	-0.14916	0.03196	-0.06231
181	C10	DYY	-0.04080	0.00116	0.06675	-0.02337	0.06799
182	C10	DZZ	0.02664	0.03501	-0.02755	-0.01638	-0.02324
183	C10	DXY	-0.06463	0.02885	-0.11032	-0.03103	0.10139
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.27649	-0.02991	0.05870	0.07743	-0.38380
187	H16	S	0.27556	0.07188	-0.03491	0.13563	-0.56041
188	H16	PX	0.00256	-0.02207	0.01008	-0.00446	-0.00504
189	H16	PY	-0.03580	-0.01039	-0.05071	0.00059	0.03778
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.25564	0.03231	-0.33475	-0.06506	0.35519
192	H18	S	-0.03152	0.13355	-0.30006	-0.19306	0.34519
193	H18	PX	-0.00710	-0.02096	-0.01411	-0.00383	0.00902
194	H18	PY	0.03849	-0.00596	-0.00588	0.00395	-0.04558
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.02871	-0.03967	-0.00292	0.00300	-0.02296
197	C9	S	0.42319	-0.52183	-0.03550	0.18153	-0.25532
198	C9	PX	-0.07277	0.00895	0.02327	-0.06194	0.04796
199	C9	PY	0.21236	0.15718	-0.00358	0.15183	0.16303
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-1.30888	1.56714	-0.00297	-0.54577	0.40380
202	C9	PX	0.24386	-0.23462	0.10161	0.20459	0.07209
203	C9	PY	-0.46923	-0.23025	-0.02020	-0.35806	-0.28556
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.00497	-0.05236	0.02080	-0.02768	-0.04877
206	C9	DYY	0.03582	-0.03904	-0.00053	0.04787	-0.02202
207	C9	DZZ	0.03291	0.01133	-0.04497	-0.02236	-0.00267
208	C9	DXY	0.05709	0.09287	-0.06027	-0.00158	-0.00247
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.06684	-0.24692	0.01435	-0.02269	-0.07856
212	H3	S	0.58276	-0.01640	-0.03052	0.32685	0.14905
213	H3	PX	0.03864	0.06118	-0.03495	-0.00234	0.02210
214	H3	PY	-0.02135	-0.01105	-0.00827	-0.03345	-0.01628

215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.01183	-0.16666	-0.03465	-0.08042	-0.13525
217	H5	S	0.19060	-0.23123	-0.00305	0.11290	-0.07953
218	H5	PX	-0.01352	-0.02666	0.01724	0.00064	-0.01634
219	H5	PY	0.00174	0.00539	-0.01336	-0.00733	-0.01217
220	H5	PZ	-0.01554	-0.01834	0.01791	0.00143	-0.00109
221	H7	S	0.01183	-0.16666	-0.03465	-0.08042	-0.13525
222	H7	S	0.19060	-0.23123	-0.00305	0.11290	-0.07953
223	H7	PX	-0.01352	-0.02666	0.01724	0.00064	-0.01634
224	H7	PY	0.00174	0.00539	-0.01336	-0.00733	-0.01217
225	H7	PZ	0.01554	0.01834	-0.01791	-0.00143	0.00109

MO:		116	117	118	119	120
Eigenvalues:		1.47318	1.48252	1.51650	1.55009	1.58637
(ev):		40.08715	40.34143	41.26607	42.18025	43.16741

		A	A	A	A	A	
1	H1	S	0.00000	-0.08782	-0.18463	0.00000	0.00000
2	H1	S	0.00000	-0.14642	-0.45293	0.00000	0.00000
3	H1	PX	0.00000	0.01095	-0.02810	0.00000	0.00000
4	H1	PY	0.00000	-0.00672	-0.01599	0.00000	0.00000
5	H1	PZ	0.01441	0.00000	0.00000	-0.11751	0.08260
6	C1	S	0.00000	-0.01273	0.00339	0.00000	0.00000
7	C1	S	0.00000	0.00838	0.05028	0.00000	0.00000
8	C1	PX	0.00000	-0.14005	0.00576	0.00000	0.00000
9	C1	PY	0.00000	0.02018	0.16580	0.00000	0.00000
10	C1	PZ	-0.02292	0.00000	0.00000	-0.08732	0.07378
11	C1	S	0.00000	0.89229	-0.06489	0.00000	0.00000
12	C1	PX	0.00000	0.97679	1.03613	0.00000	0.00000
13	C1	PY	0.00000	-2.31024	-0.25144	0.00000	0.00000
14	C1	PZ	0.01278	0.00000	0.00000	0.06685	-0.06528
15	C1	DXX	0.00000	-0.04013	-0.00255	0.00000	0.00000
16	C1	DYY	0.00000	0.01504	0.02318	0.00000	0.00000
17	C1	DZZ	0.00000	0.02785	-0.01948	0.00000	0.00000
18	C1	DXY	0.00000	-0.00663	-0.03503	0.00000	0.00000
19	C1	DXZ	-0.04134	0.00000	0.00000	-0.27508	0.15174
20	C1	DYZ	0.29314	0.00000	0.00000	-0.00356	0.19797
21	C2	S	0.00000	0.01542	0.01909	0.00000	0.00000
22	C2	S	0.00000	0.37280	0.28068	0.00000	0.00000
23	C2	PX	0.00000	-0.02837	0.14259	0.00000	0.00000
24	C2	PY	0.00000	-0.13622	0.04154	0.00000	0.00000
25	C2	PZ	-0.01632	0.00000	0.00000	-0.03230	-0.06947
26	C2	S	0.00000	-1.96039	-0.82169	0.00000	0.00000
27	C2	PX	0.00000	0.51819	-1.64223	0.00000	0.00000
28	C2	PY	0.00000	2.27039	0.68768	0.00000	0.00000
29	C2	PZ	0.02475	0.00000	0.00000	-0.06969	0.01066
30	C2	DXX	0.00000	0.11598	-0.05272	0.00000	0.00000
31	C2	DYY	0.00000	-0.06735	0.06807	0.00000	0.00000
32	C2	DZZ	0.00000	0.01648	-0.01147	0.00000	0.00000
33	C2	DXY	0.00000	0.05408	0.01380	0.00000	0.00000
34	C2	DXZ	-0.15032	0.00000	0.00000	0.16973	0.17053
35	C2	DYZ	0.23215	0.00000	0.00000	0.08673	0.01933
36	C3	S	0.00000	-0.02874	0.00934	0.00000	0.00000
37	C3	S	0.00000	-0.26349	0.12225	0.00000	0.00000

38	C3	PX	0.00000	0.10225	0.12526	0.00000	0.00000
39	C3	PY	0.00000	0.26170	0.06411	0.00000	0.00000
40	C3	PZ	-0.01522	0.00000	0.00000	0.03593	-0.02248
41	C3	S	0.00000	0.06632	-1.18154	0.00000	0.00000
42	C3	PX	0.00000	-3.57130	-1.05017	0.00000	0.00000
43	C3	PY	0.00000	-1.98264	0.60807	0.00000	0.00000
44	C3	PZ	-0.03168	0.00000	0.00000	-0.05514	-0.04242
45	C3	DXX	0.00000	-0.00570	0.01650	0.00000	0.00000
46	C3	DYY	0.00000	-0.08255	-0.02201	0.00000	0.00000
47	C3	DZZ	0.00000	0.06860	-0.00750	0.00000	0.00000
48	C3	DXY	0.00000	0.05538	-0.02313	0.00000	0.00000
49	C3	DXZ	-0.17487	0.00000	0.00000	-0.07999	0.05513
50	C3	DYZ	-0.28175	0.00000	0.00000	0.11874	-0.18349
51	C4	S	0.00000	0.02017	-0.00030	0.00000	0.00000
52	C4	S	0.00000	0.33722	-0.14553	0.00000	0.00000
53	C4	PX	0.00000	-0.26129	0.21157	0.00000	0.00000
54	C4	PY	0.00000	-0.07400	0.05234	0.00000	0.00000
55	C4	PZ	-0.04041	0.00000	0.00000	0.08178	-0.03869
56	C4	S	0.00000	-0.09336	0.67669	0.00000	0.00000
57	C4	PX	0.00000	2.38520	-0.74554	0.00000	0.00000
58	C4	PY	0.00000	0.84262	-0.77986	0.00000	0.00000
59	C4	PZ	0.06677	0.00000	0.00000	-0.17715	0.04379
60	C4	DXX	0.00000	-0.01755	-0.05110	0.00000	0.00000
61	C4	DYY	0.00000	0.07168	0.01771	0.00000	0.00000
62	C4	DZZ	0.00000	0.01036	-0.00162	0.00000	0.00000
63	C4	DXY	0.00000	-0.03925	-0.06524	0.00000	0.00000
64	C4	DXZ	0.31383	0.00000	0.00000	0.14993	0.11573
65	C4	DYZ	0.00070	0.00000	0.00000	-0.27489	0.15813
66	C5	S	0.00000	-0.02844	0.00109	0.00000	0.00000
67	C5	S	0.00000	-0.61476	0.07941	0.00000	0.00000
68	C5	PX	0.00000	-0.08086	-0.13578	0.00000	0.00000
69	C5	PY	0.00000	0.13967	-0.22160	0.00000	0.00000
70	C5	PZ	-0.02849	0.00000	0.00000	-0.06514	0.02648
71	C5	S	0.00000	1.52300	-0.87181	0.00000	0.00000
72	C5	PX	0.00000	1.39936	0.63067	0.00000	0.00000
73	C5	PY	0.00000	0.40757	0.54516	0.00000	0.00000
74	C5	PZ	0.01838	0.00000	0.00000	0.14723	-0.02610
75	C5	DXX	0.00000	-0.02453	-0.08162	0.00000	0.00000
76	C5	DYY	0.00000	-0.07437	0.04546	0.00000	0.00000
77	C5	DZZ	0.00000	0.03758	0.00890	0.00000	0.00000
78	C5	DXY	0.00000	-0.00459	-0.01108	0.00000	0.00000
79	C5	DXZ	-0.23893	0.00000	0.00000	0.01188	-0.07217
80	C5	DYZ	-0.14357	0.00000	0.00000	-0.16385	-0.04011
81	C6	S	0.00000	0.00261	-0.00881	0.00000	0.00000
82	C6	S	0.00000	0.01590	-0.28440	0.00000	0.00000
83	C6	PX	0.00000	0.44602	0.07520	0.00000	0.00000
84	C6	PY	0.00000	0.07638	-0.00344	0.00000	0.00000
85	C6	PZ	-0.00017	0.00000	0.00000	0.01945	-0.02190
86	C6	S	0.00000	-0.83586	2.61537	0.00000	0.00000
87	C6	PX	0.00000	-4.12073	-1.14317	0.00000	0.00000
88	C6	PY	0.00000	-1.31299	-0.02725	0.00000	0.00000
89	C6	PZ	-0.03445	0.00000	0.00000	0.00997	0.17687
90	C6	DXX	0.00000	-0.05847	-0.01710	0.00000	0.00000
91	C6	DYY	0.00000	0.06805	0.06494	0.00000	0.00000

92	C6	DZZ	0.00000	0.00266	-0.03797	0.00000	0.00000
93	C6	DXY	0.00000	-0.00211	-0.00711	0.00000	0.00000
94	C6	DXZ	0.31078	0.00000	0.00000	-0.00408	0.01403
95	C6	DYZ	-0.10445	0.00000	0.00000	0.14200	0.17351
96	C7	S	0.00000	-0.03367	0.00243	0.00000	0.00000
97	C7	S	0.00000	-0.47307	-0.02542	0.00000	0.00000
98	C7	PX	0.00000	0.02670	0.03286	0.00000	0.00000
99	C7	PY	0.00000	-0.02595	0.15003	0.00000	0.00000
100	C7	PZ	-0.08546	0.00000	0.00000	0.05583	0.00210
101	C7	S	0.00000	2.95027	-0.16454	0.00000	0.00000
102	C7	PX	0.00000	-1.97123	-0.72901	0.00000	0.00000
103	C7	PY	0.00000	1.21623	1.31634	0.00000	0.00000
104	C7	PZ	0.12576	0.00000	0.00000	0.01426	0.02608
105	C7	DXX	0.00000	0.02524	0.03164	0.00000	0.00000
106	C7	DYY	0.00000	-0.06441	-0.03207	0.00000	0.00000
107	C7	DZZ	0.00000	0.03761	-0.00651	0.00000	0.00000
108	C7	DXY	0.00000	0.03684	-0.05798	0.00000	0.00000
109	C7	DXZ	-0.17653	0.00000	0.00000	0.20333	0.16607
110	C7	DYZ	0.00947	0.00000	0.00000	-0.00263	0.30802
111	O1	S	0.00000	0.00788	0.01135	0.00000	0.00000
112	O1	S	0.00000	0.08318	0.32579	0.00000	0.00000
113	O1	PX	0.00000	-0.06796	-0.32039	0.00000	0.00000
114	O1	PY	0.00000	-0.11693	-0.02427	0.00000	0.00000
115	O1	PZ	0.03363	0.00000	0.00000	-0.00535	-0.02675
116	O1	S	0.00000	-0.39512	-0.80203	0.00000	0.00000
117	O1	PX	0.00000	0.04954	0.54989	0.00000	0.00000
118	O1	PY	0.00000	0.52694	-0.08493	0.00000	0.00000
119	O1	PZ	-0.08111	0.00000	0.00000	0.03999	0.01845
120	O1	DXX	0.00000	0.01944	-0.05517	0.00000	0.00000
121	O1	DYY	0.00000	0.03686	0.18331	0.00000	0.00000
122	O1	DZZ	0.00000	0.01127	0.17000	0.00000	0.00000
123	O1	DXY	0.00000	0.01406	0.09160	0.00000	0.00000
124	O1	DXZ	0.09819	0.00000	0.00000	0.22434	-0.06201
125	O1	DYZ	-0.01206	0.00000	0.00000	0.18480	-0.11423
126	H4	S	0.00000	-0.01906	0.01572	0.00000	0.00000
127	H4	S	0.00000	0.09988	0.14194	0.00000	0.00000
128	H4	PX	0.00000	-0.00440	0.02638	0.00000	0.00000
129	H4	PY	0.00000	-0.00847	0.04530	0.00000	0.00000
130	H4	PZ	0.02329	0.00000	0.00000	-0.03184	0.01175
131	N1	S	0.00000	0.00499	-0.00029	0.00000	0.00000
132	N1	S	0.00000	-0.05220	0.19890	0.00000	0.00000
133	N1	PX	0.00000	0.15540	-0.04241	0.00000	0.00000
134	N1	PY	0.00000	0.06462	0.18471	0.00000	0.00000
135	N1	PZ	-0.08639	0.00000	0.00000	0.02514	0.11935
136	N1	S	0.00000	0.21684	0.09867	0.00000	0.00000
137	N1	PX	0.00000	1.07664	0.75849	0.00000	0.00000
138	N1	PY	0.00000	-0.36650	-1.34838	0.00000	0.00000
139	N1	PZ	0.10906	0.00000	0.00000	0.03950	-0.21204
140	N1	DXX	0.00000	0.01755	0.07674	0.00000	0.00000
141	N1	DYY	0.00000	-0.03361	-0.00139	0.00000	0.00000
142	N1	DZZ	0.00000	-0.00920	-0.00362	0.00000	0.00000
143	N1	DXY	0.00000	-0.03906	0.01802	0.00000	0.00000
144	N1	DXZ	0.12709	0.00000	0.00000	-0.04521	0.08837
145	N1	DYZ	0.03649	0.00000	0.00000	-0.10084	-0.18932

146	H6	S	0.00000	0.44127	-0.27131	0.00000	0.00000
147	H6	S	0.00000	0.64761	-0.44334	0.00000	0.00000
148	H6	PX	0.00000	-0.01031	0.00784	0.00000	0.00000
149	H6	PY	0.00000	0.01662	0.00692	0.00000	0.00000
150	H6	PZ	0.02663	0.00000	0.00000	-0.09168	-0.07751
151	C8	S	0.00000	-0.00675	-0.01918	0.00000	0.00000
152	C8	S	0.00000	-0.25678	-0.39393	0.00000	0.00000
153	C8	PX	0.00000	-0.02738	-0.28421	0.00000	0.00000
154	C8	PY	0.00000	0.49280	-0.00613	0.00000	0.00000
155	C8	PZ	0.09840	0.00000	0.00000	-0.02193	-0.03054
156	C8	S	0.00000	1.66880	1.03196	0.00000	0.00000
157	C8	PX	0.00000	1.13347	2.67054	0.00000	0.00000
158	C8	PY	0.00000	-5.16351	-0.10548	0.00000	0.00000
159	C8	PZ	-0.25281	0.00000	0.00000	0.00271	0.05986
160	C8	DXX	0.00000	0.01707	-0.07091	0.00000	0.00000
161	C8	DYY	0.00000	0.00383	0.00527	0.00000	0.00000
162	C8	DZZ	0.00000	-0.02351	0.00752	0.00000	0.00000
163	C8	DXY	0.00000	-0.00380	-0.01113	0.00000	0.00000
164	C8	DXZ	-0.05024	0.00000	0.00000	-0.04037	-0.30991
165	C8	DYZ	0.17028	0.00000	0.00000	-0.17197	-0.29148
166	H8	S	0.00000	0.39283	0.27531	0.00000	0.00000
167	H8	S	0.00000	0.46221	0.29571	0.00000	0.00000
168	H8	PX	0.00000	0.04420	0.01949	0.00000	0.00000
169	H8	PY	0.00000	0.02648	0.00131	0.00000	0.00000
170	H8	PZ	-0.05269	0.00000	0.00000	0.09510	0.06850
171	C10	S	0.00000	0.02675	0.00991	0.00000	0.00000
172	C10	S	0.00000	0.48292	0.22643	0.00000	0.00000
173	C10	PX	0.00000	-0.10146	-0.04485	0.00000	0.00000
174	C10	PY	0.00000	-0.12374	0.01771	0.00000	0.00000
175	C10	PZ	0.03771	0.00000	0.00000	-0.03569	-0.07560
176	C10	S	0.00000	-5.21792	-1.18906	0.00000	0.00000
177	C10	PX	0.00000	1.00218	-0.99507	0.00000	0.00000
178	C10	PY	0.00000	-1.79957	-0.68970	0.00000	0.00000
179	C10	PZ	0.08093	0.00000	0.00000	0.00039	0.02784
180	C10	DXX	0.00000	0.11203	0.07041	0.00000	0.00000
181	C10	DYY	0.00000	-0.07848	-0.04028	0.00000	0.00000
182	C10	DZZ	0.00000	0.00462	-0.00129	0.00000	0.00000
183	C10	DXY	0.00000	0.09450	-0.05431	0.00000	0.00000
184	C10	DXZ	0.02290	0.00000	0.00000	-0.06703	-0.24496
185	C10	DYZ	-0.12798	0.00000	0.00000	0.10269	0.13597
186	H16	S	0.00000	-0.02979	0.22555	0.00000	0.00000
187	H16	S	0.00000	-0.09285	0.35553	0.00000	0.00000
188	H16	PX	0.00000	0.00215	0.01012	0.00000	0.00000
189	H16	PY	0.00000	0.03988	-0.01138	0.00000	0.00000
190	H16	PZ	0.03855	0.00000	0.00000	-0.04625	-0.12173
191	H18	S	0.00000	0.16163	-0.18783	0.00000	0.00000
192	H18	S	0.00000	0.32557	-0.26038	0.00000	0.00000
193	H18	PX	0.00000	0.01469	0.00827	0.00000	0.00000
194	H18	PY	0.00000	0.03037	0.02777	0.00000	0.00000
195	H18	PZ	0.03894	0.00000	0.00000	-0.01582	0.02604
196	C9	S	0.00000	0.01583	-0.07446	0.00000	0.00000
197	C9	S	0.00000	0.15677	-0.86602	0.00000	0.00000
198	C9	PX	0.00000	-0.00084	0.14417	0.00000	0.00000
199	C9	PY	0.00000	0.02899	0.12143	0.00000	0.00000

200	C9	PZ	-0.02747	0.00000	0.00000	-0.09547	0.03879
201	C9	S	0.00000	-0.65592	2.03324	0.00000	0.00000
202	C9	PX	0.00000	0.23361	-0.10311	0.00000	0.00000
203	C9	PY	0.00000	0.02708	-0.38281	0.00000	0.00000
204	C9	PZ	0.08071	0.00000	0.00000	0.07012	-0.03646
205	C9	DXX	0.00000	-0.00470	0.04141	0.00000	0.00000
206	C9	DYY	0.00000	0.01423	-0.09504	0.00000	0.00000
207	C9	DZZ	0.00000	-0.00133	-0.13518	0.00000	0.00000
208	C9	DXY	0.00000	-0.04078	-0.16760	0.00000	0.00000
209	C9	DXZ	-0.01109	0.00000	0.00000	-0.18024	0.08911
210	C9	DYZ	-0.08439	0.00000	0.00000	-0.31562	0.11805
211	H3	S	0.00000	0.05394	-0.17260	0.00000	0.00000
212	H3	S	0.00000	0.09573	-0.15368	0.00000	0.00000
213	H3	PX	0.00000	-0.01687	-0.06643	0.00000	0.00000
214	H3	PY	0.00000	-0.00688	-0.02551	0.00000	0.00000
215	H3	PZ	-0.03139	0.00000	0.00000	-0.12400	0.04508
216	H5	S	-0.03411	0.05138	-0.31806	-0.05220	0.01346
217	H5	S	0.10458	0.02931	-0.25321	0.05400	-0.00641
218	H5	PX	0.00671	0.00335	0.02968	0.04712	-0.02090
219	H5	PY	0.02557	-0.01017	-0.04046	0.11720	-0.04792
220	H5	PZ	-0.00093	0.00308	0.05033	0.01370	-0.00840
221	H7	S	0.03411	0.05138	-0.31806	0.05220	-0.01346
222	H7	S	-0.10458	0.02931	-0.25321	-0.05400	0.00641
223	H7	PX	-0.00671	0.00335	0.02968	-0.04712	0.02090
224	H7	PY	-0.02557	-0.01017	-0.04046	-0.11720	0.04792
225	H7	PZ	-0.00093	-0.00308	-0.05033	0.01370	-0.00840

MO:		121	122	123	124	125
Eigenvalues:		1.59404	1.61346	1.61640	1.62192	1.65269
(ev):		43.37592	43.90445	43.98446	44.13471	44.97201

		A	A	A	A	A	
1	H1	S	0.09575	0.00000	0.00000	0.19006	0.00000
2	H1	S	0.37753	0.00000	0.00000	0.33977	0.00000
3	H1	PX	0.00275	0.00000	0.00000	0.00030	0.00000
4	H1	PY	0.01825	0.00000	0.00000	0.02519	0.00000
5	H1	PZ	0.00000	0.08068	-0.03023	0.00000	0.05313
6	C1	S	0.00474	0.00000	0.00000	-0.02553	0.00000
7	C1	S	0.07641	0.00000	0.00000	-0.61363	0.00000
8	C1	PX	-0.00689	0.00000	0.00000	0.13378	0.00000
9	C1	PY	-0.15941	0.00000	0.00000	0.34206	0.00000
10	C1	PZ	0.00000	0.04663	0.00865	0.00000	0.04059
11	C1	S	0.81296	0.00000	0.00000	2.67700	0.00000
12	C1	PX	-1.32952	0.00000	0.00000	-2.02282	0.00000
13	C1	PY	1.06198	0.00000	0.00000	0.78028	0.00000
14	C1	PZ	0.00000	0.03317	-0.14884	0.00000	-0.02787
15	C1	DXX	0.02690	0.00000	0.00000	0.00844	0.00000
16	C1	DYY	-0.02672	0.00000	0.00000	-0.05480	0.00000
17	C1	DZZ	0.02604	0.00000	0.00000	0.01063	0.00000
18	C1	DXY	0.02899	0.00000	0.00000	-0.02796	0.00000
19	C1	DXZ	0.00000	0.12198	-0.03284	0.00000	0.10268
20	C1	DYZ	0.00000	0.11215	0.10835	0.00000	0.03693
21	C2	S	-0.03994	0.00000	0.00000	-0.01722	0.00000
22	C2	S	-0.42550	0.00000	0.00000	-0.24960	0.00000

23	C2	PX	0.11652	0.00000	0.00000	0.00965	0.00000
24	C2	PY	-0.26918	0.00000	0.00000	-0.08074	0.00000
25	C2	PZ	0.00000	0.00944	0.06114	0.00000	-0.13061
26	C2	S	3.98461	0.00000	0.00000	1.62680	0.00000
27	C2	PX	0.88766	0.00000	0.00000	1.75042	0.00000
28	C2	PY	-0.70818	0.00000	0.00000	-0.33118	0.00000
29	C2	PZ	0.00000	0.01936	-0.13113	0.00000	0.13479
30	C2	DXX	-0.07065	0.00000	0.00000	0.06191	0.00000
31	C2	DYY	0.02613	0.00000	0.00000	-0.07212	0.00000
32	C2	DZZ	0.06334	0.00000	0.00000	0.01756	0.00000
33	C2	DXY	-0.05533	0.00000	0.00000	-0.05481	0.00000
34	C2	DXZ	0.00000	0.08080	-0.12659	0.00000	0.31113
35	C2	DYZ	0.00000	-0.21229	-0.07953	0.00000	0.29282
36	C3	S	-0.02335	0.00000	0.00000	0.00334	0.00000
37	C3	S	-0.66182	0.00000	0.00000	-0.05597	0.00000
38	C3	PX	-0.12925	0.00000	0.00000	-0.20781	0.00000
39	C3	PY	0.14171	0.00000	0.00000	-0.02446	0.00000
40	C3	PZ	0.00000	0.00621	-0.07787	0.00000	-0.00718
41	C3	S	1.77081	0.00000	0.00000	-0.86062	0.00000
42	C3	PX	2.10930	0.00000	0.00000	-0.16274	0.00000
43	C3	PY	-0.80570	0.00000	0.00000	2.05898	0.00000
44	C3	PZ	0.00000	-0.09981	0.21609	0.00000	0.05309
45	C3	DXX	-0.10731	0.00000	0.00000	0.02896	0.00000
46	C3	DYY	0.00512	0.00000	0.00000	-0.05203	0.00000
47	C3	DZZ	0.03197	0.00000	0.00000	-0.00274	0.00000
48	C3	DXY	-0.07846	0.00000	0.00000	0.00088	0.00000
49	C3	DXZ	0.00000	0.19361	0.26701	0.00000	0.10823
50	C3	DYZ	0.00000	-0.25568	-0.14257	0.00000	-0.11419
51	C4	S	0.00550	0.00000	0.00000	0.02325	0.00000
52	C4	S	0.10796	0.00000	0.00000	0.57120	0.00000
53	C4	PX	-0.05979	0.00000	0.00000	0.17627	0.00000
54	C4	PY	-0.16301	0.00000	0.00000	0.00920	0.00000
55	C4	PZ	0.00000	0.02397	-0.04088	0.00000	0.02167
56	C4	S	-0.74268	0.00000	0.00000	-3.44493	0.00000
57	C4	PX	-0.79513	0.00000	0.00000	-2.11494	0.00000
58	C4	PY	1.59422	0.00000	0.00000	1.48722	0.00000
59	C4	PZ	0.00000	-0.05492	0.15044	0.00000	-0.08939
60	C4	DXX	-0.05759	0.00000	0.00000	0.02869	0.00000
61	C4	DYY	0.06716	0.00000	0.00000	-0.04689	0.00000
62	C4	DZZ	0.03492	0.00000	0.00000	0.02972	0.00000
63	C4	DXY	0.02864	0.00000	0.00000	0.04213	0.00000
64	C4	DXZ	0.00000	-0.18199	0.17558	0.00000	-0.05776
65	C4	DYZ	0.00000	-0.19898	0.01242	0.00000	-0.05699
66	C5	S	0.00593	0.00000	0.00000	-0.00790	0.00000
67	C5	S	0.29171	0.00000	0.00000	-0.27414	0.00000
68	C5	PX	-0.02978	0.00000	0.00000	0.03791	0.00000
69	C5	PY	-0.08931	0.00000	0.00000	0.23805	0.00000
70	C5	PZ	0.00000	-0.02999	0.02586	0.00000	-0.12164
71	C5	S	-1.23552	0.00000	0.00000	-0.26385	0.00000
72	C5	PX	0.14771	0.00000	0.00000	-0.08808	0.00000
73	C5	PY	0.08422	0.00000	0.00000	-1.53091	0.00000
74	C5	PZ	0.00000	0.07151	0.02509	0.00000	0.07037
75	C5	DXX	0.01089	0.00000	0.00000	0.01515	0.00000
76	C5	DYY	-0.08443	0.00000	0.00000	-0.02825	0.00000

77	C5	DZZ	0.08840	0.00000	0.00000	0.01831	0.00000
78	C5	DXY	-0.03279	0.00000	0.00000	-0.03576	0.00000
79	C5	DXZ	0.00000	0.27326	-0.17727	0.00000	0.20991
80	C5	DYZ	0.00000	0.11413	0.10400	0.00000	-0.42656
81	C6	S	-0.02462	0.00000	0.00000	0.01870	0.00000
82	C6	S	-0.01856	0.00000	0.00000	0.51618	0.00000
83	C6	PX	-0.33853	0.00000	0.00000	0.01425	0.00000
84	C6	PY	0.05950	0.00000	0.00000	0.39563	0.00000
85	C6	PZ	0.00000	0.02933	-0.06391	0.00000	0.04874
86	C6	S	-1.50151	0.00000	0.00000	-0.34211	0.00000
87	C6	PX	4.29752	0.00000	0.00000	0.69139	0.00000
88	C6	PY	-0.52547	0.00000	0.00000	-4.58544	0.00000
89	C6	PZ	0.00000	-0.02343	0.10147	0.00000	-0.19072
90	C6	DXX	-0.04510	0.00000	0.00000	0.05809	0.00000
91	C6	DYY	-0.13249	0.00000	0.00000	0.05911	0.00000
92	C6	DZZ	0.12138	0.00000	0.00000	-0.01036	0.00000
93	C6	DXY	-0.04779	0.00000	0.00000	-0.00634	0.00000
94	C6	DXZ	0.00000	-0.12372	-0.23039	0.00000	-0.04035
95	C6	DYZ	0.00000	0.00782	-0.23515	0.00000	-0.01556
96	C7	S	0.04294	0.00000	0.00000	0.01093	0.00000
97	C7	S	0.87913	0.00000	0.00000	0.15276	0.00000
98	C7	PX	-0.30296	0.00000	0.00000	-0.06227	0.00000
99	C7	PY	0.05853	0.00000	0.00000	0.18749	0.00000
100	C7	PZ	0.00000	-0.12939	-0.03763	0.00000	-0.06717
101	C7	S	-3.17298	0.00000	0.00000	-0.36802	0.00000
102	C7	PX	1.66306	0.00000	0.00000	-1.02146	0.00000
103	C7	PY	-1.08869	0.00000	0.00000	1.49627	0.00000
104	C7	PZ	0.00000	0.11411	-0.10983	0.00000	0.03266
105	C7	DXX	0.01359	0.00000	0.00000	0.08682	0.00000
106	C7	DYY	0.07803	0.00000	0.00000	-0.01212	0.00000
107	C7	DZZ	-0.02225	0.00000	0.00000	-0.02495	0.00000
108	C7	DXY	0.06458	0.00000	0.00000	-0.03009	0.00000
109	C7	DXZ	0.00000	-0.23926	-0.09780	0.00000	-0.16006
110	C7	DYZ	0.00000	0.21556	0.19637	0.00000	0.03836
111	O1	S	0.01245	0.00000	0.00000	-0.00651	0.00000
112	O1	S	0.24692	0.00000	0.00000	-0.32537	0.00000
113	O1	PX	-0.15803	0.00000	0.00000	0.05196	0.00000
114	O1	PY	-0.12095	0.00000	0.00000	0.22619	0.00000
115	O1	PZ	0.00000	0.08026	0.08117	0.00000	-0.09152
116	O1	S	-0.81533	0.00000	0.00000	0.40048	0.00000
117	O1	PX	0.65286	0.00000	0.00000	0.01762	0.00000
118	O1	PY	0.62486	0.00000	0.00000	-0.49346	0.00000
119	O1	PZ	0.00000	-0.09829	-0.18473	0.00000	0.21018
120	O1	DXX	0.00870	0.00000	0.00000	-0.08860	0.00000
121	O1	DYY	0.08699	0.00000	0.00000	-0.12674	0.00000
122	O1	DZZ	0.10222	0.00000	0.00000	-0.01333	0.00000
123	O1	DXY	0.04579	0.00000	0.00000	-0.04422	0.00000
124	O1	DXZ	0.00000	0.09742	0.11261	0.00000	-0.11148
125	O1	DYZ	0.00000	0.18084	-0.02053	0.00000	0.04013
126	H4	S	0.09353	0.00000	0.00000	0.27617	0.00000
127	H4	S	0.24432	0.00000	0.00000	0.36697	0.00000
128	H4	PX	0.01284	0.00000	0.00000	-0.01635	0.00000
129	H4	PY	0.02368	0.00000	0.00000	-0.00541	0.00000
130	H4	PZ	0.00000	-0.03392	0.10175	0.00000	-0.21909

131	N1	S	0.01768	0.00000	0.00000	-0.01095	0.00000
132	N1	S	0.22352	0.00000	0.00000	-0.16738	0.00000
133	N1	PX	0.28947	0.00000	0.00000	-0.05972	0.00000
134	N1	PY	-0.30668	0.00000	0.00000	-0.13101	0.00000
135	N1	PZ	0.00000	0.00957	0.01985	0.00000	-0.03010
136	N1	S	-0.72675	0.00000	0.00000	-0.00524	0.00000
137	N1	PX	-2.05956	0.00000	0.00000	1.10488	0.00000
138	N1	PY	1.97029	0.00000	0.00000	-1.52354	0.00000
139	N1	PZ	0.00000	-0.09672	-0.09268	0.00000	0.15308
140	N1	DXX	0.06950	0.00000	0.00000	0.03105	0.00000
141	N1	DYY	0.04567	0.00000	0.00000	-0.10394	0.00000
142	N1	DZZ	0.01829	0.00000	0.00000	-0.00233	0.00000
143	N1	DXY	-0.01297	0.00000	0.00000	-0.02197	0.00000
144	N1	DXZ	0.00000	0.13890	-0.22683	0.00000	-0.14300
145	N1	DYZ	0.00000	-0.03000	0.19902	0.00000	0.05750
146	H6	S	-0.08203	0.00000	0.00000	0.22272	0.00000
147	H6	S	-0.09791	0.00000	0.00000	0.41118	0.00000
148	H6	PX	-0.01508	0.00000	0.00000	-0.02603	0.00000
149	H6	PY	0.01849	0.00000	0.00000	0.00146	0.00000
150	H6	PZ	0.00000	0.00839	0.03933	0.00000	-0.17751
151	C8	S	-0.00598	0.00000	0.00000	0.00363	0.00000
152	C8	S	-0.33847	0.00000	0.00000	-0.10439	0.00000
153	C8	PX	-0.14843	0.00000	0.00000	-0.42052	0.00000
154	C8	PY	0.24590	0.00000	0.00000	-0.12760	0.00000
155	C8	PZ	0.00000	-0.00025	0.00206	0.00000	0.01487
156	C8	S	4.66409	0.00000	0.00000	-0.46778	0.00000
157	C8	PX	-0.48555	0.00000	0.00000	4.19037	0.00000
158	C8	PY	-2.42023	0.00000	0.00000	-0.61509	0.00000
159	C8	PZ	0.00000	0.05116	0.03948	0.00000	-0.05813
160	C8	DXX	0.13408	0.00000	0.00000	-0.03253	0.00000
161	C8	DYY	0.00970	0.00000	0.00000	0.00243	0.00000
162	C8	DZZ	-0.05847	0.00000	0.00000	-0.00483	0.00000
163	C8	DXY	-0.00296	0.00000	0.00000	0.02288	0.00000
164	C8	DXZ	0.00000	-0.18830	0.21489	0.00000	0.17922
165	C8	DYZ	0.00000	0.14818	-0.24245	0.00000	-0.00763
166	H8	S	-0.05948	0.00000	0.00000	0.28969	0.00000
167	H8	S	-0.37519	0.00000	0.00000	0.46272	0.00000
168	H8	PX	0.00688	0.00000	0.00000	0.03794	0.00000
169	H8	PY	0.00949	0.00000	0.00000	0.02801	0.00000
170	H8	PZ	0.00000	-0.11371	-0.09007	0.00000	-0.08871
171	C10	S	0.02357	0.00000	0.00000	0.00379	0.00000
172	C10	S	0.20734	0.00000	0.00000	-0.05387	0.00000
173	C10	PX	0.17708	0.00000	0.00000	0.04937	0.00000
174	C10	PY	-0.16403	0.00000	0.00000	-0.08448	0.00000
175	C10	PZ	0.00000	0.05374	-0.12503	0.00000	-0.01707
176	C10	S	-3.47738	0.00000	0.00000	-0.90100	0.00000
177	C10	PX	-0.13079	0.00000	0.00000	-2.01979	0.00000
178	C10	PY	-1.27698	0.00000	0.00000	-0.72432	0.00000
179	C10	PZ	0.00000	-0.04213	0.08305	0.00000	0.02400
180	C10	DXX	0.05661	0.00000	0.00000	0.06576	0.00000
181	C10	DYY	-0.10340	0.00000	0.00000	-0.05031	0.00000
182	C10	DZZ	0.02859	0.00000	0.00000	-0.01399	0.00000
183	C10	DXY	0.00768	0.00000	0.00000	-0.11250	0.00000
184	C10	DXZ	0.00000	-0.05821	0.07444	0.00000	0.17803

185	C10	DYZ	0.00000	-0.16112	0.29843	0.00000	0.08638
186	H16	S	0.20316	0.00000	0.00000	0.35243	0.00000
187	H16	S	0.24297	0.00000	0.00000	0.66018	0.00000
188	H16	PX	-0.03008	0.00000	0.00000	0.00646	0.00000
189	H16	PY	-0.00974	0.00000	0.00000	-0.02432	0.00000
190	H16	PZ	0.00000	0.00571	-0.01791	0.00000	0.06747
191	H18	S	0.02753	0.00000	0.00000	-0.36491	0.00000
192	H18	S	-0.05436	0.00000	0.00000	-0.61253	0.00000
193	H18	PX	-0.02509	0.00000	0.00000	-0.00506	0.00000
194	H18	PY	0.02110	0.00000	0.00000	0.03963	0.00000
195	H18	PZ	0.00000	0.06861	-0.11634	0.00000	-0.08782
196	C9	S	0.02099	0.00000	0.00000	-0.01785	0.00000
197	C9	S	0.24938	0.00000	0.00000	-0.19406	0.00000
198	C9	PX	0.07987	0.00000	0.00000	-0.02146	0.00000
199	C9	PY	-0.10217	0.00000	0.00000	0.10038	0.00000
200	C9	PZ	0.00000	-0.07901	-0.02089	0.00000	0.03135
201	C9	S	-0.99438	0.00000	0.00000	0.50418	0.00000
202	C9	PX	0.15071	0.00000	0.00000	-0.02249	0.00000
203	C9	PY	0.48180	0.00000	0.00000	-0.37956	0.00000
204	C9	PZ	0.00000	0.15109	0.10365	0.00000	-0.15807
205	C9	DXX	0.03950	0.00000	0.00000	-0.08100	0.00000
206	C9	DYY	-0.03588	0.00000	0.00000	0.00994	0.00000
207	C9	DZZ	0.00458	0.00000	0.00000	0.05416	0.00000
208	C9	DXY	-0.12616	0.00000	0.00000	0.10487	0.00000
209	C9	DXZ	0.00000	-0.12700	-0.04172	0.00000	0.04991
210	C9	DYZ	0.00000	-0.19626	-0.09076	0.00000	0.10099
211	H3	S	0.07140	0.00000	0.00000	-0.00130	0.00000
212	H3	S	-0.11404	0.00000	0.00000	0.14681	0.00000
213	H3	PX	-0.06477	0.00000	0.00000	0.07705	0.00000
214	H3	PY	0.00572	0.00000	0.00000	0.00484	0.00000
215	H3	PZ	0.00000	-0.07445	-0.02772	0.00000	0.02531
216	H5	S	0.12546	-0.04399	0.00366	-0.08564	-0.00742
217	H5	S	0.09300	0.10690	0.04996	-0.08509	-0.08160
218	H5	PX	0.01502	0.03259	0.01346	-0.03284	-0.01971
219	H5	PY	-0.00360	0.07551	0.02630	0.00023	-0.03387
220	H5	PZ	0.01961	0.01051	0.00471	-0.02299	-0.00702
221	H7	S	0.12546	0.04399	-0.00366	-0.08564	0.00742
222	H7	S	0.09300	-0.10690	-0.04996	-0.08509	0.08160
223	H7	PX	0.01502	-0.03259	-0.01346	-0.03284	0.01971
224	H7	PY	-0.00360	-0.07551	-0.02630	0.00023	0.03387
225	H7	PZ	-0.01961	0.01051	0.00471	0.02299	-0.00702

MO:	126	127	128	129	130
Eigenvalues:	1.66549	1.68081	1.68528	1.70352	1.71993
(ev):	45.32025	45.73720	45.85883	46.35520	46.80183

		A	A	A	A	A	
1	H1	S	0.16851	0.00000	0.55819	0.00000	0.00000
2	H1	S	0.18463	0.00000	1.07200	0.00000	0.00000
3	H1	PX	-0.01046	0.00000	0.02693	0.00000	0.00000
4	H1	PY	0.02803	0.00000	0.01841	0.00000	0.00000
5	H1	PZ	0.00000	-0.03610	0.00000	0.04791	-0.15354
6	C1	S	0.04540	0.00000	-0.00356	0.00000	0.00000
7	C1	S	0.76507	0.00000	-0.26109	0.00000	0.00000

8	C1	PX	-0.05190	0.00000	0.18168	0.00000	0.00000
9	C1	PY	-0.13805	0.00000	-0.00799	0.00000	0.00000
10	C1	PZ	0.00000	0.01762	0.00000	0.00043	-0.16004
11	C1	S	-5.05081	0.00000	-0.31330	0.00000	0.00000
12	C1	PX	0.41693	0.00000	-2.97723	0.00000	0.00000
13	C1	PY	1.27707	0.00000	0.62287	0.00000	0.00000
14	C1	PZ	0.00000	-0.15417	0.00000	0.04643	0.24269
15	C1	DXX	0.05354	0.00000	0.09130	0.00000	0.00000
16	C1	DYY	0.05468	0.00000	-0.10491	0.00000	0.00000
17	C1	DZZ	-0.06250	0.00000	0.02380	0.00000	0.00000
18	C1	DXY	0.07426	0.00000	0.04491	0.00000	0.00000
19	C1	DXZ	0.00000	0.00019	0.00000	-0.02568	-0.36026
20	C1	DYZ	0.00000	0.00305	0.00000	0.22613	0.06477
21	C2	S	0.02364	0.00000	-0.01561	0.00000	0.00000
22	C2	S	0.48565	0.00000	-0.43786	0.00000	0.00000
23	C2	PX	0.03204	0.00000	-0.19584	0.00000	0.00000
24	C2	PY	0.15841	0.00000	0.05151	0.00000	0.00000
25	C2	PZ	0.00000	-0.09710	0.00000	0.04184	-0.03846
26	C2	S	-2.29989	0.00000	1.56749	0.00000	0.00000
27	C2	PX	-1.62578	0.00000	1.99916	0.00000	0.00000
28	C2	PY	-0.66699	0.00000	1.16861	0.00000	0.00000
29	C2	PZ	0.00000	0.14598	0.00000	0.04918	0.00739
30	C2	DXX	-0.00907	0.00000	-0.04783	0.00000	0.00000
31	C2	DYY	0.01439	0.00000	-0.01606	0.00000	0.00000
32	C2	DZZ	-0.02447	0.00000	0.04487	0.00000	0.00000
33	C2	DXY	0.00505	0.00000	0.09884	0.00000	0.00000
34	C2	DXZ	0.00000	0.31183	0.00000	-0.05631	0.08238
35	C2	DYZ	0.00000	-0.12785	0.00000	-0.17700	-0.08315
36	C3	S	-0.00610	0.00000	0.01911	0.00000	0.00000
37	C3	S	-0.48581	0.00000	0.21190	0.00000	0.00000
38	C3	PX	-0.44044	0.00000	-0.45149	0.00000	0.00000
39	C3	PY	0.12484	0.00000	-0.23514	0.00000	0.00000
40	C3	PZ	0.00000	-0.02844	0.00000	-0.04338	0.05506
41	C3	S	2.01149	0.00000	-0.50347	0.00000	0.00000
42	C3	PX	4.31556	0.00000	3.72735	0.00000	0.00000
43	C3	PY	0.30181	0.00000	0.96192	0.00000	0.00000
44	C3	PZ	0.00000	0.19802	0.00000	0.11123	-0.13586
45	C3	DXX	-0.01375	0.00000	0.09158	0.00000	0.00000
46	C3	DYY	0.08572	0.00000	-0.03850	0.00000	0.00000
47	C3	DZZ	-0.08712	0.00000	-0.01424	0.00000	0.00000
48	C3	DXY	-0.01797	0.00000	-0.01645	0.00000	0.00000
49	C3	DXZ	0.00000	0.06161	0.00000	-0.28310	0.12367
50	C3	DYZ	0.00000	0.06696	0.00000	-0.19199	0.02329
51	C4	S	-0.04221	0.00000	0.00504	0.00000	0.00000
52	C4	S	-0.84244	0.00000	0.01445	0.00000	0.00000
53	C4	PX	-0.05393	0.00000	-0.29679	0.00000	0.00000
54	C4	PY	0.33044	0.00000	-0.08075	0.00000	0.00000
55	C4	PZ	0.00000	-0.02370	0.00000	-0.00872	-0.01564
56	C4	S	2.18340	0.00000	-0.74310	0.00000	0.00000
57	C4	PX	0.96231	0.00000	0.07850	0.00000	0.00000
58	C4	PY	-2.67242	0.00000	0.99082	0.00000	0.00000
59	C4	PZ	0.00000	0.14134	0.00000	-0.11106	-0.21071
60	C4	DXX	-0.01010	0.00000	-0.02502	0.00000	0.00000
61	C4	DYY	-0.07620	0.00000	0.03641	0.00000	0.00000

62	C4	DZZ	0.00891	0.00000	0.01933	0.00000	0.00000
63	C4	DXY	-0.03385	0.00000	0.04246	0.00000	0.00000
64	C4	DXZ	0.00000	0.23641	0.00000	-0.05608	0.20100
65	C4	DYZ	0.00000	0.23815	0.00000	-0.18295	-0.28085
66	C5	S	-0.00044	0.00000	0.01362	0.00000	0.00000
67	C5	S	-0.04449	0.00000	0.48267	0.00000	0.00000
68	C5	PX	-0.04661	0.00000	0.21643	0.00000	0.00000
69	C5	PY	0.00841	0.00000	-0.12449	0.00000	0.00000
70	C5	PZ	0.00000	0.06272	0.00000	0.05693	0.06988
71	C5	S	0.98274	0.00000	-1.87787	0.00000	0.00000
72	C5	PX	-0.09947	0.00000	-1.32521	0.00000	0.00000
73	C5	PY	-0.14455	0.00000	1.97502	0.00000	0.00000
74	C5	PZ	0.00000	-0.07582	0.00000	-0.03948	-0.01080
75	C5	DXX	-0.03972	0.00000	0.00679	0.00000	0.00000
76	C5	DYY	0.06818	0.00000	-0.05002	0.00000	0.00000
77	C5	DZZ	-0.04106	0.00000	0.05021	0.00000	0.00000
78	C5	DXY	0.02109	0.00000	0.05809	0.00000	0.00000
79	C5	DXZ	0.00000	-0.21220	0.00000	0.07592	-0.13301
80	C5	DYZ	0.00000	0.05872	0.00000	0.19930	0.00958
81	C6	S	-0.03509	0.00000	-0.00234	0.00000	0.00000
82	C6	S	-0.55143	0.00000	-0.02906	0.00000	0.00000
83	C6	PX	0.03515	0.00000	0.30693	0.00000	0.00000
84	C6	PY	-0.03055	0.00000	-0.19651	0.00000	0.00000
85	C6	PZ	0.00000	0.09108	0.00000	0.04003	0.00979
86	C6	S	4.30492	0.00000	2.09993	0.00000	0.00000
87	C6	PX	1.03298	0.00000	0.03805	0.00000	0.00000
88	C6	PY	1.92582	0.00000	0.59630	0.00000	0.00000
89	C6	PZ	0.00000	-0.27570	0.00000	-0.19614	0.02813
90	C6	DXX	0.01207	0.00000	0.02885	0.00000	0.00000
91	C6	DYY	0.00973	0.00000	-0.02396	0.00000	0.00000
92	C6	DZZ	-0.04125	0.00000	0.01520	0.00000	0.00000
93	C6	DXY	-0.00233	0.00000	0.08731	0.00000	0.00000
94	C6	DXZ	0.00000	-0.24472	0.00000	0.16066	-0.21843
95	C6	DYZ	0.00000	0.31873	0.00000	0.27281	-0.01027
96	C7	S	0.03038	0.00000	0.00455	0.00000	0.00000
97	C7	S	0.31190	0.00000	-0.11458	0.00000	0.00000
98	C7	PX	0.05111	0.00000	0.06413	0.00000	0.00000
99	C7	PY	0.05040	0.00000	-0.03923	0.00000	0.00000
100	C7	PZ	0.00000	-0.05267	0.00000	-0.00388	-0.04755
101	C7	S	-3.33786	0.00000	-1.63008	0.00000	0.00000
102	C7	PX	-1.12820	0.00000	-0.79721	0.00000	0.00000
103	C7	PY	-1.41535	0.00000	-0.98191	0.00000	0.00000
104	C7	PZ	0.00000	-0.00968	0.00000	0.02749	0.05590
105	C7	DXX	0.12773	0.00000	0.01494	0.00000	0.00000
106	C7	DYY	-0.06154	0.00000	-0.04505	0.00000	0.00000
107	C7	DZZ	-0.05582	0.00000	0.02754	0.00000	0.00000
108	C7	DXY	0.03187	0.00000	-0.03045	0.00000	0.00000
109	C7	DXZ	0.00000	-0.16577	0.00000	-0.02829	-0.09718
110	C7	DYZ	0.00000	-0.07806	0.00000	-0.03983	0.03474
111	O1	S	-0.00445	0.00000	0.00508	0.00000	0.00000
112	O1	S	-0.00541	0.00000	0.14400	0.00000	0.00000
113	O1	PX	0.27309	0.00000	-0.20443	0.00000	0.00000
114	O1	PY	-0.05340	0.00000	-0.08577	0.00000	0.00000
115	O1	PZ	0.00000	0.03963	0.00000	-0.04553	-0.14717

116	O1	S	0.62886	0.00000	-0.40346	0.00000	0.00000
117	O1	PX	-0.91614	0.00000	0.58216	0.00000	0.00000
118	O1	PY	-0.32952	0.00000	0.46321	0.00000	0.00000
119	O1	PZ	0.00000	-0.20498	0.00000	0.21113	0.48525
120	O1	DXX	0.14052	0.00000	-0.01589	0.00000	0.00000
121	O1	DYY	-0.01799	0.00000	0.07859	0.00000	0.00000
122	O1	DZZ	-0.13660	0.00000	0.06038	0.00000	0.00000
123	O1	DXY	-0.08382	0.00000	0.02354	0.00000	0.00000
124	O1	DXZ	0.00000	0.15044	0.00000	-0.13134	-0.24789
125	O1	DYZ	0.00000	-0.21699	0.00000	0.19028	0.23218
126	H4	S	0.01274	0.00000	-0.40492	0.00000	0.00000
127	H4	S	-0.10272	0.00000	-0.68887	0.00000	0.00000
128	H4	PX	-0.01679	0.00000	0.02244	0.00000	0.00000
129	H4	PY	-0.02763	0.00000	-0.00429	0.00000	0.00000
130	H4	PZ	0.00000	0.10626	0.00000	0.05104	0.07204
131	N1	S	-0.00144	0.00000	0.01859	0.00000	0.00000
132	N1	S	0.24132	0.00000	0.24913	0.00000	0.00000
133	N1	PX	0.08803	0.00000	0.08288	0.00000	0.00000
134	N1	PY	0.09550	0.00000	-0.01921	0.00000	0.00000
135	N1	PZ	0.00000	0.06906	0.00000	0.07580	0.00775
136	N1	S	0.26317	0.00000	-1.22721	0.00000	0.00000
137	N1	PX	-0.18513	0.00000	-0.47734	0.00000	0.00000
138	N1	PY	-0.10857	0.00000	-0.37986	0.00000	0.00000
139	N1	PZ	0.00000	0.09586	0.00000	0.18203	-0.08186
140	N1	DXX	0.06157	0.00000	0.02550	0.00000	0.00000
141	N1	DYY	0.02927	0.00000	0.05359	0.00000	0.00000
142	N1	DZZ	-0.01743	0.00000	0.03698	0.00000	0.00000
143	N1	DXY	-0.00381	0.00000	0.02339	0.00000	0.00000
144	N1	DXZ	0.00000	-0.07818	0.00000	-0.13478	0.00765
145	N1	DYZ	0.00000	-0.18977	0.00000	-0.23836	0.03466
146	H6	S	-0.20573	0.00000	0.44840	0.00000	0.00000
147	H6	S	-0.40230	0.00000	0.70990	0.00000	0.00000
148	H6	PX	0.01897	0.00000	-0.02913	0.00000	0.00000
149	H6	PY	0.01211	0.00000	-0.01835	0.00000	0.00000
150	H6	PZ	0.00000	-0.12707	0.00000	0.08013	-0.04197
151	C8	S	-0.01494	0.00000	-0.00553	0.00000	0.00000
152	C8	S	-0.45188	0.00000	-0.15027	0.00000	0.00000
153	C8	PX	-0.20067	0.00000	-0.07846	0.00000	0.00000
154	C8	PY	0.01900	0.00000	-0.25835	0.00000	0.00000
155	C8	PZ	0.00000	-0.01881	0.00000	0.00997	-0.01181
156	C8	S	1.51665	0.00000	-0.87062	0.00000	0.00000
157	C8	PX	0.88938	0.00000	-0.63612	0.00000	0.00000
158	C8	PY	-0.96385	0.00000	2.61431	0.00000	0.00000
159	C8	PZ	0.00000	0.06505	0.00000	-0.15390	0.09643
160	C8	DXX	-0.01248	0.00000	-0.06189	0.00000	0.00000
161	C8	DYY	0.02131	0.00000	-0.05819	0.00000	0.00000
162	C8	DZZ	-0.03501	0.00000	0.08308	0.00000	0.00000
163	C8	DXY	-0.01535	0.00000	-0.03544	0.00000	0.00000
164	C8	DXZ	0.00000	0.05771	0.00000	0.12164	-0.04495
165	C8	DYZ	0.00000	0.18734	0.00000	-0.11047	0.10135
166	H8	S	0.53355	0.00000	0.33972	0.00000	0.00000
167	H8	S	0.65196	0.00000	0.37525	0.00000	0.00000
168	H8	PX	0.02354	0.00000	0.02375	0.00000	0.00000
169	H8	PY	-0.03144	0.00000	-0.03759	0.00000	0.00000

170	H8	PZ	0.00000	-0.08865	0.00000	-0.00180	-0.05100
171	C10	S	0.01676	0.00000	-0.00979	0.00000	0.00000
172	C10	S	0.21621	0.00000	-0.03738	0.00000	0.00000
173	C10	PX	0.02475	0.00000	-0.02328	0.00000	0.00000
174	C10	PY	-0.01604	0.00000	0.13591	0.00000	0.00000
175	C10	PZ	0.00000	0.07767	0.00000	-0.02960	0.03710
176	C10	S	-1.71725	0.00000	2.25270	0.00000	0.00000
177	C10	PX	-0.42307	0.00000	-0.30762	0.00000	0.00000
178	C10	PY	-0.90127	0.00000	0.86479	0.00000	0.00000
179	C10	PZ	0.00000	-0.08985	0.00000	0.05705	-0.05958
180	C10	DXX	0.07442	0.00000	-0.06617	0.00000	0.00000
181	C10	DYY	-0.03550	0.00000	0.03945	0.00000	0.00000
182	C10	DZZ	-0.02961	0.00000	0.04984	0.00000	0.00000
183	C10	DXY	-0.01385	0.00000	-0.03195	0.00000	0.00000
184	C10	DXZ	0.00000	0.19505	0.00000	0.31519	-0.14786
185	C10	DYZ	0.00000	-0.14189	0.00000	0.17395	-0.13298
186	H16	S	0.15817	0.00000	0.01187	0.00000	0.00000
187	H16	S	0.14199	0.00000	0.05032	0.00000	0.00000
188	H16	PX	-0.00757	0.00000	0.00892	0.00000	0.00000
189	H16	PY	-0.00474	0.00000	-0.01647	0.00000	0.00000
190	H16	PZ	0.00000	0.11275	0.00000	0.13259	-0.05821
191	H18	S	-0.07303	0.00000	-0.04594	0.00000	0.00000
192	H18	S	-0.20072	0.00000	-0.03155	0.00000	0.00000
193	H18	PX	0.00233	0.00000	-0.00457	0.00000	0.00000
194	H18	PY	0.01726	0.00000	-0.00798	0.00000	0.00000
195	H18	PZ	0.00000	-0.02897	0.00000	-0.18301	0.10433
196	C9	S	0.00735	0.00000	0.01506	0.00000	0.00000
197	C9	S	0.11357	0.00000	0.17776	0.00000	0.00000
198	C9	PX	-0.10007	0.00000	0.07919	0.00000	0.00000
199	C9	PY	-0.07254	0.00000	-0.03207	0.00000	0.00000
200	C9	PZ	0.00000	-0.00636	0.00000	0.01313	0.07119
201	C9	S	0.37220	0.00000	-0.86014	0.00000	0.00000
202	C9	PX	-0.28168	0.00000	0.15951	0.00000	0.00000
203	C9	PY	0.00325	0.00000	0.34255	0.00000	0.00000
204	C9	PZ	0.00000	0.14747	0.00000	-0.16843	-0.44117
205	C9	DXX	-0.05233	0.00000	0.02921	0.00000	0.00000
206	C9	DYY	0.07704	0.00000	-0.03604	0.00000	0.00000
207	C9	DZZ	0.03090	0.00000	-0.00101	0.00000	0.00000
208	C9	DXY	0.18389	0.00000	-0.13171	0.00000	0.00000
209	C9	DXZ	0.00000	-0.01084	0.00000	0.03581	0.13988
210	C9	DYZ	0.00000	-0.08795	0.00000	0.11053	0.30611
211	H3	S	-0.05175	0.00000	0.03998	0.00000	0.00000
212	H3	S	-0.08665	0.00000	-0.03495	0.00000	0.00000
213	H3	PX	0.06707	0.00000	-0.06990	0.00000	0.00000
214	H3	PY	0.00859	0.00000	-0.00491	0.00000	0.00000
215	H3	PZ	0.00000	-0.01504	0.00000	0.02107	0.07685
216	H5	S	0.01148	0.03908	0.08372	-0.04149	-0.05000
217	H5	S	0.03361	0.05694	0.07838	-0.06063	-0.19823
218	H5	PX	-0.02342	0.01977	0.01623	-0.02939	-0.07776
219	H5	PY	0.03149	0.01998	-0.00234	-0.03413	-0.10237
220	H5	PZ	-0.03630	0.00513	0.01969	-0.00845	-0.02332
221	H7	S	0.01148	-0.03908	0.08372	0.04149	0.05000
222	H7	S	0.03361	-0.05694	0.07838	0.06063	0.19823
223	H7	PX	-0.02342	-0.01977	0.01623	0.02939	0.07776

224	H7	PY	0.03149	-0.01998	-0.00234	0.03413	0.10237
225	H7	PZ	0.03630	0.00513	-0.01969	-0.00845	-0.02332

MO:		131	132	133	134	135
Eigenvalues:		1.76128	1.77360	1.88956	1.93003	1.98351
(ev):		47.92702	48.26220	51.41768	52.51890	53.97413

		A	A	A	A	A	
1	H1	S	0.00000	-0.22188	-0.05629	0.13897	-0.18629
2	H1	S	0.00000	-0.04031	-0.00271	0.35563	-0.13177
3	H1	PX	0.00000	-0.02408	-0.00126	0.02052	-0.02359
4	H1	PY	0.00000	0.05217	-0.02240	-0.07853	-0.04362
5	H1	PZ	-0.05805	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.00000	0.03289	-0.02192	0.01814	0.00359
7	C1	S	0.00000	0.53373	-0.09084	0.17671	0.14808
8	C1	PX	0.00000	-0.15607	-0.02254	0.09716	-0.00597
9	C1	PY	0.00000	-0.01057	-0.00245	-0.13244	-0.10437
10	C1	PZ	-0.04569	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.00000	-3.64290	1.49353	-2.64644	-0.09275
12	C1	PX	0.00000	0.81929	-0.64320	0.20772	0.36247
13	C1	PY	0.00000	2.76291	0.69742	-0.94982	0.32023
14	C1	PZ	0.08445	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.00000	0.03574	0.04454	0.09123	0.07717
16	C1	DYY	0.00000	-0.00472	-0.16847	-0.08849	-0.07915
17	C1	DZZ	0.00000	-0.03859	0.17266	-0.02208	0.01672
18	C1	DXY	0.00000	-0.01500	-0.06618	-0.09555	0.01344
19	C1	DXZ	-0.08250	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	-0.08329	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00000	0.03044	-0.00171	0.00368	-0.00445
22	C2	S	0.00000	0.59337	0.22177	0.25140	0.00531
23	C2	PX	0.00000	0.18706	0.15622	0.12660	0.02977
24	C2	PY	0.00000	-0.02230	-0.11123	-0.19916	-0.01323
25	C2	PZ	-0.00571	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.00000	-3.69143	0.43162	-1.07691	-0.01978
27	C2	PX	0.00000	-2.45783	-0.03245	-0.65366	-0.69030
28	C2	PY	0.00000	-0.16981	-0.04949	-0.07354	-1.32415
29	C2	PZ	-0.05238	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.00000	0.00718	-0.06570	-0.01459	-0.10720
31	C2	DYY	0.00000	0.02409	-0.02097	-0.04606	0.00422
32	C2	DZZ	0.00000	-0.01996	0.11811	0.07602	0.13308
33	C2	DXY	0.00000	-0.03249	0.09497	0.11436	0.12304
34	C2	DXZ	-0.02798	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.02779	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.00000	-0.01418	0.02639	-0.00216	0.01425
37	C3	S	0.00000	-0.50427	0.49625	-0.22690	0.27599
38	C3	PX	0.00000	0.02003	0.06645	0.14335	-0.08072
39	C3	PY	0.00000	-0.58057	0.10281	-0.13267	0.08518
40	C3	PZ	0.02715	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.00000	2.28403	-1.62373	0.40692	-3.04955
42	C3	PX	0.00000	-0.72130	1.02791	-1.23867	0.81201
43	C3	PY	0.00000	6.02401	0.41785	1.33322	0.46253
44	C3	PZ	-0.15073	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.00000	0.00365	0.17751	0.14714	-0.04868
46	C3	DYY	0.00000	-0.01494	-0.19919	-0.16832	-0.04062

47	C3	DZZ	0.00000	-0.03529	0.04374	0.02464	0.15126
48	C3	DXY	0.00000	-0.00401	-0.12725	-0.07468	-0.08073
49	C3	DXZ	0.19684	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.08427	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00000	0.03347	0.00786	-0.00321	-0.00817
52	C4	S	0.00000	0.38116	0.28106	-0.02786	-0.02676
53	C4	PX	0.00000	-0.02269	0.04175	-0.20224	-0.00371
54	C4	PY	0.00000	-0.22077	0.19773	-0.19734	0.05890
55	C4	PZ	0.00126	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.00000	-1.49259	-0.96965	0.17156	1.06810
57	C4	PX	0.00000	0.18445	-1.56105	3.11144	-0.54722
58	C4	PY	0.00000	2.79761	-0.03889	1.16493	-0.28304
59	C4	PZ	-0.02215	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.00000	-0.02634	-0.15691	-0.01752	-0.09637
61	C4	DYY	0.00000	0.16439	0.03293	-0.01933	0.08496
62	C4	DZZ	0.00000	-0.09312	0.15904	0.00397	0.04270
63	C4	DXY	0.00000	0.04163	-0.05707	-0.18388	-0.04817
64	C4	DXZ	0.03880	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	-0.02599	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.00000	-0.03049	0.00090	-0.02631	0.01226
67	C5	S	0.00000	-0.69620	0.05520	-0.19228	0.27626
68	C5	PX	0.00000	-0.17775	0.02268	0.13806	0.03579
69	C5	PY	0.00000	-0.00499	0.00569	0.20490	-0.08760
70	C5	PZ	0.00422	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.00000	3.41289	-0.81334	2.84668	-0.05980
72	C5	PX	0.00000	2.19485	-0.22353	1.40949	-0.86003
73	C5	PY	0.00000	-1.91610	-0.34170	-1.07785	-0.03422
74	C5	PZ	0.00788	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.00000	0.01065	-0.16352	-0.10235	-0.09808
76	C5	DYY	0.00000	-0.02365	0.02719	0.07880	0.07639
77	C5	DZZ	0.00000	-0.01875	0.15166	0.05899	0.02344
78	C5	DXY	0.00000	-0.04392	-0.03626	-0.03640	-0.04442
79	C5	DXZ	-0.04947	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	-0.03016	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00000	0.00889	-0.00637	0.01703	-0.01113
82	C6	S	0.00000	0.13133	-0.08129	0.37500	0.07503
83	C6	PX	0.00000	0.10668	-0.13019	-0.11564	-0.15407
84	C6	PY	0.00000	-0.13964	0.01416	0.06943	-0.06381
85	C6	PZ	-0.01395	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00000	2.55040	3.06611	0.06141	-2.32265
87	C6	PX	0.00000	-1.41900	1.59398	-0.40578	1.87942
88	C6	PY	0.00000	-0.43439	-1.64632	-1.48185	3.44351
89	C6	PZ	0.19711	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.00000	0.01789	-0.08010	-0.03907	-0.11486
91	C6	DYY	0.00000	0.07395	0.05107	0.06958	-0.15587
92	C6	DZZ	0.00000	-0.05527	0.03367	-0.01169	0.36897
93	C6	DXY	0.00000	0.00543	0.21519	0.21334	0.03021
94	C6	DXZ	-0.02585	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	-0.12630	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00000	-0.00183	0.00516	0.00753	-0.01957
97	C7	S	0.00000	-0.03278	-0.00418	-0.02518	-0.42367
98	C7	PX	0.00000	-0.02545	-0.06062	0.00617	0.02888
99	C7	PY	0.00000	0.20734	0.00397	0.12948	-0.13085
100	C7	PZ	0.06320	0.00000	0.00000	0.00000	0.00000

101	C7	S	0.00000	1.84004	0.12453	0.12734	2.29331
102	C7	PX	0.00000	-1.00912	0.61204	0.20288	-2.37140
103	C7	PY	0.00000	0.83387	-0.57614	0.52383	0.47385
104	C7	PZ	-0.09727	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.00000	0.00153	-0.19977	-0.12991	-0.01452
106	C7	DYY	0.00000	0.01722	0.12954	0.10064	-0.07995
107	C7	DZZ	0.00000	-0.00930	0.04890	0.02801	0.17577
108	C7	DXY	0.00000	-0.08174	0.04831	0.01508	-0.08384
109	C7	DXZ	0.21815	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.23940	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00000	-0.00643	-0.01387	0.05872	0.00388
112	O1	S	0.00000	-0.07366	-0.19921	0.63385	0.06668
113	O1	PX	0.00000	-0.18809	-0.05709	0.28583	-0.00811
114	O1	PY	0.00000	-0.19489	-0.10585	0.12861	-0.06196
115	O1	PZ	-0.01401	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00000	0.01197	0.73270	-2.50599	-0.13326
117	O1	PX	0.00000	1.07112	0.46518	-1.42096	0.14093
118	O1	PY	0.00000	1.29298	0.41311	-0.39967	0.34937
119	O1	PZ	0.04381	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.00000	-0.05212	-0.11032	0.30815	-0.00230
121	O1	DYY	0.00000	-0.01601	-0.05131	0.19746	0.04480
122	O1	DZZ	0.00000	-0.03125	0.01898	-0.00357	-0.01032
123	O1	DXY	0.00000	-0.05866	-0.12233	0.21600	-0.03159
124	O1	DXZ	-0.01948	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.01043	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.00000	0.31521	0.08919	0.17391	-0.14830
127	H4	S	0.00000	0.67989	0.09722	0.44026	-0.18647
128	H4	PX	0.00000	-0.01491	0.02615	-0.01315	0.02725
129	H4	PY	0.00000	0.03838	0.02626	-0.00318	-0.00783
130	H4	PZ	0.00790	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.00000	0.00334	0.08153	0.01435	-0.08700
132	N1	S	0.00000	-0.05745	1.01957	0.02745	-1.29721
133	N1	PX	0.00000	-0.14029	0.08259	-0.01491	0.09267
134	N1	PY	0.00000	0.00435	-0.01891	-0.04172	-0.06824
135	N1	PZ	-0.09482	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.00000	-0.62349	-5.42373	-1.06153	7.19966
137	N1	PX	0.00000	0.74918	-1.67930	0.10905	0.85801
138	N1	PY	0.00000	-1.30852	-0.78215	-0.91176	1.81129
139	N1	PZ	-0.13483	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.00000	-0.07873	0.11246	-0.12805	-0.28168
141	N1	DYY	0.00000	0.00570	0.19158	0.04244	-0.28698
142	N1	DZZ	0.00000	0.03865	0.04713	0.07627	0.22550
143	N1	DXY	0.00000	-0.00808	-0.15139	-0.18723	0.05185
144	N1	DXZ	0.34769	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.03428	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.00000	-0.21413	-0.01203	-0.09914	-0.24106
147	H6	S	0.00000	-0.57029	-0.05666	-0.10741	-0.33979
148	H6	PX	0.00000	0.01490	0.01372	0.04012	0.04903
149	H6	PY	0.00000	0.01168	-0.01983	-0.05398	-0.07644
150	H6	PZ	-0.00256	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.00000	-0.00923	0.01302	0.00995	0.01921
152	C8	S	0.00000	-0.04892	0.08659	0.07350	0.43761
153	C8	PX	0.00000	-0.12627	0.01219	-0.07883	-0.10871
154	C8	PY	0.00000	-0.20279	-0.05250	-0.14021	0.08020

155	C8	PZ	-0.02715	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.00000	-1.86436	0.61847	-0.98674	-2.57796
157	C8	PX	0.00000	0.78446	-2.30724	0.55344	1.62453
158	C8	PY	0.00000	3.13767	1.68899	2.09835	-2.50495
159	C8	PZ	0.17372	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.00000	-0.07652	0.13469	0.07620	-0.10235
161	C8	DYY	0.00000	-0.04528	-0.13814	-0.12413	-0.06844
162	C8	DZZ	0.00000	0.07355	0.00035	0.01714	0.21241
163	C8	DXY	0.00000	0.01891	0.03006	0.09160	-0.02451
164	C8	DXZ	-0.30860	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.03477	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.00000	0.11888	0.04624	0.11878	0.31817
167	H8	S	0.00000	0.24079	-0.33573	-0.12629	0.67148
168	H8	PX	0.00000	0.01919	0.03037	0.03051	0.04189
169	H8	PY	0.00000	-0.01629	-0.00591	0.01143	-0.05524
170	H8	PZ	0.09793	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00000	-0.01546	-0.00620	-0.01234	0.00275
172	C10	S	0.00000	0.01979	0.05492	0.01938	-0.10203
173	C10	PX	0.00000	-0.05213	-0.03393	-0.03790	0.01581
174	C10	PY	0.00000	0.22061	0.14619	0.18794	-0.06390
175	C10	PZ	0.02564	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.00000	2.70893	1.36583	1.80492	-1.17880
177	C10	PX	0.00000	-0.77495	0.79893	-0.53947	-0.59157
178	C10	PY	0.00000	0.90481	0.67882	0.55267	-0.42071
179	C10	PZ	-0.06982	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.00000	-0.03425	-0.04796	0.00627	-0.00411
181	C10	DYY	0.00000	0.03119	0.00008	-0.00618	-0.03633
182	C10	DZZ	0.00000	0.03742	0.08358	0.04972	0.09115
183	C10	DXY	0.00000	-0.05058	0.03391	-0.01601	-0.00587
184	C10	DXZ	0.47851	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00589	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.00000	0.01316	-0.15200	-0.00830	0.13135
187	H16	S	0.00000	0.19742	-0.26120	0.14066	0.25365
188	H16	PX	0.00000	0.01569	0.00439	0.01889	0.02447
189	H16	PY	0.00000	-0.01086	0.00431	0.01824	0.01577
190	H16	PZ	0.27469	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.00000	-0.12383	0.14620	-0.10019	-0.10901
192	H18	S	0.00000	-0.17685	0.25908	-0.14385	-0.14189
193	H18	PX	0.00000	-0.00230	-0.02470	-0.01459	-0.00597
194	H18	PY	0.00000	-0.00518	0.00065	0.00984	0.01488
195	H18	PZ	-0.23021	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00000	0.07625	-0.00830	0.00494	-0.00081
197	C9	S	0.00000	0.87661	-0.11980	-0.04626	-0.02934
198	C9	PX	0.00000	0.12214	0.04698	-0.17689	0.01374
199	C9	PY	0.00000	-0.15464	0.10156	-0.10865	0.00838
200	C9	PZ	0.00890	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.00000	-3.17215	-0.20040	1.34302	-0.05517
202	C9	PX	0.00000	0.56601	0.36763	-0.63082	0.13601
203	C9	PY	0.00000	1.10981	-0.39377	0.27851	-0.09599
204	C9	PZ	-0.04374	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	0.00000	-0.10657	-0.30974	0.35305	-0.12446
206	C9	DYY	0.00000	0.03237	0.12065	-0.05743	0.06220
207	C9	DZZ	0.00000	0.13439	0.18067	-0.24220	0.06449
208	C9	DXY	0.00000	-0.06075	0.15690	-0.00508	0.07596

209	C9	DXZ	0.01711	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.03353	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.00000	0.18945	0.05406	-0.18872	0.01158
212	H3	S	0.00000	-0.08306	0.24360	-0.34527	0.05169
213	H3	PX	0.00000	-0.01489	0.16396	-0.07963	0.08242
214	H3	PY	0.00000	0.01917	0.00987	-0.00484	0.00799
215	H3	PZ	0.01026	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.00206	0.35679	-0.04896	0.01931	-0.00624
217	H5	S	-0.02007	0.30600	-0.08960	-0.10861	-0.04371
218	H5	PX	-0.00839	-0.03465	-0.10387	0.08944	-0.04895
219	H5	PY	-0.01047	0.02545	-0.03075	0.00183	-0.01598
220	H5	PZ	-0.00272	-0.02144	-0.05465	0.03906	-0.02522
221	H7	S	0.00206	0.35679	-0.04896	0.01931	-0.00624
222	H7	S	0.02007	0.30600	-0.08960	-0.10861	-0.04371
223	H7	PX	0.00839	-0.03465	-0.10387	0.08944	-0.04895
224	H7	PY	0.01047	0.02545	-0.03075	0.00183	-0.01598
225	H7	PZ	-0.00272	0.02144	0.05465	-0.03906	0.02522

MO:	136	137	138	139	140
Eigenvalues:	2.03285	2.07072	2.10565	2.10726	2.12833
(ev):	55.31678	56.34722	57.29768	57.34162	57.91471

		A	A	A	A	A	
1	H1	S	-0.03448	-0.00721	0.17825	0.00000	0.23073
2	H1	S	0.08424	0.38995	0.13455	0.00000	0.47675
3	H1	PX	0.02129	-0.01379	0.09304	0.00000	0.02346
4	H1	PY	0.01617	0.01124	-0.07421	0.00000	0.03635
5	H1	PZ	0.00000	0.00000	0.00000	-0.24925	0.00000
6	C1	S	-0.01942	-0.01913	-0.01747	0.00000	-0.01097
7	C1	S	-0.24978	-0.23415	-0.04903	0.00000	-0.51555
8	C1	PX	-0.01437	-0.02442	-0.07614	0.00000	0.18270
9	C1	PY	-0.04443	0.11912	0.08463	0.00000	0.13625
10	C1	PZ	0.00000	0.00000	0.00000	0.00206	0.00000
11	C1	S	0.56215	0.63208	2.12566	0.00000	0.89898
12	C1	PX	-0.53362	-1.32361	-1.03065	0.00000	-1.73184
13	C1	PY	0.55078	0.59393	0.10710	0.00000	0.15503
14	C1	PZ	0.00000	0.00000	0.00000	0.54326	0.00000
15	C1	DXX	0.03150	0.05553	-0.05695	0.00000	0.02851
16	C1	DYY	0.09710	0.06638	0.00226	0.00000	0.09033
17	C1	DZZ	-0.09148	-0.02696	0.05990	0.00000	-0.18561
18	C1	DXY	-0.00610	0.17987	-0.15152	0.00000	-0.15165
19	C1	DXZ	0.00000	0.00000	0.00000	-0.31069	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.42950	0.00000
21	C2	S	-0.01365	0.01165	-0.01535	0.00000	0.00634
22	C2	S	0.04959	0.50570	-0.23220	0.00000	0.12467
23	C2	PX	0.07250	0.22370	0.02937	0.00000	0.06567
24	C2	PY	-0.02608	-0.00310	-0.04059	0.00000	-0.14202
25	C2	PZ	0.00000	0.00000	0.00000	0.01620	0.00000
26	C2	S	0.83916	-0.77106	1.09378	0.00000	-0.55301
27	C2	PX	-0.55355	-1.17286	0.75032	0.00000	-0.49157
28	C2	PY	-1.35388	-1.69391	-0.52256	0.00000	-1.05235
29	C2	PZ	0.00000	0.00000	0.00000	-0.13725	0.00000
30	C2	DXX	-0.06816	0.00318	-0.07924	0.00000	-0.21487
31	C2	DYY	0.08812	-0.08685	0.05457	0.00000	0.13514

32	C2	DZZ	-0.05563	0.10579	0.09327	0.00000	0.03228
33	C2	DXY	0.06123	-0.12544	-0.16307	0.00000	0.00472
34	C2	DXZ	0.00000	0.00000	0.00000	-0.08891	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.14446	0.00000
36	C3	S	0.03410	0.05226	0.01674	0.00000	0.03701
37	C3	S	0.20335	0.70247	0.24908	0.00000	0.23368
38	C3	PX	0.04510	-0.23067	0.02949	0.00000	0.08096
39	C3	PY	0.09415	-0.13942	-0.09311	0.00000	-0.14688
40	C3	PZ	0.00000	0.00000	0.00000	-0.04023	0.00000
41	C3	S	-4.34098	-6.41876	-1.98770	0.00000	-5.23912
42	C3	PX	2.04117	2.62263	0.23932	0.00000	1.02869
43	C3	PY	0.95943	3.30769	0.52916	0.00000	3.33352
44	C3	PZ	0.00000	0.00000	0.00000	-0.85225	0.00000
45	C3	DXX	0.23600	-0.06188	0.08297	0.00000	0.03713
46	C3	DYY	-0.03397	-0.02975	-0.09744	0.00000	0.05690
47	C3	DZZ	-0.26662	-0.00725	0.04716	0.00000	-0.18925
48	C3	DXY	0.07952	-0.18937	0.08991	0.00000	0.19302
49	C3	DXZ	0.00000	0.00000	0.00000	-0.01238	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.04772	0.00000
51	C4	S	0.00392	0.01356	0.00386	0.00000	0.01169
52	C4	S	-0.05992	-0.03159	-0.27160	0.00000	0.21100
53	C4	PX	-0.13273	0.14943	0.20262	0.00000	-0.05012
54	C4	PY	0.03681	-0.00319	0.08662	0.00000	-0.02290
55	C4	PZ	0.00000	0.00000	0.00000	0.00743	0.00000
56	C4	S	-1.57040	-2.57958	0.99230	0.00000	-1.05173
57	C4	PX	-0.10874	-0.60283	-2.27189	0.00000	-0.18199
58	C4	PY	-0.98423	0.65645	2.07045	0.00000	2.62256
59	C4	PZ	0.00000	0.00000	0.00000	-0.23692	0.00000
60	C4	DXX	0.05621	0.08204	0.21792	0.00000	0.05418
61	C4	DYY	-0.00396	-0.01121	-0.01206	0.00000	0.04858
62	C4	DZZ	-0.09088	-0.07921	-0.25609	0.00000	-0.17682
63	C4	DXY	0.06085	0.25109	0.13333	0.00000	-0.17212
64	C4	DXZ	0.00000	0.00000	0.00000	-0.22570	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.04719	0.00000
66	C5	S	-0.00346	-0.01136	0.02266	0.00000	-0.01030
67	C5	S	-0.09338	-0.33730	0.08408	0.00000	-0.13239
68	C5	PX	-0.02960	-0.14071	-0.13890	0.00000	0.09555
69	C5	PY	-0.02784	-0.01203	-0.11831	0.00000	0.07490
70	C5	PZ	0.00000	0.00000	0.00000	-0.03768	0.00000
71	C5	S	1.07778	2.35907	-1.61752	0.00000	1.68230
72	C5	PX	-0.31146	0.82408	-0.61103	0.00000	0.33090
73	C5	PY	0.40231	-1.33629	-0.57910	0.00000	-1.51124
74	C5	PZ	0.00000	0.00000	0.00000	0.04699	0.00000
75	C5	DXX	0.02595	0.18740	0.26238	0.00000	-0.10495
76	C5	DYY	0.09224	-0.12665	-0.16645	0.00000	0.10356
77	C5	DZZ	-0.16361	-0.02398	-0.13518	0.00000	-0.00695
78	C5	DXY	-0.00292	-0.00927	0.15535	0.00000	0.11165
79	C5	DXZ	0.00000	0.00000	0.00000	-0.07117	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.01026	0.00000
81	C6	S	-0.01956	-0.03695	0.01610	0.00000	-0.02773
82	C6	S	-0.46839	-0.31063	-0.07208	0.00000	-0.41972
83	C6	PX	-0.29634	-0.01067	-0.03963	0.00000	-0.14666
84	C6	PY	0.02175	0.07796	-0.08085	0.00000	0.05143
85	C6	PZ	0.00000	0.00000	0.00000	0.00468	0.00000

86	C6	S	0.74896	4.92261	-0.85754	0.00000	2.94850
87	C6	PX	3.47371	3.80549	1.35323	0.00000	2.93571
88	C6	PY	1.81077	-1.04675	0.15515	0.00000	-0.61196
89	C6	PZ	0.00000	0.00000	0.00000	0.45460	0.00000
90	C6	DXX	0.17530	-0.16320	0.02764	0.00000	0.23644
91	C6	DYY	-0.10381	0.02439	-0.09072	0.00000	-0.13939
92	C6	DZZ	-0.08069	0.19921	0.04222	0.00000	-0.01182
93	C6	DXY	0.15134	-0.01514	0.00561	0.00000	0.02107
94	C6	DXZ	0.00000	0.00000	0.00000	0.23247	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.10797	0.00000
96	C7	S	-0.02561	-0.03306	-0.00325	0.00000	-0.04075
97	C7	S	-0.61724	-0.46556	-0.23577	0.00000	-0.16601
98	C7	PX	0.17831	-0.00891	0.03287	0.00000	-0.15200
99	C7	PY	0.02746	-0.11014	0.11935	0.00000	-0.04144
100	C7	PZ	0.00000	0.00000	0.00000	-0.02748	0.00000
101	C7	S	2.85837	5.31405	1.25287	0.00000	5.11123
102	C7	PX	-2.63996	-3.14134	-0.59520	0.00000	-2.57323
103	C7	PY	-0.42153	-0.34975	-0.10347	0.00000	0.24508
104	C7	PZ	0.00000	0.00000	0.00000	0.59243	0.00000
105	C7	DXX	0.02752	-0.12835	-0.05873	0.00000	0.13748
106	C7	DYY	0.11769	0.01172	0.07021	0.00000	-0.17717
107	C7	DZZ	-0.12555	0.16343	0.03745	0.00000	0.14348
108	C7	DXY	0.13079	-0.20453	0.16985	0.00000	-0.14731
109	C7	DXZ	0.00000	0.00000	0.00000	-0.43207	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.19020	0.00000
111	O1	S	-0.05763	-0.00178	0.04418	0.00000	0.03133
112	O1	S	-0.78193	-0.17534	0.74869	0.00000	0.43789
113	O1	PX	-0.09522	0.00449	-0.14016	0.00000	-0.01551
114	O1	PY	0.08103	0.23142	-0.11974	0.00000	-0.17182
115	O1	PZ	0.00000	0.00000	0.00000	0.00973	0.00000
116	O1	S	2.74907	0.29491	-2.71966	0.00000	-1.88109
117	O1	PX	0.49055	-0.12603	0.54307	0.00000	0.11576
118	O1	PY	-0.49113	-0.74541	0.91635	0.00000	0.91641
119	O1	PZ	0.00000	0.00000	0.00000	-0.00855	0.00000
120	O1	DXX	-0.32759	0.05998	0.39227	0.00000	0.10067
121	O1	DYY	-0.25084	-0.06651	0.29019	0.00000	0.17800
122	O1	DZZ	0.01768	-0.06624	-0.19134	0.00000	-0.01601
123	O1	DXY	0.02611	-0.10222	-0.23070	0.00000	0.13118
124	O1	DXZ	0.00000	0.00000	0.00000	-0.15048	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.15309	0.00000
126	H4	S	-0.25746	0.09322	0.18628	0.00000	0.22275
127	H4	S	-0.25951	0.38222	0.06122	0.00000	0.26451
128	H4	PX	0.04730	-0.07815	-0.13265	0.00000	-0.01627
129	H4	PY	0.00397	-0.06226	-0.05955	0.00000	0.06567
130	H4	PZ	0.00000	0.00000	0.00000	0.03748	0.00000
131	N1	S	-0.03781	0.05386	-0.01068	0.00000	0.01365
132	N1	S	-0.49112	0.56409	-0.10941	0.00000	0.13969
133	N1	PX	0.08456	-0.01806	0.08891	0.00000	-0.02956
134	N1	PY	-0.01982	-0.06892	-0.00829	0.00000	0.02635
135	N1	PZ	0.00000	0.00000	0.00000	0.03211	0.00000
136	N1	S	2.71623	-3.21965	0.64585	0.00000	-0.96737
137	N1	PX	-0.37964	-1.21221	-0.36573	0.00000	-0.47553
138	N1	PY	1.26511	0.01602	0.47881	0.00000	0.31147
139	N1	PZ	0.00000	0.00000	0.00000	-0.04398	0.00000

140	N1	DXX	-0.10198	0.12334	-0.09700	0.00000	0.22217
141	N1	DYY	-0.06362	0.02542	-0.01897	0.00000	-0.09688
142	N1	DZZ	-0.01327	0.02734	0.10784	0.00000	-0.07688
143	N1	DXY	-0.24342	-0.02922	-0.07525	0.00000	-0.03767
144	N1	DXZ	0.00000	0.00000	0.00000	0.09051	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.20354	0.00000
146	H6	S	-0.21959	-0.16069	0.17855	0.00000	0.04915
147	H6	S	-0.37741	-0.50846	0.05504	0.00000	-0.25545
148	H6	PX	0.02269	0.00485	-0.07138	0.00000	-0.02751
149	H6	PY	-0.05362	-0.02451	-0.02898	0.00000	-0.06372
150	H6	PZ	0.00000	0.00000	0.00000	0.00742	0.00000
151	C8	S	0.02196	0.02079	0.01376	0.00000	0.00844
152	C8	S	0.11055	0.59617	0.09381	0.00000	0.24401
153	C8	PX	-0.03287	0.02380	-0.05848	0.00000	0.07374
154	C8	PY	-0.09972	0.21029	-0.09768	0.00000	0.16669
155	C8	PZ	0.00000	0.00000	0.00000	-0.01769	0.00000
156	C8	S	-1.59171	-1.40113	-0.61659	0.00000	-0.81212
157	C8	PX	-0.34136	-2.39707	-0.27558	0.00000	-1.20472
158	C8	PY	-2.19811	-2.75568	-0.10204	0.00000	-3.17120
159	C8	PZ	0.00000	0.00000	0.00000	-0.39478	0.00000
160	C8	DXX	0.24502	0.14046	0.07842	0.00000	0.04411
161	C8	DYY	-0.04858	-0.18139	-0.05080	0.00000	-0.00696
162	C8	DZZ	-0.26958	0.08222	-0.03080	0.00000	-0.06965
163	C8	DXY	0.10922	-0.14347	0.18549	0.00000	-0.34206
164	C8	DXZ	0.00000	0.00000	0.00000	-0.12092	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	-0.08632	0.00000
166	H8	S	0.27341	0.26092	0.07871	0.00000	-0.03590
167	H8	S	0.72590	0.66012	0.07460	0.00000	0.60466
168	H8	PX	0.05971	0.04874	0.05117	0.00000	0.01455
169	H8	PY	0.05328	-0.15815	0.13337	0.00000	-0.04120
170	H8	PZ	0.00000	0.00000	0.00000	-0.25810	0.00000
171	C10	S	-0.00968	0.00742	-0.00345	0.00000	0.00374
172	C10	S	-0.09720	0.01645	0.00606	0.00000	-0.11704
173	C10	PX	0.02566	-0.06013	0.02663	0.00000	-0.03224
174	C10	PY	-0.04340	-0.03203	0.05673	0.00000	-0.20323
175	C10	PZ	0.00000	0.00000	0.00000	-0.00895	0.00000
176	C10	S	-0.82189	-1.27583	0.18309	0.00000	-1.75730
177	C10	PX	0.30374	1.49318	0.11266	0.00000	0.86807
178	C10	PY	-0.42899	-0.18857	0.02126	0.00000	-0.44100
179	C10	PZ	0.00000	0.00000	0.00000	0.17644	0.00000
180	C10	DXX	0.18124	-0.02434	0.10830	0.00000	-0.07608
181	C10	DYY	-0.03297	-0.03282	-0.08347	0.00000	0.10982
182	C10	DZZ	-0.16646	0.10168	0.00001	0.00000	-0.08044
183	C10	DXY	0.03032	0.15130	-0.07213	0.00000	0.22473
184	C10	DXZ	0.00000	0.00000	0.00000	-0.05276	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.21613	0.00000
186	H16	S	-0.16312	-0.11662	-0.16277	0.00000	0.09435
187	H16	S	-0.08668	-0.46007	0.01547	0.00000	-0.31654
188	H16	PX	-0.02594	0.02848	-0.03840	0.00000	0.05477
189	H16	PY	0.05332	0.01223	0.03832	0.00000	-0.02553
190	H16	PZ	0.00000	0.00000	0.00000	-0.05409	0.00000
191	H18	S	-0.07205	0.14321	0.05328	0.00000	-0.05727
192	H18	S	0.01140	0.47442	-0.00808	0.00000	0.31061

193	H18	PX	-0.02974	-0.02161	-0.06524	0.00000	0.07039
194	H18	PY	0.06063	0.05749	0.02486	0.00000	0.04550
195	H18	PZ	0.00000	0.00000	0.00000	-0.07067	0.00000
196	C9	S	0.02235	-0.00710	-0.02380	0.00000	0.00776
197	C9	S	0.26556	-0.01795	-0.28826	0.00000	0.03869
198	C9	PX	0.08222	-0.04296	0.04885	0.00000	0.03835
199	C9	PY	0.01108	-0.00436	0.05331	0.00000	-0.02238
200	C9	PZ	0.00000	0.00000	0.00000	0.00622	0.00000
201	C9	S	-1.24455	0.32265	0.55968	0.00000	-0.21714
202	C9	PX	0.22658	-0.26653	0.03223	0.00000	0.13574
203	C9	PY	0.27810	0.14373	-0.20047	0.00000	-0.01304
204	C9	PZ	0.00000	0.00000	0.00000	0.12362	0.00000
205	C9	DXX	0.02964	0.15804	-0.13671	0.00000	-0.05399
206	C9	DYY	-0.09019	-0.06322	0.14065	0.00000	0.01224
207	C9	DZZ	0.06480	-0.09212	-0.04586	0.00000	0.01953
208	C9	DXY	-0.13743	-0.11995	0.04306	0.00000	0.13047
209	C9	DXZ	0.00000	0.00000	0.00000	0.02521	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.05684	0.00000
211	H3	S	0.13263	-0.08223	-0.13510	0.00000	0.08020
212	H3	S	0.06284	-0.08895	0.03811	0.00000	-0.01309
213	H3	PX	-0.08092	-0.15055	0.01286	0.00000	0.12924
214	H3	PY	0.01139	-0.02649	-0.04476	0.00000	0.03725
215	H3	PZ	0.00000	0.00000	0.00000	0.02424	0.00000
216	H5	S	0.08440	0.00085	-0.03417	0.06195	0.02934
217	H5	S	0.17209	0.03433	-0.13043	0.03865	-0.05227
218	H5	PX	0.03023	0.07611	-0.02956	0.07033	-0.05022
219	H5	PY	0.03074	0.03617	-0.01901	0.07033	-0.01467
220	H5	PZ	0.02305	0.03512	-0.02572	-0.00068	-0.02844
221	H7	S	0.08440	0.00085	-0.03417	-0.06195	0.02934
222	H7	S	0.17209	0.03433	-0.13043	-0.03865	-0.05227
223	H7	PX	0.03023	0.07611	-0.02956	-0.07033	-0.05022
224	H7	PY	0.03074	0.03617	-0.01901	-0.07033	-0.01467
225	H7	PZ	-0.02305	-0.03512	0.02572	-0.00068	0.02844

MO:	141	142	143	144	145
Eigenvalues:	2.16374	2.16713	2.17488	2.17972	2.21319
(ev):	58.87839	58.97055	59.18163	59.31313	60.22393

		A	A	A	A	A	
1	H1	S	0.17763	0.00000	0.22691	-0.32980	0.00000
2	H1	S	-0.51849	0.00000	0.29965	-0.06370	0.00000
3	H1	PX	0.08963	0.00000	0.05662	-0.03069	0.00000
4	H1	PY	0.01433	0.00000	0.00184	-0.12010	0.00000
5	H1	PZ	0.00000	-0.17654	0.00000	0.00000	-0.07086
6	C1	S	0.01484	0.00000	0.00385	-0.00212	0.00000
7	C1	S	0.21476	0.00000	-0.26185	0.13677	0.00000
8	C1	PX	-0.07084	0.00000	0.09117	0.04394	0.00000
9	C1	PY	-0.14740	0.00000	0.03492	-0.28627	0.00000
10	C1	PZ	0.00000	0.01409	0.00000	0.00000	0.02604
11	C1	S	-1.00866	0.00000	-1.32729	-0.22142	0.00000
12	C1	PX	1.18872	0.00000	-0.78791	0.56419	0.00000
13	C1	PY	0.12823	0.00000	0.32984	0.45213	0.00000
14	C1	PZ	0.00000	0.29955	0.00000	0.00000	0.09289
15	C1	DXX	-0.25805	0.00000	-0.03253	0.22211	0.00000

16	C1	DYY	0.16253	0.00000	0.07574	-0.18841	0.00000
17	C1	DZZ	0.14687	0.00000	-0.01151	-0.04794	0.00000
18	C1	DXY	-0.12071	0.00000	-0.14835	0.01066	0.00000
19	C1	DXZ	0.00000	-0.33103	0.00000	0.00000	-0.15910
20	C1	DYZ	0.00000	0.20695	0.00000	0.00000	0.16736
21	C2	S	0.00370	0.00000	0.02714	0.00961	0.00000
22	C2	S	0.09322	0.00000	0.41730	-0.10509	0.00000
23	C2	PX	0.10347	0.00000	0.10261	-0.07807	0.00000
24	C2	PY	-0.02725	0.00000	-0.02777	0.04794	0.00000
25	C2	PZ	0.00000	0.04100	0.00000	0.00000	-0.01664
26	C2	S	0.23103	0.00000	-1.61310	-0.84827	0.00000
27	C2	PX	-0.06229	0.00000	-1.79777	0.13401	0.00000
28	C2	PY	0.99189	0.00000	-1.27371	0.19627	0.00000
29	C2	PZ	0.00000	0.15897	0.00000	0.00000	-0.17268
30	C2	DXX	-0.19397	0.00000	-0.00375	-0.20007	0.00000
31	C2	DYY	0.14294	0.00000	-0.01651	0.19980	0.00000
32	C2	DZZ	0.10767	0.00000	-0.03507	-0.00844	0.00000
33	C2	DXY	-0.01936	0.00000	-0.09052	-0.25694	0.00000
34	C2	DXZ	0.00000	0.28900	0.00000	0.00000	-0.15069
35	C2	DYZ	0.00000	-0.30696	0.00000	0.00000	0.02768
36	C3	S	-0.00463	0.00000	0.03487	-0.01246	0.00000
37	C3	S	-0.44673	0.00000	0.71360	-0.10667	0.00000
38	C3	PX	0.10126	0.00000	-0.10456	-0.03832	0.00000
39	C3	PY	0.08747	0.00000	-0.32422	0.17174	0.00000
40	C3	PZ	0.00000	0.00993	0.00000	0.00000	0.00895
41	C3	S	3.79486	0.00000	-5.27719	0.82740	0.00000
42	C3	PX	-0.69916	0.00000	1.85011	-0.59696	0.00000
43	C3	PY	-2.16063	0.00000	3.59313	-0.51620	0.00000
44	C3	PZ	0.00000	0.11195	0.00000	0.00000	0.04388
45	C3	DXX	0.01136	0.00000	-0.02602	0.22995	0.00000
46	C3	DYY	-0.02284	0.00000	-0.01939	-0.16297	0.00000
47	C3	DZZ	0.07022	0.00000	0.06162	-0.04916	0.00000
48	C3	DXY	0.08066	0.00000	0.17239	-0.25588	0.00000
49	C3	DXZ	0.00000	-0.28929	0.00000	0.00000	0.06338
50	C3	DYZ	0.00000	-0.13679	0.00000	0.00000	-0.09794
51	C4	S	0.01042	0.00000	0.02244	0.00291	0.00000
52	C4	S	-0.19777	0.00000	0.17250	-0.04731	0.00000
53	C4	PX	-0.00379	0.00000	-0.13322	0.08780	0.00000
54	C4	PY	0.12520	0.00000	0.05093	-0.00884	0.00000
55	C4	PZ	0.00000	-0.10475	0.00000	0.00000	-0.03043
56	C4	S	-0.02677	0.00000	-2.36528	-0.04804	0.00000
57	C4	PX	0.28051	0.00000	1.49114	0.25397	0.00000
58	C4	PY	-2.97318	0.00000	0.18486	-0.33591	0.00000
59	C4	PZ	0.00000	-0.54353	0.00000	0.00000	-0.18606
60	C4	DXX	0.26443	0.00000	0.02136	-0.01744	0.00000
61	C4	DYY	-0.42375	0.00000	-0.09287	0.02216	0.00000
62	C4	DZZ	0.25839	0.00000	0.04449	-0.01457	0.00000
63	C4	DXY	-0.03349	0.00000	-0.15617	-0.12697	0.00000
64	C4	DXZ	0.00000	0.07951	0.00000	0.00000	-0.07170
65	C4	DYZ	0.00000	0.13231	0.00000	0.00000	0.01659
66	C5	S	0.01714	0.00000	-0.02271	-0.00426	0.00000
67	C5	S	-0.13016	0.00000	-0.27802	-0.03478	0.00000
68	C5	PX	-0.11943	0.00000	0.01866	0.14271	0.00000
69	C5	PY	0.03135	0.00000	0.00522	0.10864	0.00000

70	C5	PZ	0.00000	0.03086	0.00000	0.00000	-0.00134
71	C5	S	-1.02198	0.00000	3.49724	0.22159	0.00000
72	C5	PX	0.14250	0.00000	1.31114	0.07908	0.00000
73	C5	PY	1.07829	0.00000	-0.90316	-0.31857	0.00000
74	C5	PZ	0.00000	0.23641	0.00000	0.00000	0.14979
75	C5	DXX	-0.05968	0.00000	-0.06693	-0.06352	0.00000
76	C5	DYY	-0.04655	0.00000	0.04410	-0.02657	0.00000
77	C5	DZZ	0.11449	0.00000	0.12104	0.12685	0.00000
78	C5	DXY	0.25713	0.00000	0.05784	0.25466	0.00000
79	C5	DXZ	0.00000	0.41017	0.00000	0.00000	0.02564
80	C5	DYZ	0.00000	0.11767	0.00000	0.00000	-0.08237
81	C6	S	0.02447	0.00000	-0.02474	0.00591	0.00000
82	C6	S	0.18714	0.00000	-0.50177	-0.22561	0.00000
83	C6	PX	0.04851	0.00000	-0.10652	0.04783	0.00000
84	C6	PY	-0.07072	0.00000	0.03800	-0.10119	0.00000
85	C6	PZ	0.00000	-0.09362	0.00000	0.00000	0.02908
86	C6	S	-1.19706	0.00000	4.45622	-0.65287	0.00000
87	C6	PX	-1.61570	0.00000	2.66825	-1.09255	0.00000
88	C6	PY	0.25322	0.00000	0.11165	0.52167	0.00000
89	C6	PZ	0.00000	-0.40499	0.00000	0.00000	0.15008
90	C6	DXX	0.06972	0.00000	-0.09656	0.16566	0.00000
91	C6	DYY	-0.08363	0.00000	-0.02176	-0.07466	0.00000
92	C6	DZZ	0.03430	0.00000	0.17476	-0.11118	0.00000
93	C6	DXY	0.14674	0.00000	-0.15124	-0.16340	0.00000
94	C6	DXZ	0.00000	0.04169	0.00000	0.00000	-0.10773
95	C6	DYZ	0.00000	-0.17887	0.00000	0.00000	0.04298
96	C7	S	0.02848	0.00000	-0.02117	-0.00915	0.00000
97	C7	S	0.47412	0.00000	-0.47359	-0.15256	0.00000
98	C7	PX	-0.11969	0.00000	0.04166	-0.01231	0.00000
99	C7	PY	-0.01109	0.00000	0.12634	-0.20331	0.00000
100	C7	PZ	0.00000	0.01462	0.00000	0.00000	-0.01663
101	C7	S	-3.93981	0.00000	5.14135	0.51475	0.00000
102	C7	PX	2.23350	0.00000	-3.02092	-0.48979	0.00000
103	C7	PY	0.00720	0.00000	-0.43066	0.30554	0.00000
104	C7	PZ	0.00000	0.01013	0.00000	0.00000	-0.25570
105	C7	DXX	-0.06315	0.00000	0.14233	-0.25933	0.00000
106	C7	DYY	-0.04217	0.00000	-0.15894	0.26877	0.00000
107	C7	DZZ	0.13452	0.00000	0.10701	-0.00328	0.00000
108	C7	DXY	-0.00835	0.00000	0.14342	0.00149	0.00000
109	C7	DXZ	0.00000	-0.02430	0.00000	0.00000	0.21424
110	C7	DYZ	0.00000	-0.10053	0.00000	0.00000	0.18096
111	O1	S	-0.05934	0.00000	-0.01379	-0.00725	0.00000
112	O1	S	-0.52991	0.00000	-0.26741	-0.20666	0.00000
113	O1	PX	0.01077	0.00000	0.05576	0.05061	0.00000
114	O1	PY	-0.11179	0.00000	-0.03679	0.02060	0.00000
115	O1	PZ	0.00000	-0.08389	0.00000	0.00000	0.09096
116	O1	S	2.70098	0.00000	0.86170	0.61075	0.00000
117	O1	PX	-0.05230	0.00000	-0.29551	-0.14704	0.00000
118	O1	PY	-0.83815	0.00000	-0.25116	-0.17709	0.00000
119	O1	PZ	0.00000	0.22127	0.00000	0.00000	-0.16057
120	O1	DXX	-0.10089	0.00000	-0.12177	-0.07677	0.00000
121	O1	DYY	-0.33040	0.00000	-0.12943	-0.07470	0.00000
122	O1	DZZ	0.11255	0.00000	0.10508	0.03579	0.00000
123	O1	DXY	-0.09137	0.00000	0.19415	0.08414	0.00000

124	O1	DXZ	0.00000	-0.00187	0.00000	0.00000	-0.52813
125	O1	DYZ	0.00000	-0.36607	0.00000	0.00000	-0.21113
126	H4	S	0.17321	0.00000	0.11985	0.29457	0.00000
127	H4	S	-0.21268	0.00000	0.28493	-0.00979	0.00000
128	H4	PX	-0.07109	0.00000	-0.02154	-0.06172	0.00000
129	H4	PY	0.03957	0.00000	0.05855	0.09498	0.00000
130	H4	PZ	0.00000	-0.10687	0.00000	0.00000	-0.07675
131	N1	S	-0.00349	0.00000	0.00888	-0.00812	0.00000
132	N1	S	-0.05711	0.00000	0.51193	-0.21174	0.00000
133	N1	PX	0.03919	0.00000	0.23807	-0.11218	0.00000
134	N1	PY	0.12407	0.00000	-0.06707	0.04059	0.00000
135	N1	PZ	0.00000	-0.11003	0.00000	0.00000	0.07413
136	N1	S	0.59194	0.00000	-1.45956	0.99564	0.00000
137	N1	PX	0.32650	0.00000	-0.78165	0.56799	0.00000
138	N1	PY	-0.51741	0.00000	0.23623	0.23036	0.00000
139	N1	PZ	0.00000	0.28544	0.00000	0.00000	-0.24860
140	N1	DXX	-0.09924	0.00000	-0.00750	0.16556	0.00000
141	N1	DYY	-0.02999	0.00000	0.01792	-0.10296	0.00000
142	N1	DZZ	0.14484	0.00000	0.13842	-0.05182	0.00000
143	N1	DXY	-0.11653	0.00000	0.14994	0.31141	0.00000
144	N1	DXZ	0.00000	0.18983	0.00000	0.00000	-0.28725
145	N1	DYZ	0.00000	0.28185	0.00000	0.00000	-0.05206
146	H6	S	0.18983	0.00000	-0.22078	0.34358	0.00000
147	H6	S	-0.00190	0.00000	-0.61456	0.02509	0.00000
148	H6	PX	-0.06259	0.00000	0.02284	-0.12534	0.00000
149	H6	PY	-0.06219	0.00000	0.01236	0.03426	0.00000
150	H6	PZ	0.00000	-0.10628	0.00000	0.00000	0.10425
151	C8	S	0.00379	0.00000	0.02205	-0.00043	0.00000
152	C8	S	-0.04681	0.00000	0.36320	-0.05460	0.00000
153	C8	PX	-0.02965	0.00000	-0.08546	-0.01301	0.00000
154	C8	PY	0.01129	0.00000	0.16877	-0.04643	0.00000
155	C8	PZ	0.00000	-0.03450	0.00000	0.00000	0.06904
156	C8	S	0.77233	0.00000	-1.36579	-0.20244	0.00000
157	C8	PX	1.23507	0.00000	-1.43423	0.08582	0.00000
158	C8	PY	1.81042	0.00000	-2.73687	-0.88397	0.00000
159	C8	PZ	0.00000	-0.16952	0.00000	0.00000	0.43555
160	C8	DXX	-0.07491	0.00000	-0.22323	-0.00242	0.00000
161	C8	DYY	-0.11212	0.00000	0.12854	0.02936	0.00000
162	C8	DZZ	0.23945	0.00000	0.11878	-0.01715	0.00000
163	C8	DXY	-0.05580	0.00000	0.17703	-0.00036	0.00000
164	C8	DXZ	0.00000	-0.02334	0.00000	0.00000	0.07708
165	C8	DYZ	0.00000	0.01056	0.00000	0.00000	-0.00379
166	H8	S	-0.05865	0.00000	0.06336	0.30185	0.00000
167	H8	S	-0.51416	0.00000	0.69522	0.03204	0.00000
168	H8	PX	-0.00399	0.00000	0.00994	0.09913	0.00000
169	H8	PY	-0.02126	0.00000	0.09958	-0.08923	0.00000
170	H8	PZ	0.00000	0.02632	0.00000	0.00000	0.14593
171	C10	S	0.00897	0.00000	0.01024	0.00183	0.00000
172	C10	S	0.13512	0.00000	-0.01885	-0.05316	0.00000
173	C10	PX	-0.02188	0.00000	0.03180	0.00887	0.00000
174	C10	PY	0.13202	0.00000	-0.08934	-0.08401	0.00000
175	C10	PZ	0.00000	0.00221	0.00000	0.00000	-0.01138
176	C10	S	0.67635	0.00000	-1.44600	-0.57304	0.00000
177	C10	PX	-0.93708	0.00000	1.24851	0.31112	0.00000

178	C10	PY	0.14443	0.00000	-0.18040	-0.12077	0.00000
179	C10	PZ	0.00000	0.10143	0.00000	0.00000	-0.23894
180	C10	DXX	-0.15772	0.00000	0.00151	0.05696	0.00000
181	C10	DYY	0.01829	0.00000	-0.07928	-0.04139	0.00000
182	C10	DZZ	0.22137	0.00000	0.08431	-0.02182	0.00000
183	C10	DXY	0.05301	0.00000	-0.26734	-0.04772	0.00000
184	C10	DXZ	0.00000	-0.02138	0.00000	0.00000	0.06118
185	C10	DYZ	0.00000	0.14884	0.00000	0.00000	-0.31038
186	H16	S	0.30279	0.00000	-0.29484	-0.12333	0.00000
187	H16	S	0.24931	0.00000	-0.28172	-0.02941	0.00000
188	H16	PX	0.08459	0.00000	-0.13786	-0.02236	0.00000
189	H16	PY	-0.00947	0.00000	-0.09866	0.01717	0.00000
190	H16	PZ	0.00000	-0.03630	0.00000	0.00000	0.09577
191	H18	S	-0.11194	0.00000	0.47404	0.08268	0.00000
192	H18	S	-0.23997	0.00000	0.27457	0.10213	0.00000
193	H18	PX	0.06139	0.00000	-0.14559	-0.02598	0.00000
194	H18	PY	-0.05656	0.00000	-0.02542	0.00880	0.00000
195	H18	PZ	0.00000	-0.06147	0.00000	0.00000	0.12699
196	C9	S	-0.00530	0.00000	0.01647	0.01416	0.00000
197	C9	S	-0.02777	0.00000	0.13743	0.11371	0.00000
198	C9	PX	0.02996	0.00000	0.00936	-0.01604	0.00000
199	C9	PY	0.06966	0.00000	-0.00548	-0.03595	0.00000
200	C9	PZ	0.00000	-0.00001	0.00000	0.00000	0.03746
201	C9	S	-0.06514	0.00000	-0.33730	-0.22133	0.00000
202	C9	PX	-0.04888	0.00000	-0.03045	-0.02016	0.00000
203	C9	PY	-0.11415	0.00000	0.11941	0.20463	0.00000
204	C9	PZ	0.00000	0.06083	0.00000	0.00000	0.29296
205	C9	DXX	0.00558	0.00000	0.09298	0.06281	0.00000
206	C9	DYY	-0.01701	0.00000	-0.07786	-0.03070	0.00000
207	C9	DZZ	0.00920	0.00000	-0.00279	-0.00408	0.00000
208	C9	DXY	-0.10949	0.00000	0.02555	0.01527	0.00000
209	C9	DXZ	0.00000	0.11252	0.00000	0.00000	0.09306
210	C9	DYZ	0.00000	-0.05278	0.00000	0.00000	-0.20117
211	H3	S	-0.01692	0.00000	0.08275	0.02397	0.00000
212	H3	S	0.10566	0.00000	-0.03386	-0.07637	0.00000
213	H3	PX	-0.14990	0.00000	0.01713	0.01220	0.00000
214	H3	PY	-0.04498	0.00000	0.03449	0.02302	0.00000
215	H3	PZ	0.00000	-0.00093	0.00000	0.00000	-0.02264
216	H5	S	-0.03317	0.09517	0.04111	0.06799	0.20963
217	H5	S	0.09288	-0.02413	0.05001	0.00466	-0.00844
218	H5	PX	0.06999	0.03451	0.02447	0.01792	0.25349
219	H5	PY	0.01970	0.00748	0.00527	0.00755	0.16822
220	H5	PZ	0.02756	-0.02004	0.00943	0.00873	0.01942
221	H7	S	-0.03317	-0.09517	0.04111	0.06799	-0.20963
222	H7	S	0.09288	0.02413	0.05001	0.00466	0.00844
223	H7	PX	0.06999	-0.03451	0.02447	0.01792	-0.25349
224	H7	PY	0.01970	-0.00748	0.00527	0.00755	-0.16822
225	H7	PZ	-0.02756	-0.02004	-0.00943	-0.00873	0.01942

MO:	146	147	148	149	150
Eigenvalues:	2.22326	2.23489	2.28694	2.28708	2.29163
(ev):	60.49797	60.81459	62.23095	62.23476	62.35851

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1	H1	S	0.00000	-0.14262	0.05545	0.00000	-0.32355
2	H1	S	0.00000	0.10920	0.02209	0.00000	-0.15533
3	H1	PX	0.00000	0.00743	0.02900	0.00000	-0.17584
4	H1	PY	0.00000	-0.04910	-0.08020	0.00000	0.10110
5	H1	PZ	-0.10012	0.00000	0.00000	-0.17317	0.00000
6	C1	S	0.00000	-0.01564	-0.01127	0.00000	-0.00923
7	C1	S	0.00000	0.08324	-0.11613	0.00000	-0.17923
8	C1	PX	0.00000	-0.07662	0.05182	0.00000	0.01184
9	C1	PY	0.00000	-0.01172	-0.09587	0.00000	0.12565
10	C1	PZ	-0.04574	0.00000	0.00000	0.04721	0.00000
11	C1	S	0.00000	1.23753	0.09068	0.00000	0.62291
12	C1	PX	0.00000	-0.32440	-0.02964	0.00000	0.77007
13	C1	PY	0.00000	0.41149	-0.73678	0.00000	-1.12088
14	C1	PZ	0.37905	0.00000	0.00000	0.21300	0.00000
15	C1	DXX	0.00000	0.11449	0.04976	0.00000	0.14000
16	C1	DYY	0.00000	-0.12222	0.04634	0.00000	0.08658
17	C1	DZZ	0.00000	0.03181	-0.11426	0.00000	-0.29991
18	C1	DXY	0.00000	-0.01598	-0.09458	0.00000	0.31565
19	C1	DXZ	-0.16008	0.00000	0.00000	-0.12043	0.00000
20	C1	DYZ	-0.01069	0.00000	0.00000	-0.17838	0.00000
21	C2	S	0.00000	-0.01021	-0.01557	0.00000	0.01791
22	C2	S	0.00000	0.02991	-0.02704	0.00000	0.20309
23	C2	PX	0.00000	0.02400	0.05183	0.00000	0.05392
24	C2	PY	0.00000	-0.04283	0.11349	0.00000	0.03087
25	C2	PZ	-0.00270	0.00000	0.00000	0.05408	0.00000
26	C2	S	0.00000	0.02461	1.46213	0.00000	-0.58117
27	C2	PX	0.00000	0.27605	0.54060	0.00000	0.19349
28	C2	PY	0.00000	0.13986	-0.35456	0.00000	0.55505
29	C2	PZ	-0.60043	0.00000	0.00000	0.30111	0.00000
30	C2	DXX	0.00000	-0.11521	0.18901	0.00000	-0.32451
31	C2	DYY	0.00000	0.11906	-0.09810	0.00000	0.04077
32	C2	DZZ	0.00000	-0.03716	-0.04459	0.00000	0.40468
33	C2	DXY	0.00000	0.15704	-0.22375	0.00000	-0.06573
34	C2	DXZ	-0.37202	0.00000	0.00000	0.20171	0.00000
35	C2	DYZ	-0.09878	0.00000	0.00000	0.12251	0.00000
36	C3	S	0.00000	-0.00385	-0.00558	0.00000	-0.00981
37	C3	S	0.00000	0.01130	-0.10471	0.00000	-0.30696
38	C3	PX	0.00000	0.10261	-0.04779	0.00000	0.25933
39	C3	PY	0.00000	0.13823	0.17075	0.00000	-0.02023
40	C3	PZ	0.02248	0.00000	0.00000	-0.06661	0.00000
41	C3	S	0.00000	-0.31730	0.69871	0.00000	0.63687
42	C3	PX	0.00000	-0.22680	-0.08602	0.00000	-1.27629
43	C3	PY	0.00000	-0.26922	-1.68604	0.00000	-1.26735
44	C3	PZ	-0.38881	0.00000	0.00000	-0.10073	0.00000
45	C3	DXX	0.00000	0.18989	0.06226	0.00000	-0.09192
46	C3	DYY	0.00000	-0.15143	-0.08921	0.00000	0.20949
47	C3	DZZ	0.00000	-0.02753	0.02492	0.00000	-0.16339
48	C3	DXY	0.00000	-0.00935	0.07548	0.00000	-0.02873
49	C3	DXZ	0.11844	0.00000	0.00000	-0.04162	0.00000
50	C3	DYZ	0.02549	0.00000	0.00000	-0.24228	0.00000
51	C4	S	0.00000	-0.01272	-0.01064	0.00000	-0.01157
52	C4	S	0.00000	-0.14827	-0.29194	0.00000	-0.06457
53	C4	PX	0.00000	-0.03507	0.03600	0.00000	0.15596
54	C4	PY	0.00000	-0.02753	0.20076	0.00000	-0.01163

55	C4	PZ	-0.03058	0.00000	0.00000	-0.01952	0.00000
56	C4	S	0.00000	-0.30986	0.44543	0.00000	1.61324
57	C4	PX	0.00000	-1.10601	1.07104	0.00000	0.01006
58	C4	PY	0.00000	0.55712	-0.71487	0.00000	-0.24502
59	C4	PZ	-0.57581	0.00000	0.00000	-0.04072	0.00000
60	C4	DXX	0.00000	-0.00175	-0.02875	0.00000	-0.11008
61	C4	DYY	0.00000	0.16341	0.19599	0.00000	0.16438
62	C4	DZZ	0.00000	-0.20820	-0.28547	0.00000	0.00202
63	C4	DXY	0.00000	0.13209	-0.00216	0.00000	0.09184
64	C4	DXZ	0.19865	0.00000	0.00000	-0.21192	0.00000
65	C4	DYZ	0.05764	0.00000	0.00000	0.04857	0.00000
66	C5	S	0.00000	-0.00483	-0.01189	0.00000	0.02199
67	C5	S	0.00000	-0.27282	0.01389	0.00000	0.31286
68	C5	PX	0.00000	-0.06786	0.02057	0.00000	0.13724
69	C5	PY	0.00000	0.16745	-0.08260	0.00000	0.00507
70	C5	PZ	0.01363	0.00000	0.00000	-0.03900	0.00000
71	C5	S	0.00000	-0.34653	0.38336	0.00000	-1.13048
72	C5	PX	0.00000	-0.14358	0.14150	0.00000	-0.56951
73	C5	PY	0.00000	-0.70230	1.05220	0.00000	0.29609
74	C5	PZ	0.61032	0.00000	0.00000	-0.23353	0.00000
75	C5	DXX	0.00000	-0.01733	0.34243	0.00000	-0.06001
76	C5	DYY	0.00000	0.11661	-0.16752	0.00000	-0.12644
77	C5	DZZ	0.00000	-0.19297	-0.15833	0.00000	0.21443
78	C5	DXY	0.00000	-0.09927	-0.07877	0.00000	0.11292
79	C5	DXZ	0.33381	0.00000	0.00000	0.01329	0.00000
80	C5	DYZ	-0.22428	0.00000	0.00000	0.25059	0.00000
81	C6	S	0.00000	-0.00822	0.00963	0.00000	0.01492
82	C6	S	0.00000	-0.09486	-0.06074	0.00000	0.18128
83	C6	PX	0.00000	-0.14946	0.00417	0.00000	0.16987
84	C6	PY	0.00000	0.14807	-0.02822	0.00000	0.09276
85	C6	PZ	0.03261	0.00000	0.00000	-0.02195	0.00000
86	C6	S	0.00000	0.44052	-0.86673	0.00000	-1.31187
87	C6	PX	0.00000	0.29657	0.35912	0.00000	-1.33146
88	C6	PY	0.00000	-1.03465	-0.59231	0.00000	0.59692
89	C6	PZ	0.55354	0.00000	0.00000	-0.12485	0.00000
90	C6	DXX	0.00000	0.13158	-0.03655	0.00000	0.08737
91	C6	DYY	0.00000	-0.08033	-0.01462	0.00000	-0.16385
92	C6	DZZ	0.00000	-0.02727	-0.05126	0.00000	0.07726
93	C6	DXY	0.00000	0.13688	-0.00497	0.00000	0.08181
94	C6	DXZ	-0.07557	0.00000	0.00000	0.30208	0.00000
95	C6	DYZ	0.10995	0.00000	0.00000	-0.02602	0.00000
96	C7	S	0.00000	-0.00552	0.01671	0.00000	-0.00647
97	C7	S	0.00000	-0.00599	0.21415	0.00000	-0.24068
98	C7	PX	0.00000	-0.06307	-0.07705	0.00000	0.19865
99	C7	PY	0.00000	-0.13142	0.07705	0.00000	0.03032
100	C7	PZ	-0.00198	0.00000	0.00000	-0.03157	0.00000
101	C7	S	0.00000	0.67845	-1.81043	0.00000	-0.37445
102	C7	PX	0.00000	-0.47447	1.01594	0.00000	0.24962
103	C7	PY	0.00000	0.20844	-0.19031	0.00000	0.21167
104	C7	PZ	0.06569	0.00000	0.00000	-0.18427	0.00000
105	C7	DXX	0.00000	0.07335	-0.10877	0.00000	0.15703
106	C7	DYY	0.00000	-0.00417	0.10476	0.00000	-0.11339
107	C7	DZZ	0.00000	-0.03304	0.06131	0.00000	-0.16364
108	C7	DXY	0.00000	0.09858	0.04856	0.00000	-0.02590

109	C7	DXZ	-0.01253	0.00000	0.00000	0.17405	0.00000
110	C7	DYZ	0.13680	0.00000	0.00000	0.38342	0.00000
111	O1	S	0.00000	-0.00087	0.00592	0.00000	0.01867
112	O1	S	0.00000	-0.17456	-0.16914	0.00000	0.16099
113	O1	PX	0.00000	-0.07638	-0.01933	0.00000	0.08736
114	O1	PY	0.00000	0.18982	-0.00852	0.00000	0.08114
115	O1	PZ	-0.14290	0.00000	0.00000	-0.07038	0.00000
116	O1	S	0.00000	0.17012	0.36439	0.00000	-0.70638
117	O1	PX	0.00000	0.34458	-0.09333	0.00000	-0.34453
118	O1	PY	0.00000	-0.18218	0.15829	0.00000	0.00598
119	O1	PZ	0.35488	0.00000	0.00000	0.13747	0.00000
120	O1	DXX	0.00000	0.08385	-0.21205	0.00000	-0.01294
121	O1	DYY	0.00000	0.01881	0.02111	0.00000	0.04634
122	O1	DZZ	0.00000	-0.19774	0.09725	0.00000	0.05424
123	O1	DXY	0.00000	-0.20744	0.34796	0.00000	0.02648
124	O1	DXZ	0.38158	0.00000	0.00000	0.26644	0.00000
125	O1	DYZ	-0.20639	0.00000	0.00000	-0.01321	0.00000
126	H4	S	0.00000	-0.04077	-0.25563	0.00000	0.13418
127	H4	S	0.00000	0.21070	-0.18691	0.00000	-0.22905
128	H4	PX	0.00000	0.05707	-0.05829	0.00000	-0.06410
129	H4	PY	0.00000	-0.03109	-0.10870	0.00000	0.01214
130	H4	PZ	-0.30750	0.00000	0.00000	0.17430	0.00000
131	N1	S	0.00000	-0.00261	0.00184	0.00000	-0.01192
132	N1	S	0.00000	0.11416	-0.00346	0.00000	0.07831
133	N1	PX	0.00000	0.10745	-0.01187	0.00000	0.16143
134	N1	PY	0.00000	-0.00027	0.06176	0.00000	0.17205
135	N1	PZ	0.08147	0.00000	0.00000	0.04574	0.00000
136	N1	S	0.00000	-0.19365	0.14197	0.00000	0.62420
137	N1	PX	0.00000	0.23397	0.07848	0.00000	0.06391
138	N1	PY	0.00000	-0.22015	-0.27617	0.00000	-0.09102
139	N1	PZ	-0.28508	0.00000	0.00000	-0.09803	0.00000
140	N1	DXX	0.00000	0.10466	-0.12484	0.00000	-0.13111
141	N1	DYY	0.00000	-0.02221	0.06576	0.00000	0.09370
142	N1	DZZ	0.00000	-0.01896	0.08005	0.00000	0.08051
143	N1	DXY	0.00000	0.08447	-0.14249	0.00000	-0.24711
144	N1	DXZ	-0.16591	0.00000	0.00000	-0.27708	0.00000
145	N1	DYZ	-0.22851	0.00000	0.00000	0.14154	0.00000
146	H6	S	0.00000	0.06676	-0.05414	0.00000	0.37777
147	H6	S	0.00000	0.10865	0.05190	0.00000	0.04620
148	H6	PX	0.00000	0.02643	-0.04708	0.00000	-0.13825
149	H6	PY	0.00000	-0.09897	0.10092	0.00000	-0.03079
150	H6	PZ	0.31567	0.00000	0.00000	-0.19892	0.00000
151	C8	S	0.00000	0.01236	0.02005	0.00000	0.00093
152	C8	S	0.00000	-0.18351	0.05039	0.00000	-0.04822
153	C8	PX	0.00000	-0.09911	-0.08694	0.00000	0.09224
154	C8	PY	0.00000	0.27013	0.09022	0.00000	0.04629
155	C8	PZ	0.03569	0.00000	0.00000	0.08933	0.00000
156	C8	S	0.00000	-0.06457	0.20905	0.00000	-0.04628
157	C8	PX	0.00000	0.58701	0.80044	0.00000	0.26896
158	C8	PY	0.00000	-1.99822	0.02995	0.00000	0.58477
159	C8	PZ	0.13333	0.00000	0.00000	0.43544	0.00000
160	C8	DXX	0.00000	-0.26843	0.03895	0.00000	-0.03501
161	C8	DYY	0.00000	0.20651	-0.13312	0.00000	0.01877
162	C8	DZZ	0.00000	-0.02009	0.15449	0.00000	0.00379

163	C8	DXY	0.00000	-0.10297	0.05700	0.00000	0.15612
164	C8	DXZ	-0.01594	0.00000	0.00000	0.18346	0.00000
165	C8	DYZ	-0.03582	0.00000	0.00000	-0.03745	0.00000
166	H8	S	0.00000	0.01534	0.04206	0.00000	-0.15275
167	H8	S	0.00000	0.12594	-0.29576	0.00000	0.02778
168	H8	PX	0.00000	0.00516	0.03844	0.00000	-0.10481
169	H8	PY	0.00000	-0.00766	-0.04340	0.00000	-0.01071
170	H8	PZ	-0.02374	0.00000	0.00000	0.15561	0.00000
171	C10	S	0.00000	0.00967	0.02038	0.00000	0.00144
172	C10	S	0.00000	-0.04722	0.21398	0.00000	0.07172
173	C10	PX	0.00000	0.02769	0.02086	0.00000	-0.03776
174	C10	PY	0.00000	-0.14991	0.12029	0.00000	0.07034
175	C10	PZ	-0.00790	0.00000	0.00000	-0.02986	0.00000
176	C10	S	0.00000	-1.57495	-0.55195	0.00000	0.31208
177	C10	PX	0.00000	0.03730	-0.61483	0.00000	-0.00989
178	C10	PY	0.00000	-0.00865	-0.14183	0.00000	0.20492
179	C10	PZ	-0.08641	0.00000	0.00000	-0.26461	0.00000
180	C10	DXX	0.00000	-0.39387	-0.25250	0.00000	-0.04440
181	C10	DYY	0.00000	0.24288	0.01467	0.00000	-0.02289
182	C10	DZZ	0.00000	0.16786	0.38877	0.00000	0.10693
183	C10	DXY	0.00000	-0.20136	0.05644	0.00000	-0.14908
184	C10	DXZ	0.01857	0.00000	0.00000	0.06973	0.00000
185	C10	DYZ	-0.12634	0.00000	0.00000	-0.32850	0.00000
186	H16	S	0.00000	0.25310	0.35354	0.00000	-0.02913
187	H16	S	0.00000	0.04068	0.19553	0.00000	0.01448
188	H16	PX	0.00000	-0.01216	0.13923	0.00000	-0.05190
189	H16	PY	0.00000	-0.28081	-0.01383	0.00000	-0.09046
190	H16	PZ	0.04198	0.00000	0.00000	0.10888	0.00000
191	H18	S	0.00000	0.32680	0.02719	0.00000	0.15364
192	H18	S	0.00000	0.03711	-0.17355	0.00000	-0.01726
193	H18	PX	0.00000	0.06668	0.12033	0.00000	-0.06208
194	H18	PY	0.00000	-0.23026	-0.18226	0.00000	-0.05516
195	H18	PZ	0.05313	0.00000	0.00000	0.18007	0.00000
196	C9	S	0.00000	0.00322	0.00616	0.00000	-0.01362
197	C9	S	0.00000	0.01309	0.02957	0.00000	-0.04230
198	C9	PX	0.00000	0.01703	0.04176	0.00000	-0.09452
199	C9	PY	0.00000	0.01301	0.01643	0.00000	-0.03352
200	C9	PZ	-0.03611	0.00000	0.00000	-0.01701	0.00000
201	C9	S	0.00000	-0.20096	-0.19854	0.00000	0.53428
202	C9	PX	0.00000	-0.00741	0.06689	0.00000	-0.05241
203	C9	PY	0.00000	0.22057	-0.22671	0.00000	-0.26607
204	C9	PZ	-0.12269	0.00000	0.00000	-0.13082	0.00000
205	C9	DXX	0.00000	0.01321	0.08145	0.00000	0.01664
206	C9	DYY	0.00000	0.05813	-0.18403	0.00000	-0.08522
207	C9	DZZ	0.00000	-0.06211	0.10129	0.00000	0.05658
208	C9	DXY	0.00000	-0.07499	0.12355	0.00000	0.03186
209	C9	DXZ	0.06043	0.00000	0.00000	-0.05714	0.00000
210	C9	DYZ	0.08081	0.00000	0.00000	0.09321	0.00000
211	H3	S	0.00000	-0.08852	0.24417	0.00000	0.06265
212	H3	S	0.00000	-0.02414	0.02218	0.00000	0.00261
213	H3	PX	0.00000	-0.12255	0.20387	0.00000	0.04465
214	H3	PY	0.00000	-0.04177	0.14033	0.00000	0.03897
215	H3	PZ	0.01672	0.00000	0.00000	0.08726	0.00000
216	H5	S	-0.04518	0.07523	-0.05001	-0.10269	-0.10195

217	H5	S	-0.00978	0.00703	0.03150	0.02199	-0.03996
218	H5	PX	-0.15578	0.04413	-0.05476	-0.14918	-0.03883
219	H5	PY	-0.10848	0.04504	-0.01555	-0.02798	0.00730
220	H5	PZ	-0.05101	0.00688	-0.00682	-0.03433	0.00314
221	H7	S	0.04518	0.07523	-0.05001	0.10269	-0.10195
222	H7	S	0.00978	0.00703	0.03150	-0.02199	-0.03996
223	H7	PX	0.15578	0.04413	-0.05476	0.14918	-0.03883
224	H7	PY	0.10848	0.04504	-0.01555	0.02798	0.00730
225	H7	PZ	-0.05101	-0.00688	0.00682	-0.03433	-0.00314

M0:	151	152	153	154	155
Eigenvalues:	2.31790	2.32310	2.34457	2.34735	2.35830
(ev):	63.07317	63.21490	63.79889	63.87459	64.17265

			A	A	A	A	A
1	H1	S	-0.10218	0.00000	-0.04429	0.15793	0.00000
2	H1	S	-0.05713	0.00000	-0.05055	0.04742	0.00000
3	H1	PX	-0.03593	0.00000	-0.02036	0.03362	0.00000
4	H1	PY	0.00104	0.00000	0.00266	-0.03762	0.00000
5	H1	PZ	0.00000	0.01196	0.00000	0.00000	0.10022
6	C1	S	-0.01126	0.00000	0.01630	-0.00818	0.00000
7	C1	S	-0.09348	0.00000	0.30023	-0.14682	0.00000
8	C1	PX	0.04051	0.00000	-0.16126	0.00947	0.00000
9	C1	PY	-0.01030	0.00000	0.13040	-0.00369	0.00000
10	C1	PZ	0.00000	0.02198	0.00000	0.00000	-0.00188
11	C1	S	1.06292	0.00000	-2.09647	0.45790	0.00000
12	C1	PX	0.14116	0.00000	0.68630	-0.35288	0.00000
13	C1	PY	-0.42762	0.00000	0.12908	-0.86313	0.00000
14	C1	PZ	0.00000	-0.09559	0.00000	0.00000	-0.14130
15	C1	DXX	0.00667	0.00000	0.13099	-0.04157	0.00000
16	C1	DYY	0.06462	0.00000	-0.09748	0.09182	0.00000
17	C1	DZZ	-0.13955	0.00000	0.01468	-0.05834	0.00000
18	C1	DXY	0.08181	0.00000	-0.08337	-0.03060	0.00000
19	C1	DXZ	0.00000	0.03043	0.00000	0.00000	0.05965
20	C1	DYZ	0.00000	0.04740	0.00000	0.00000	-0.04512
21	C2	S	-0.02246	0.00000	0.01662	-0.01739	0.00000
22	C2	S	-0.38735	0.00000	0.27070	-0.20345	0.00000
23	C2	PX	-0.12490	0.00000	0.01627	-0.03188	0.00000
24	C2	PY	-0.08303	0.00000	0.16912	-0.11372	0.00000
25	C2	PZ	0.00000	-0.01003	0.00000	0.00000	0.01162
26	C2	S	1.07827	0.00000	-1.22323	0.48053	0.00000
27	C2	PX	1.34448	0.00000	-0.56250	0.29786	0.00000
28	C2	PY	1.15707	0.00000	-0.62651	-0.02070	0.00000
29	C2	PZ	0.00000	-0.01861	0.00000	0.00000	0.06138
30	C2	DXX	-0.13714	0.00000	-0.10269	0.10378	0.00000
31	C2	DYY	0.25548	0.00000	0.05018	0.06160	0.00000
32	C2	DZZ	-0.19259	0.00000	0.08446	-0.23037	0.00000
33	C2	DXY	0.13216	0.00000	-0.11690	0.00798	0.00000
34	C2	DXZ	0.00000	-0.01331	0.00000	0.00000	0.01922
35	C2	DYZ	0.00000	-0.02544	0.00000	0.00000	0.05879
36	C3	S	-0.01042	0.00000	0.00985	-0.00356	0.00000
37	C3	S	-0.22571	0.00000	0.12268	-0.13996	0.00000
38	C3	PX	-0.01797	0.00000	0.14780	-0.05489	0.00000
39	C3	PY	0.17636	0.00000	-0.13586	0.08516	0.00000

40	C3	PZ	0.00000	0.00086	0.00000	0.00000	-0.01781
41	C3	S	3.21289	0.00000	0.67411	-1.36979	0.00000
42	C3	PX	-0.65456	0.00000	0.23230	-0.54183	0.00000
43	C3	PY	-2.53555	0.00000	0.98940	-0.03694	0.00000
44	C3	PZ	0.00000	0.09392	0.00000	0.00000	0.07759
45	C3	DXX	-0.16036	0.00000	0.05850	0.00835	0.00000
46	C3	DYY	0.02649	0.00000	-0.10878	0.04205	0.00000
47	C3	DZZ	0.11817	0.00000	0.17438	-0.15187	0.00000
48	C3	DXY	0.07713	0.00000	0.22726	-0.05501	0.00000
49	C3	DXZ	0.00000	-0.00296	0.00000	0.00000	0.06194
50	C3	DYZ	0.00000	0.02331	0.00000	0.00000	0.04422
51	C4	S	-0.02974	0.00000	-0.00278	0.00500	0.00000
52	C4	S	-0.22169	0.00000	-0.21590	0.06718	0.00000
53	C4	PX	0.01206	0.00000	-0.17415	-0.06744	0.00000
54	C4	PY	0.02050	0.00000	0.03219	-0.07813	0.00000
55	C4	PZ	0.00000	0.00388	0.00000	0.00000	0.03028
56	C4	S	1.07872	0.00000	0.45565	-0.21355	0.00000
57	C4	PX	-0.60658	0.00000	1.18946	1.15878	0.00000
58	C4	PY	-0.54962	0.00000	-0.18739	1.06320	0.00000
59	C4	PZ	0.00000	0.03984	0.00000	0.00000	0.05086
60	C4	DXX	0.04904	0.00000	-0.26377	0.04764	0.00000
61	C4	DYY	0.17046	0.00000	0.22940	-0.12615	0.00000
62	C4	DZZ	-0.25109	0.00000	0.01934	0.01751	0.00000
63	C4	DXY	0.01077	0.00000	0.11859	-0.01135	0.00000
64	C4	DXZ	0.00000	0.03461	0.00000	0.00000	-0.03599
65	C4	DYZ	0.00000	0.03010	0.00000	0.00000	-0.20498
66	C5	S	-0.01252	0.00000	-0.00377	-0.01859	0.00000
67	C5	S	-0.26033	0.00000	-0.07360	-0.19217	0.00000
68	C5	PX	-0.01211	0.00000	0.12450	0.03808	0.00000
69	C5	PY	0.23405	0.00000	0.09811	0.08683	0.00000
70	C5	PZ	0.00000	0.00854	0.00000	0.00000	-0.03112
71	C5	S	-1.58327	0.00000	1.52175	1.12825	0.00000
72	C5	PX	-0.58638	0.00000	0.18979	0.53560	0.00000
73	C5	PY	0.04998	0.00000	-0.36855	-0.35242	0.00000
74	C5	PZ	0.00000	0.01903	0.00000	0.00000	-0.07280
75	C5	DXX	-0.08394	0.00000	0.02371	0.06377	0.00000
76	C5	DYY	0.28009	0.00000	-0.05171	0.06139	0.00000
77	C5	DZZ	-0.36440	0.00000	0.07954	-0.16078	0.00000
78	C5	DXY	-0.03784	0.00000	-0.14043	0.06170	0.00000
79	C5	DXZ	0.00000	-0.00439	0.00000	0.00000	-0.02507
80	C5	DYZ	0.00000	-0.03198	0.00000	0.00000	0.04386
81	C6	S	0.01376	0.00000	0.01108	-0.01328	0.00000
82	C6	S	0.41536	0.00000	-0.13070	-0.07756	0.00000
83	C6	PX	0.05031	0.00000	-0.05637	-0.03339	0.00000
84	C6	PY	0.17692	0.00000	-0.07515	0.02689	0.00000
85	C6	PZ	0.00000	0.00264	0.00000	0.00000	0.01269
86	C6	S	-0.78433	0.00000	0.72518	0.10033	0.00000
87	C6	PX	-1.39364	0.00000	0.28489	0.33720	0.00000
88	C6	PY	-1.86918	0.00000	0.51621	-1.00103	0.00000
89	C6	PZ	0.00000	-0.03131	0.00000	0.00000	-0.03428
90	C6	DXX	0.10175	0.00000	0.17521	-0.00282	0.00000
91	C6	DYY	-0.17204	0.00000	-0.23954	0.12020	0.00000
92	C6	DZZ	0.00051	0.00000	0.09373	-0.16980	0.00000
93	C6	DXY	-0.03739	0.00000	-0.07084	0.00894	0.00000

94	C6	DXZ	0.00000	-0.05410	0.00000	0.00000	0.05298
95	C6	DYZ	0.00000	-0.00372	0.00000	0.00000	0.00665
96	C7	S	0.03211	0.00000	0.01722	-0.01054	0.00000
97	C7	S	0.58603	0.00000	0.35061	-0.13599	0.00000
98	C7	PX	-0.14056	0.00000	-0.16288	0.02449	0.00000
99	C7	PY	0.07779	0.00000	0.14505	-0.04390	0.00000
100	C7	PZ	0.00000	0.00449	0.00000	0.00000	-0.00018
101	C7	S	-3.84203	0.00000	-0.47942	1.28469	0.00000
102	C7	PX	2.58942	0.00000	0.57121	-0.73433	0.00000
103	C7	PY	-0.23949	0.00000	-0.65146	0.61989	0.00000
104	C7	PZ	0.00000	-0.01658	0.00000	0.00000	-0.02140
105	C7	DXX	-0.14162	0.00000	0.00572	-0.06494	0.00000
106	C7	DYY	0.00688	0.00000	-0.15349	0.10456	0.00000
107	C7	DZZ	0.11406	0.00000	0.23478	-0.02854	0.00000
108	C7	DXY	-0.04677	0.00000	0.22207	-0.16586	0.00000
109	C7	DXZ	0.00000	-0.00116	0.00000	0.00000	0.01274
110	C7	DYZ	0.00000	-0.05984	0.00000	0.00000	-0.00684
111	O1	S	-0.00280	0.00000	-0.00275	-0.01397	0.00000
112	O1	S	-0.25887	0.00000	0.07557	0.61348	0.00000
113	O1	PX	-0.11076	0.00000	0.31045	0.37728	0.00000
114	O1	PY	0.04654	0.00000	0.31528	0.03086	0.00000
115	O1	PZ	0.00000	0.00693	0.00000	0.00000	0.05642
116	O1	S	0.50485	0.00000	-0.05018	-1.11766	0.00000
117	O1	PX	0.23377	0.00000	-0.64166	-0.57186	0.00000
118	O1	PY	-0.01879	0.00000	-0.41989	0.18136	0.00000
119	O1	PZ	0.00000	-0.02636	0.00000	0.00000	-0.11273
120	O1	DXX	-0.02395	0.00000	-0.09414	-0.10911	0.00000
121	O1	DYY	-0.01851	0.00000	0.03699	0.14464	0.00000
122	O1	DZZ	-0.11244	0.00000	0.06020	0.15705	0.00000
123	O1	DXY	-0.01187	0.00000	-0.06784	0.01876	0.00000
124	O1	DXZ	0.00000	-0.04139	0.00000	0.00000	0.06200
125	O1	DYZ	0.00000	0.02594	0.00000	0.00000	-0.03097
126	H4	S	-0.10196	0.00000	-0.08177	0.04808	0.00000
127	H4	S	0.01557	0.00000	0.06534	0.11186	0.00000
128	H4	PX	0.16823	0.00000	0.02467	0.04986	0.00000
129	H4	PY	0.05708	0.00000	-0.02999	0.04640	0.00000
130	H4	PZ	0.00000	-0.03128	0.00000	0.00000	0.10371
131	N1	S	0.02177	0.00000	0.00190	0.00132	0.00000
132	N1	S	0.57437	0.00000	0.31053	-0.13652	0.00000
133	N1	PX	0.04172	0.00000	0.05169	-0.04223	0.00000
134	N1	PY	0.23104	0.00000	0.13955	-0.05326	0.00000
135	N1	PZ	0.00000	-0.00840	0.00000	0.00000	0.00075
136	N1	S	-2.38375	0.00000	-0.58595	0.04343	0.00000
137	N1	PX	-0.16259	0.00000	-0.25211	0.25308	0.00000
138	N1	PY	-1.14137	0.00000	-0.06237	-0.23542	0.00000
139	N1	PZ	0.00000	0.02270	0.00000	0.00000	0.01872
140	N1	DXX	0.03242	0.00000	0.07568	-0.03698	0.00000
141	N1	DYY	0.02155	0.00000	-0.05044	0.00425	0.00000
142	N1	DZZ	0.07143	0.00000	0.07749	-0.01058	0.00000
143	N1	DXY	0.04264	0.00000	0.05747	-0.01108	0.00000
144	N1	DXZ	0.00000	0.02908	0.00000	0.00000	0.01375
145	N1	DYZ	0.00000	-0.00266	0.00000	0.00000	-0.01187
146	H6	S	0.23511	0.00000	0.07771	-0.07137	0.00000
147	H6	S	0.44772	0.00000	-0.21672	0.11513	0.00000

148	H6	PX	0.03705	0.00000	-0.07329	0.05674	0.00000
149	H6	PY	-0.16931	0.00000	0.05666	-0.06508	0.00000
150	H6	PZ	0.00000	0.02330	0.00000	0.00000	-0.04036
151	C8	S	0.00749	0.00000	0.00287	0.01109	0.00000
152	C8	S	0.20854	0.00000	-0.00947	0.19701	0.00000
153	C8	PX	0.07629	0.00000	-0.01863	0.00852	0.00000
154	C8	PY	-0.12343	0.00000	-0.14076	0.12295	0.00000
155	C8	PZ	0.00000	-0.00986	0.00000	0.00000	-0.00103
156	C8	S	1.57230	0.00000	0.14324	-0.34317	0.00000
157	C8	PX	0.29353	0.00000	-0.40376	0.39495	0.00000
158	C8	PY	1.55837	0.00000	0.96670	-1.49622	0.00000
159	C8	PZ	0.00000	-0.03771	0.00000	0.00000	-0.01102
160	C8	DXX	-0.00515	0.00000	-0.13286	0.07324	0.00000
161	C8	DYY	-0.17474	0.00000	0.01752	-0.07051	0.00000
162	C8	DZZ	0.34784	0.00000	0.12141	0.04991	0.00000
163	C8	DXY	0.08431	0.00000	-0.02021	0.00094	0.00000
164	C8	DXZ	0.00000	-0.01874	0.00000	0.00000	0.03440
165	C8	DYZ	0.00000	0.00865	0.00000	0.00000	0.00798
166	H8	S	-0.07470	0.00000	-0.02469	0.07404	0.00000
167	H8	S	-0.71213	0.00000	-0.22346	0.17377	0.00000
168	H8	PX	-0.01515	0.00000	0.03116	0.01929	0.00000
169	H8	PY	-0.05780	0.00000	0.13554	-0.12114	0.00000
170	H8	PZ	0.00000	-0.00509	0.00000	0.00000	-0.00941
171	C10	S	0.01982	0.00000	-0.00678	0.01684	0.00000
172	C10	S	0.19679	0.00000	-0.04410	0.09109	0.00000
173	C10	PX	-0.05462	0.00000	0.06253	-0.06789	0.00000
174	C10	PY	0.11728	0.00000	0.03369	-0.03206	0.00000
175	C10	PZ	0.00000	0.00361	0.00000	0.00000	-0.00006
176	C10	S	0.29022	0.00000	0.81678	-1.26180	0.00000
177	C10	PX	0.05485	0.00000	-0.33654	0.47886	0.00000
178	C10	PY	-0.30405	0.00000	0.00116	-0.26769	0.00000
179	C10	PZ	0.00000	0.02729	0.00000	0.00000	0.00704
180	C10	DXX	0.20362	0.00000	0.07762	-0.04016	0.00000
181	C10	DYY	-0.31723	0.00000	0.01916	-0.10843	0.00000
182	C10	DZZ	0.17917	0.00000	-0.16779	0.24602	0.00000
183	C10	DXY	-0.01297	0.00000	0.15023	-0.11245	0.00000
184	C10	DXZ	0.00000	-0.00672	0.00000	0.00000	0.00075
185	C10	DYZ	0.00000	0.03352	0.00000	0.00000	0.00695
186	H16	S	-0.13365	0.00000	0.02344	-0.03386	0.00000
187	H16	S	-0.03408	0.00000	0.04732	-0.09885	0.00000
188	H16	PX	-0.05297	0.00000	0.07387	-0.06578	0.00000
189	H16	PY	0.08918	0.00000	0.23994	-0.19189	0.00000
190	H16	PZ	0.00000	-0.01132	0.00000	0.00000	-0.00967
191	H18	S	0.03789	0.00000	-0.22880	0.24160	0.00000
192	H18	S	-0.08537	0.00000	-0.14806	0.14982	0.00000
193	H18	PX	-0.17326	0.00000	0.12941	-0.15888	0.00000
194	H18	PY	0.17039	0.00000	0.01860	0.03098	0.00000
195	H18	PZ	0.00000	-0.02147	0.00000	0.00000	0.00436
196	C9	S	-0.00134	0.00000	0.00848	0.00199	0.00000
197	C9	S	-0.02778	0.00000	0.20376	0.15817	0.00000
198	C9	PX	0.05071	0.00000	-0.18831	-0.18337	0.00000
199	C9	PY	0.03998	0.00000	-0.09415	-0.09963	0.00000
200	C9	PZ	0.00000	0.01380	0.00000	0.00000	-0.11625
201	C9	S	-0.16944	0.00000	0.15926	0.20921	0.00000

202	C9	PX	-0.01050	0.00000	0.12820	0.36969	0.00000
203	C9	PY	-0.15471	0.00000	0.27924	0.17886	0.00000
204	C9	PZ	0.00000	-0.04469	0.00000	0.00000	0.61065
205	C9	DXX	0.06164	0.00000	-0.12340	-0.31077	0.00000
206	C9	DYY	-0.02682	0.00000	-0.05852	-0.02135	0.00000
207	C9	DZZ	-0.03265	0.00000	0.17717	0.28026	0.00000
208	C9	DXY	0.09132	0.00000	-0.28075	-0.37895	0.00000
209	C9	DXZ	0.00000	-0.05582	0.00000	0.00000	0.51986
210	C9	DYZ	0.00000	0.01657	0.00000	0.00000	-0.29111
211	H3	S	0.08501	0.00000	-0.07361	-0.09880	0.00000
212	H3	S	0.07049	0.00000	-0.11819	-0.05713	0.00000
213	H3	PX	0.02271	0.00000	-0.16083	-0.05122	0.00000
214	H3	PY	0.03922	0.00000	-0.03629	-0.07011	0.00000
215	H3	PZ	0.00000	0.59478	0.00000	0.00000	-0.22409
216	H5	S	0.03086	-0.03442	-0.11672	-0.20813	0.46738
217	H5	S	0.01625	-0.00744	0.02332	0.00008	-0.02118
218	H5	PX	0.04155	-0.21764	-0.11720	-0.22788	-0.14042
219	H5	PY	0.04497	0.45744	0.01645	-0.10570	-0.06778
220	H5	PZ	-0.00746	-0.25048	0.02935	0.02715	-0.39593
221	H7	S	0.03086	0.03442	-0.11672	-0.20813	-0.46738
222	H7	S	0.01625	0.00744	0.02332	0.00008	0.02118
223	H7	PX	0.04155	0.21764	-0.11720	-0.22788	0.14042
224	H7	PY	0.04497	-0.45744	0.01645	-0.10570	0.06778
225	H7	PZ	0.00746	-0.25048	-0.02935	-0.02715	-0.39593

M0:	156	157	158	159	160
Eigenvalues:	2.38941	2.40058	2.43816	2.44064	2.45653
(ev):	65.01916	65.32302	66.34566	66.41335	66.84554

		A	A	A	A	A	
1	H1	S	0.09481	0.00035	0.03272	0.00000	-0.05830
2	H1	S	-0.21783	0.21816	0.14406	0.00000	0.06162
3	H1	PX	0.03142	-0.04213	0.02906	0.00000	0.01828
4	H1	PY	0.07018	0.17535	0.01756	0.00000	-0.12263
5	H1	PZ	0.00000	0.00000	0.00000	-0.12102	0.00000
6	C1	S	0.01703	0.00844	-0.00909	0.00000	0.00637
7	C1	S	0.30134	-0.04085	-0.03642	0.00000	0.06574
8	C1	PX	-0.12504	-0.06456	0.00589	0.00000	0.03995
9	C1	PY	0.07102	0.24832	-0.05105	0.00000	-0.20223
10	C1	PZ	0.00000	0.00000	0.00000	-0.01161	0.00000
11	C1	S	-1.07822	0.18418	1.12917	0.00000	-1.91109
12	C1	PX	0.78632	-0.35856	-0.52643	0.00000	0.42978
13	C1	PY	-0.38170	-0.04304	0.18597	0.00000	0.86380
14	C1	PZ	0.00000	0.00000	0.00000	0.02794	0.00000
15	C1	DXX	-0.12035	-0.08534	0.01065	0.00000	-0.00714
16	C1	DYY	0.02037	0.03658	-0.07054	0.00000	0.06577
17	C1	DZZ	0.16973	0.09508	0.09385	0.00000	-0.08838
18	C1	DXY	-0.05393	0.12860	-0.06723	0.00000	0.05869
19	C1	DXZ	0.00000	0.00000	0.00000	0.02139	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.04625	0.00000
21	C2	S	0.01124	-0.00003	-0.01181	0.00000	0.00884
22	C2	S	0.25078	-0.13698	0.07408	0.00000	0.18390
23	C2	PX	0.03707	-0.11679	0.09122	0.00000	0.04939
24	C2	PY	0.26840	0.09188	-0.00196	0.00000	-0.04293

25	C2	PZ	0.00000	0.00000	0.00000	0.02795	0.00000
26	C2	S	-0.51880	-0.45052	0.92115	0.00000	-0.63745
27	C2	PX	-0.31468	-0.09825	0.40083	0.00000	-0.53552
28	C2	PY	-0.20981	-1.54381	-0.14041	0.00000	0.78883
29	C2	PZ	0.00000	0.00000	0.00000	-0.01259	0.00000
30	C2	DXX	0.00972	0.04790	0.04982	0.00000	-0.13510
31	C2	DYY	-0.04485	0.05928	0.00024	0.00000	0.06050
32	C2	DZZ	0.13670	-0.16247	-0.01741	0.00000	0.09339
33	C2	DXY	-0.04392	-0.13052	-0.05580	0.00000	0.01988
34	C2	DXZ	0.00000	0.00000	0.00000	0.04027	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	-0.00185	0.00000
36	C3	S	0.00469	0.01227	-0.02384	0.00000	0.00589
37	C3	S	-0.31355	0.06327	-0.28354	0.00000	0.05112
38	C3	PX	0.15094	-0.00962	0.15879	0.00000	-0.09793
39	C3	PY	0.07245	-0.06839	0.22257	0.00000	-0.13512
40	C3	PZ	0.00000	0.00000	0.00000	-0.00282	0.00000
41	C3	S	0.95837	-2.99933	-0.21182	0.00000	2.21198
42	C3	PX	-0.94251	0.68442	-0.60440	0.00000	0.66195
43	C3	PY	-0.19998	1.84762	-0.58018	0.00000	0.27333
44	C3	PZ	0.00000	0.00000	0.00000	0.01599	0.00000
45	C3	DXX	0.08050	-0.01149	0.30751	0.00000	-0.16703
46	C3	DYY	-0.08331	0.11692	-0.04917	0.00000	-0.02044
47	C3	DZZ	0.02568	-0.17433	-0.31782	0.00000	0.24972
48	C3	DXY	0.12307	0.20306	-0.02590	0.00000	-0.08869
49	C3	DXZ	0.00000	0.00000	0.00000	0.56676	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.06921	0.00000
51	C4	S	0.01073	0.01651	0.00359	0.00000	-0.00904
52	C4	S	0.04282	0.38718	0.02154	0.00000	-0.30255
53	C4	PX	-0.03009	-0.03557	0.02929	0.00000	0.06647
54	C4	PY	0.02638	-0.19413	-0.02905	0.00000	0.00897
55	C4	PZ	0.00000	0.00000	0.00000	-0.01891	0.00000
56	C4	S	0.43702	-0.48616	-0.96809	0.00000	-0.47297
57	C4	PX	0.73147	-0.32308	-0.25251	0.00000	1.05813
58	C4	PY	-0.38874	1.31697	0.44540	0.00000	-1.25858
59	C4	PZ	0.00000	0.00000	0.00000	-0.04623	0.00000
60	C4	DXX	-0.15388	-0.23940	-0.05959	0.00000	0.10054
61	C4	DYY	0.05285	0.02121	0.02958	0.00000	-0.01132
62	C4	DZZ	0.13869	0.27398	-0.03968	0.00000	-0.11344
63	C4	DXY	0.11820	0.04142	0.04804	0.00000	-0.00040
64	C4	DXZ	0.00000	0.00000	0.00000	0.12491	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.00526	0.00000
66	C5	S	0.00694	-0.00139	-0.00323	0.00000	-0.01552
67	C5	S	0.03623	0.10513	-0.03346	0.00000	-0.26459
68	C5	PX	0.05433	0.15906	0.02858	0.00000	-0.04707
69	C5	PY	-0.02001	0.03416	0.02957	0.00000	0.05579
70	C5	PZ	0.00000	0.00000	0.00000	0.00971	0.00000
71	C5	S	0.51715	1.20447	0.02791	0.00000	0.63062
72	C5	PX	0.10495	-0.51296	0.17583	0.00000	0.77376
73	C5	PY	0.54187	-1.09203	0.05318	0.00000	0.52582
74	C5	PZ	0.00000	0.00000	0.00000	0.02322	0.00000
75	C5	DXX	0.13572	-0.13196	0.13649	0.00000	0.15350
76	C5	DYY	-0.20124	0.06554	-0.12554	0.00000	0.01395
77	C5	DZZ	0.09595	0.10259	-0.00161	0.00000	-0.19114
78	C5	DXY	-0.22809	-0.10089	-0.02768	0.00000	0.05689

79	C5	DXZ	0.00000	0.00000	0.00000	0.11741	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.08793	0.00000
81	C6	S	0.00840	-0.00969	-0.01959	0.00000	0.01848
82	C6	S	0.00439	-0.44862	-0.31780	0.00000	0.38608
83	C6	PX	-0.05334	-0.10559	-0.16456	0.00000	0.18398
84	C6	PY	-0.19628	-0.05603	0.00448	0.00000	0.03894
85	C6	PZ	0.00000	0.00000	0.00000	0.04173	0.00000
86	C6	S	-0.53147	0.66740	0.21243	0.00000	0.45605
87	C6	PX	-0.71583	2.08146	0.70291	0.00000	-1.13378
88	C6	PY	0.58411	0.82097	-1.37951	0.00000	0.23708
89	C6	PZ	0.00000	0.00000	0.00000	0.05089	0.00000
90	C6	DXX	0.24426	0.22016	0.05107	0.00000	-0.11141
91	C6	DYY	-0.09473	-0.15995	0.14784	0.00000	-0.08733
92	C6	DZZ	-0.10972	-0.05686	-0.27577	0.00000	0.23852
93	C6	DXY	0.11473	-0.23159	0.21286	0.00000	0.02447
94	C6	DXZ	0.00000	0.00000	0.00000	0.36576	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.15473	0.00000
96	C7	S	0.00610	-0.01717	-0.00752	0.00000	0.01294
97	C7	S	0.41562	-0.32048	-0.02983	0.00000	0.15315
98	C7	PX	-0.17164	0.02537	-0.06510	0.00000	0.02703
99	C7	PY	-0.04680	0.17244	-0.18221	0.00000	0.01877
100	C7	PZ	0.00000	0.00000	0.00000	-0.10895	0.00000
101	C7	S	-0.79357	3.14890	0.26718	0.00000	-1.70317
102	C7	PX	0.58509	-1.86693	-0.07945	0.00000	0.78899
103	C7	PY	0.44057	-0.26775	0.86506	0.00000	-0.53780
104	C7	PZ	0.00000	0.00000	0.00000	-0.15760	0.00000
105	C7	DXX	-0.08828	-0.07506	0.20864	0.00000	-0.04379
106	C7	DYY	0.01291	0.15155	-0.16805	0.00000	-0.00171
107	C7	DZZ	0.15141	0.04664	-0.10574	0.00000	0.00087
108	C7	DXY	-0.06498	0.06728	-0.14138	0.00000	0.06261
109	C7	DXZ	0.00000	0.00000	0.00000	0.13396	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	-0.02608	0.00000
111	O1	S	0.01581	0.02044	0.00144	0.00000	-0.02373
112	O1	S	0.00574	0.18244	-0.05715	0.00000	-0.23389
113	O1	PX	-0.03249	-0.02353	-0.02228	0.00000	0.11374
114	O1	PY	0.02480	0.06506	0.06338	0.00000	0.06735
115	O1	PZ	0.00000	0.00000	0.00000	0.00051	0.00000
116	O1	S	-0.20415	-1.02254	0.05518	0.00000	1.27596
117	O1	PX	-0.18928	-0.10830	0.12079	0.00000	-0.22246
118	O1	PY	-0.09681	-0.09129	-0.15758	0.00000	-0.56155
119	O1	PZ	0.00000	0.00000	0.00000	0.02209	0.00000
120	O1	DXX	-0.01223	0.05856	-0.07727	0.00000	-0.28883
121	O1	DYY	0.00797	0.05614	0.04037	0.00000	-0.04447
122	O1	DZZ	0.05270	-0.00226	0.02830	0.00000	0.20244
123	O1	DXY	0.06629	-0.09943	0.02935	0.00000	0.20730
124	O1	DXZ	0.00000	0.00000	0.00000	-0.04325	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.02217	0.00000
126	H4	S	-0.21082	-0.03210	-0.01475	0.00000	-0.05076
127	H4	S	-0.07995	0.07797	0.04902	0.00000	0.03320
128	H4	PX	-0.02925	0.11790	-0.04601	0.00000	-0.00302
129	H4	PY	-0.13310	0.10125	-0.04838	0.00000	-0.03049
130	H4	PZ	0.00000	0.00000	0.00000	0.00321	0.00000
131	N1	S	-0.00232	-0.00897	-0.01581	0.00000	0.01611
132	N1	S	-0.23318	-0.12379	0.11485	0.00000	0.22752

133	N1	PX	-0.13892	-0.02734	0.26801	0.00000	-0.05979
134	N1	PY	0.13043	0.14784	-0.21365	0.00000	0.07461
135	N1	PZ	0.00000	0.00000	0.00000	0.01330	0.00000
136	N1	S	0.79491	1.03923	0.20705	0.00000	-1.27918
137	N1	PX	0.55070	-0.13288	0.20790	0.00000	-0.28335
138	N1	PY	-0.41101	0.55065	-0.30540	0.00000	-0.23582
139	N1	PZ	0.00000	0.00000	0.00000	0.17593	0.00000
140	N1	DXX	0.10283	0.02177	-0.12689	0.00000	0.03170
141	N1	DYY	-0.15531	-0.02669	0.03618	0.00000	0.00752
142	N1	DZZ	0.03192	0.05183	0.07001	0.00000	-0.01532
143	N1	DXY	-0.02446	-0.04618	0.05610	0.00000	-0.02840
144	N1	DXZ	0.00000	0.00000	0.00000	0.34232	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.14855	0.00000
146	H6	S	-0.01251	-0.08009	0.00118	0.00000	0.08980
147	H6	S	-0.08165	-0.16292	0.06385	0.00000	-0.09380
148	H6	PX	-0.08275	-0.00530	-0.03979	0.00000	-0.01544
149	H6	PY	0.13653	0.07387	0.05525	0.00000	-0.12439
150	H6	PZ	0.00000	0.00000	0.00000	0.04384	0.00000
151	C8	S	-0.00126	0.02281	0.01948	0.00000	-0.02055
152	C8	S	-0.09737	0.15477	0.43259	0.00000	-0.28627
153	C8	PX	0.08071	-0.01130	-0.02367	0.00000	-0.01833
154	C8	PY	-0.03741	0.00402	0.03854	0.00000	-0.00541
155	C8	PZ	0.00000	0.00000	0.00000	-0.05773	0.00000
156	C8	S	-0.06127	-1.05960	0.37359	0.00000	0.22129
157	C8	PX	0.26035	-0.53811	1.58983	0.00000	-0.74809
158	C8	PY	0.65555	-1.81187	-2.19754	0.00000	2.36074
159	C8	PZ	0.00000	0.00000	0.00000	-0.16848	0.00000
160	C8	DXX	0.02110	0.17929	-0.45050	0.00000	0.07653
161	C8	DYY	-0.08652	-0.13563	0.20296	0.00000	-0.02367
162	C8	DZZ	0.05568	0.00483	0.36922	0.00000	-0.15776
163	C8	DXY	-0.27009	0.11851	0.02839	0.00000	-0.03837
164	C8	DXZ	0.00000	0.00000	0.00000	0.51862	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.32612	0.00000
166	H8	S	0.06562	0.16258	-0.15635	0.00000	0.01796
167	H8	S	-0.17200	0.36963	0.11113	0.00000	-0.17993
168	H8	PX	0.05540	0.09461	-0.12671	0.00000	-0.00096
169	H8	PY	0.01905	0.00881	-0.28404	0.00000	0.10418
170	H8	PZ	0.00000	0.00000	0.00000	0.25018	0.00000
171	C10	S	-0.00483	0.02584	0.01184	0.00000	-0.02460
172	C10	S	-0.03402	0.20190	-0.11931	0.00000	-0.05710
173	C10	PX	-0.16443	0.02134	0.06990	0.00000	-0.02239
174	C10	PY	-0.01160	0.04507	-0.20682	0.00000	0.11929
175	C10	PZ	0.00000	0.00000	0.00000	0.06204	0.00000
176	C10	S	0.53622	-1.37332	-1.85123	0.00000	2.00166
177	C10	PX	0.59310	0.31222	-0.34474	0.00000	-0.10250
178	C10	PY	0.30379	-0.35682	-1.03828	0.00000	0.82085
179	C10	PZ	0.00000	0.00000	0.00000	0.17028	0.00000
180	C10	DXX	0.06394	-0.12778	0.16538	0.00000	-0.03441
181	C10	DYY	-0.01754	-0.10331	-0.19816	0.00000	0.20142
182	C10	DZZ	-0.06429	0.39984	-0.04878	0.00000	-0.23548
183	C10	DXY	-0.13138	0.04575	0.02837	0.00000	-0.02701
184	C10	DXZ	0.00000	0.00000	0.00000	0.02513	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.19542	0.00000
186	H16	S	-0.19776	0.13421	-0.00202	0.00000	-0.05472

187	H16	S	-0.26291	-0.05349	0.19170	0.00000	-0.03486
188	H16	PX	-0.22292	0.11924	0.00011	0.00000	-0.03497
189	H16	PY	-0.39609	0.03015	0.27055	0.00000	-0.07656
190	H16	PZ	0.00000	0.00000	0.00000	-0.31455	0.00000
191	H18	S	0.13731	0.15252	-0.07654	0.00000	-0.07523
192	H18	S	0.25179	0.07221	-0.24889	0.00000	0.03963
193	H18	PX	-0.35134	0.06141	0.02510	0.00000	0.02869
194	H18	PY	0.30865	-0.16142	0.06474	0.00000	0.00580
195	H18	PZ	0.00000	0.00000	0.00000	-0.02630	0.00000
196	C9	S	-0.00556	-0.00686	0.00316	0.00000	0.01617
197	C9	S	-0.03321	0.00423	0.05180	0.00000	0.27610
198	C9	PX	-0.01877	-0.04964	0.02198	0.00000	0.00677
199	C9	PY	-0.01013	-0.11695	-0.09029	0.00000	-0.23219
200	C9	PZ	0.00000	0.00000	0.00000	0.01334	0.00000
201	C9	S	0.24905	0.32951	-0.11071	0.00000	-0.38970
202	C9	PX	-0.18020	-0.32140	-0.15099	0.00000	-0.26864
203	C9	PY	-0.07691	0.33238	0.39473	0.00000	0.91779
204	C9	PZ	0.00000	0.00000	0.00000	-0.04535	0.00000
205	C9	DXX	0.10333	0.02775	-0.01844	0.00000	-0.08176
206	C9	DYY	-0.00698	0.29677	0.20070	0.00000	0.31460
207	C9	DZZ	-0.08460	-0.31725	-0.18175	0.00000	-0.25431
208	C9	DXY	0.08435	0.03233	-0.05016	0.00000	-0.19068
209	C9	DXZ	0.00000	0.00000	0.00000	-0.00004	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.01259	0.00000
211	H3	S	-0.00202	-0.30782	-0.20525	0.00000	-0.36237
212	H3	S	-0.01799	-0.07592	-0.07585	0.00000	-0.21861
213	H3	PX	0.08397	0.11738	0.16011	0.00000	0.36155
214	H3	PY	0.01967	-0.15475	-0.10128	0.00000	-0.18464
215	H3	PZ	0.00000	0.00000	0.00000	0.02377	0.00000
216	H5	S	0.00834	0.17021	0.14048	-0.00598	0.23379
217	H5	S	0.00232	-0.05393	0.01218	-0.02128	0.10750
218	H5	PX	0.02971	0.09292	0.03829	0.03694	0.03172
219	H5	PY	-0.02290	-0.10824	-0.12001	0.02163	-0.26928
220	H5	PZ	-0.00645	-0.02264	-0.01463	0.02715	-0.01456
221	H7	S	0.00834	0.17021	0.14048	0.00598	0.23379
222	H7	S	0.00232	-0.05393	0.01218	0.02128	0.10750
223	H7	PX	0.02971	0.09292	0.03829	-0.03694	0.03172
224	H7	PY	-0.02290	-0.10824	-0.12001	-0.02163	-0.26928
225	H7	PZ	0.00645	0.02264	0.01463	0.02715	0.01456

M0:	161	162	163	164	165
Eigenvalues:	2.47655	2.52504	2.52866	2.55727	2.60320
(ev):	67.39045	68.70988	68.80824	69.58695	70.83661

		A	A	A	A	A	
1	H1	S	-0.22887	0.00000	-0.04773	0.00000	0.00000
2	H1	S	0.35499	0.00000	-0.13486	0.00000	0.00000
3	H1	PX	-0.04542	0.00000	0.06107	0.00000	0.00000
4	H1	PY	-0.15085	0.00000	-0.07586	0.00000	0.00000
5	H1	PZ	0.00000	0.20268	0.00000	0.08744	0.39747
6	C1	S	-0.02280	0.00000	-0.03047	0.00000	0.00000
7	C1	S	-0.32963	0.00000	-0.28429	0.00000	0.00000
8	C1	PX	0.16686	0.00000	0.11427	0.00000	0.00000
9	C1	PY	-0.06254	0.00000	-0.04012	0.00000	0.00000

10	C1	PZ	0.00000	-0.10372	0.00000	-0.01461	-0.08272
11	C1	S	0.99711	0.00000	1.06038	0.00000	0.00000
12	C1	PX	-1.08684	0.00000	0.17386	0.00000	0.00000
13	C1	PY	2.06581	0.00000	-0.15947	0.00000	0.00000
14	C1	PZ	0.00000	-0.11696	0.00000	-0.05549	-0.08933
15	C1	DXX	0.33022	0.00000	-0.06944	0.00000	0.00000
16	C1	DYY	-0.22764	0.00000	0.31237	0.00000	0.00000
17	C1	DZZ	-0.25733	0.00000	-0.33667	0.00000	0.00000
18	C1	DXY	-0.18658	0.00000	-0.08820	0.00000	0.00000
19	C1	DXZ	0.00000	0.09135	0.00000	0.12032	-0.17079
20	C1	DYZ	0.00000	-0.06880	0.00000	-0.39383	0.17788
21	C2	S	-0.00641	0.00000	0.03898	0.00000	0.00000
22	C2	S	-0.21994	0.00000	0.22832	0.00000	0.00000
23	C2	PX	-0.02158	0.00000	-0.04471	0.00000	0.00000
24	C2	PY	-0.07756	0.00000	0.20810	0.00000	0.00000
25	C2	PZ	0.00000	0.04920	0.00000	-0.07694	0.02667
26	C2	S	0.96023	0.00000	-0.62612	0.00000	0.00000
27	C2	PX	0.55078	0.00000	-0.20068	0.00000	0.00000
28	C2	PY	-0.74291	0.00000	0.98883	0.00000	0.00000
29	C2	PZ	0.00000	0.04217	0.00000	-0.12235	0.08008
30	C2	DXX	0.20630	0.00000	-0.12578	0.00000	0.00000
31	C2	DYY	-0.21220	0.00000	-0.25932	0.00000	0.00000
32	C2	DZZ	-0.04030	0.00000	0.46240	0.00000	0.00000
33	C2	DXY	-0.12501	0.00000	0.34527	0.00000	0.00000
34	C2	DXZ	0.00000	0.12731	0.00000	0.11642	-0.02792
35	C2	DYZ	0.00000	-0.18486	0.00000	-0.42074	0.28290
36	C3	S	-0.01287	0.00000	-0.02466	0.00000	0.00000
37	C3	S	0.08110	0.00000	-0.39194	0.00000	0.00000
38	C3	PX	-0.06316	0.00000	-0.03569	0.00000	0.00000
39	C3	PY	0.19895	0.00000	-0.09690	0.00000	0.00000
40	C3	PZ	0.00000	-0.04729	0.00000	-0.10575	-0.02621
41	C3	S	1.20097	0.00000	1.90953	0.00000	0.00000
42	C3	PX	1.54774	0.00000	-1.68096	0.00000	0.00000
43	C3	PY	0.10095	0.00000	-1.01049	0.00000	0.00000
44	C3	PZ	0.00000	-0.13042	0.00000	-0.02929	-0.02509
45	C3	DXX	-0.05817	0.00000	0.04848	0.00000	0.00000
46	C3	DYY	0.09784	0.00000	0.04994	0.00000	0.00000
47	C3	DZZ	0.01505	0.00000	-0.17585	0.00000	0.00000
48	C3	DXY	0.13558	0.00000	0.02321	0.00000	0.00000
49	C3	DXZ	0.00000	0.10660	0.00000	-0.35610	-0.06833
50	C3	DYZ	0.00000	0.40444	0.00000	-0.03035	0.39190
51	C4	S	-0.02319	0.00000	-0.02217	0.00000	0.00000
52	C4	S	-0.29418	0.00000	-0.04971	0.00000	0.00000
53	C4	PX	-0.11435	0.00000	-0.18047	0.00000	0.00000
54	C4	PY	0.09193	0.00000	0.04436	0.00000	0.00000
55	C4	PZ	0.00000	0.01628	0.00000	0.11641	-0.11536
56	C4	S	-0.86762	0.00000	0.37019	0.00000	0.00000
57	C4	PX	-1.82595	0.00000	-0.47532	0.00000	0.00000
58	C4	PY	-0.44849	0.00000	-0.52860	0.00000	0.00000
59	C4	PZ	0.00000	0.06574	0.00000	0.10584	-0.05784
60	C4	DXX	-0.00620	0.00000	0.26047	0.00000	0.00000
61	C4	DYY	0.13810	0.00000	-0.09772	0.00000	0.00000
62	C4	DZZ	-0.22344	0.00000	-0.17816	0.00000	0.00000
63	C4	DXY	-0.27319	0.00000	-0.07456	0.00000	0.00000

64	C4	DXZ	0.00000	0.41164	0.00000	0.19770	-0.03632
65	C4	DYZ	0.00000	-0.02034	0.00000	0.05777	-0.29592
66	C5	S	0.01022	0.00000	0.02716	0.00000	0.00000
67	C5	S	0.40102	0.00000	0.13521	0.00000	0.00000
68	C5	PX	-0.01983	0.00000	-0.13916	0.00000	0.00000
69	C5	PY	-0.19532	0.00000	-0.17951	0.00000	0.00000
70	C5	PZ	0.00000	0.06074	0.00000	0.08918	-0.05872
71	C5	S	-1.27394	0.00000	-1.35455	0.00000	0.00000
72	C5	PX	-0.94238	0.00000	-0.15270	0.00000	0.00000
73	C5	PY	-0.03241	0.00000	0.75812	0.00000	0.00000
74	C5	PZ	0.00000	0.03684	0.00000	0.13801	-0.10935
75	C5	DXX	-0.14688	0.00000	-0.19138	0.00000	0.00000
76	C5	DYY	0.08047	0.00000	-0.00632	0.00000	0.00000
77	C5	DZZ	0.15108	0.00000	0.17889	0.00000	0.00000
78	C5	DXY	0.12432	0.00000	-0.28522	0.00000	0.00000
79	C5	DXZ	0.00000	0.16251	0.00000	-0.21251	0.18611
80	C5	DYZ	0.00000	0.08886	0.00000	-0.29550	0.15539
81	C6	S	-0.00333	0.00000	0.00293	0.00000	0.00000
82	C6	S	0.02922	0.00000	0.20191	0.00000	0.00000
83	C6	PX	0.07060	0.00000	-0.21441	0.00000	0.00000
84	C6	PY	-0.07342	0.00000	0.29605	0.00000	0.00000
85	C6	PZ	0.00000	-0.02927	0.00000	-0.12667	0.01039
86	C6	S	0.08527	0.00000	-1.00430	0.00000	0.00000
87	C6	PX	1.05718	0.00000	-2.28000	0.00000	0.00000
88	C6	PY	-0.21031	0.00000	-0.23906	0.00000	0.00000
89	C6	PZ	0.00000	-0.02914	0.00000	-0.13601	-0.00668
90	C6	DXX	-0.10854	0.00000	0.11096	0.00000	0.00000
91	C6	DYY	0.09815	0.00000	-0.10595	0.00000	0.00000
92	C6	DZZ	-0.05656	0.00000	0.02571	0.00000	0.00000
93	C6	DXY	-0.06099	0.00000	-0.10533	0.00000	0.00000
94	C6	DXZ	0.00000	0.43547	0.00000	0.04373	0.03636
95	C6	DYZ	0.00000	0.02910	0.00000	0.22791	0.13783
96	C7	S	0.00658	0.00000	-0.00506	0.00000	0.00000
97	C7	S	0.20306	0.00000	-0.03295	0.00000	0.00000
98	C7	PX	-0.10863	0.00000	0.03251	0.00000	0.00000
99	C7	PY	-0.01114	0.00000	-0.02667	0.00000	0.00000
100	C7	PZ	0.00000	0.09233	0.00000	-0.00566	0.05180
101	C7	S	-1.32938	0.00000	-0.28190	0.00000	0.00000
102	C7	PX	0.48940	0.00000	0.53680	0.00000	0.00000
103	C7	PY	-0.56262	0.00000	0.48994	0.00000	0.00000
104	C7	PZ	0.00000	0.19321	0.00000	-0.00315	0.07848
105	C7	DXX	0.16516	0.00000	-0.17988	0.00000	0.00000
106	C7	DYY	-0.13062	0.00000	0.20100	0.00000	0.00000
107	C7	DZZ	-0.04354	0.00000	-0.02570	0.00000	0.00000
108	C7	DXY	0.02151	0.00000	-0.04346	0.00000	0.00000
109	C7	DXZ	0.00000	0.04047	0.00000	-0.03491	0.04313
110	C7	DYZ	0.00000	0.18290	0.00000	0.45816	0.33908
111	O1	S	-0.03313	0.00000	-0.02528	0.00000	0.00000
112	O1	S	-0.53600	0.00000	-0.13079	0.00000	0.00000
113	O1	PX	-0.02436	0.00000	-0.01224	0.00000	0.00000
114	O1	PY	0.14068	0.00000	-0.05959	0.00000	0.00000
115	O1	PZ	0.00000	0.02867	0.00000	0.04056	-0.05212
116	O1	S	1.82151	0.00000	0.80921	0.00000	0.00000
117	O1	PX	0.76931	0.00000	0.49352	0.00000	0.00000

118	O1	PY	-0.19577	0.00000	0.18051	0.00000	0.00000
119	O1	PZ	0.00000	-0.04309	0.00000	-0.14585	0.25349
120	O1	DXX	0.00684	0.00000	0.05638	0.00000	0.00000
121	O1	DYY	-0.10844	0.00000	-0.08542	0.00000	0.00000
122	O1	DZZ	-0.14361	0.00000	-0.06108	0.00000	0.00000
123	O1	DXY	-0.15397	0.00000	0.02565	0.00000	0.00000
124	O1	DXZ	0.00000	-0.10827	0.00000	-0.08706	0.11688
125	O1	DYZ	0.00000	0.07793	0.00000	0.19753	-0.33232
126	H4	S	0.08016	0.00000	-0.13618	0.00000	0.00000
127	H4	S	-0.16141	0.00000	-0.06095	0.00000	0.00000
128	H4	PX	-0.13418	0.00000	-0.11102	0.00000	0.00000
129	H4	PY	0.01151	0.00000	-0.26517	0.00000	0.00000
130	H4	PZ	0.00000	-0.06770	0.00000	-0.17834	0.21575
131	N1	S	0.00427	0.00000	-0.01113	0.00000	0.00000
132	N1	S	-0.04610	0.00000	-0.08386	0.00000	0.00000
133	N1	PX	-0.08174	0.00000	-0.01939	0.00000	0.00000
134	N1	PY	-0.00387	0.00000	0.13165	0.00000	0.00000
135	N1	PZ	0.00000	-0.00254	0.00000	0.00770	0.01029
136	N1	S	-0.19944	0.00000	0.50397	0.00000	0.00000
137	N1	PX	-0.21413	0.00000	0.85290	0.00000	0.00000
138	N1	PY	-0.07922	0.00000	-0.29268	0.00000	0.00000
139	N1	PZ	0.00000	0.11460	0.00000	0.14221	-0.02267
140	N1	DXX	-0.12618	0.00000	0.27637	0.00000	0.00000
141	N1	DYY	0.03884	0.00000	-0.00569	0.00000	0.00000
142	N1	DZZ	0.02431	0.00000	-0.21496	0.00000	0.00000
143	N1	DXY	-0.18239	0.00000	0.28071	0.00000	0.00000
144	N1	DXZ	0.00000	0.11420	0.00000	-0.04472	-0.21065
145	N1	DYZ	0.00000	0.09051	0.00000	0.37126	0.14771
146	H6	S	-0.10261	0.00000	0.03911	0.00000	0.00000
147	H6	S	0.05667	0.00000	0.10814	0.00000	0.00000
148	H6	PX	0.01202	0.00000	-0.02510	0.00000	0.00000
149	H6	PY	0.16976	0.00000	0.14562	0.00000	0.00000
150	H6	PZ	0.00000	-0.01707	0.00000	0.22778	-0.00391
151	C8	S	0.00588	0.00000	-0.00009	0.00000	0.00000
152	C8	S	0.05876	0.00000	-0.11477	0.00000	0.00000
153	C8	PX	-0.03282	0.00000	0.15281	0.00000	0.00000
154	C8	PY	-0.05345	0.00000	-0.11493	0.00000	0.00000
155	C8	PZ	0.00000	0.02921	0.00000	0.03106	0.05251
156	C8	S	0.30157	0.00000	0.35812	0.00000	0.00000
157	C8	PX	-0.08506	0.00000	0.59970	0.00000	0.00000
158	C8	PY	0.23865	0.00000	-0.15360	0.00000	0.00000
159	C8	PZ	0.00000	-0.00223	0.00000	-0.01828	-0.03460
160	C8	DXX	0.12154	0.00000	-0.04891	0.00000	0.00000
161	C8	DYY	-0.13134	0.00000	0.05296	0.00000	0.00000
162	C8	DZZ	0.06544	0.00000	0.06281	0.00000	0.00000
163	C8	DXY	-0.11713	0.00000	0.08795	0.00000	0.00000
164	C8	DXZ	0.00000	0.18143	0.00000	0.07784	-0.10444
165	C8	DYZ	0.00000	-0.32286	0.00000	0.28137	0.30520
166	H8	S	-0.12275	0.00000	0.04081	0.00000	0.00000
167	H8	S	-0.01515	0.00000	-0.23795	0.00000	0.00000
168	H8	PX	-0.06466	0.00000	0.08123	0.00000	0.00000
169	H8	PY	0.05689	0.00000	0.00368	0.00000	0.00000
170	H8	PZ	0.00000	-0.44615	0.00000	0.15159	-0.17404
171	C10	S	0.01249	0.00000	0.01514	0.00000	0.00000

172	C10	S	0.12165	0.00000	0.07723	0.00000	0.00000
173	C10	PX	-0.03926	0.00000	-0.00499	0.00000	0.00000
174	C10	PY	0.05076	0.00000	-0.05013	0.00000	0.00000
175	C10	PZ	0.00000	-0.10159	0.00000	0.06440	0.10242
176	C10	S	-0.12407	0.00000	-0.55218	0.00000	0.00000
177	C10	PX	0.12518	0.00000	-0.07906	0.00000	0.00000
178	C10	PY	-0.13856	0.00000	-0.28611	0.00000	0.00000
179	C10	PZ	0.00000	-0.16313	0.00000	0.09814	0.14977
180	C10	DXX	-0.02820	0.00000	0.05733	0.00000	0.00000
181	C10	DYY	-0.07320	0.00000	-0.17575	0.00000	0.00000
182	C10	DZZ	0.15770	0.00000	0.15881	0.00000	0.00000
183	C10	DXY	0.10034	0.00000	-0.08802	0.00000	0.00000
184	C10	DXZ	0.00000	0.03829	0.00000	0.02338	0.00453
185	C10	DYZ	0.00000	-0.10893	0.00000	0.05550	-0.01943
186	H16	S	0.08362	0.00000	-0.03273	0.00000	0.00000
187	H16	S	-0.14356	0.00000	0.11290	0.00000	0.00000
188	H16	PX	-0.02601	0.00000	0.03284	0.00000	0.00000
189	H16	PY	-0.18871	0.00000	0.16849	0.00000	0.00000
190	H16	PZ	0.00000	0.24786	0.00000	-0.22432	-0.31538
191	H18	S	-0.00697	0.00000	0.08941	0.00000	0.00000
192	H18	S	0.05973	0.00000	-0.09598	0.00000	0.00000
193	H18	PX	-0.14273	0.00000	0.02530	0.00000	0.00000
194	H18	PY	0.16272	0.00000	-0.11685	0.00000	0.00000
195	H18	PZ	0.00000	0.31628	0.00000	-0.13005	-0.31650
196	C9	S	0.02489	0.00000	0.00610	0.00000	0.00000
197	C9	S	0.08755	0.00000	-0.04681	0.00000	0.00000
198	C9	PX	0.17154	0.00000	0.15952	0.00000	0.00000
199	C9	PY	-0.01904	0.00000	0.04090	0.00000	0.00000
200	C9	PZ	0.00000	0.00972	0.00000	-0.00857	0.01087
201	C9	S	-0.93982	0.00000	-0.46616	0.00000	0.00000
202	C9	PX	0.22460	0.00000	0.24329	0.00000	0.00000
203	C9	PY	0.57957	0.00000	0.08501	0.00000	0.00000
204	C9	PZ	0.00000	-0.04116	0.00000	0.09678	-0.23394
205	C9	DXX	-0.24458	0.00000	-0.20052	0.00000	0.00000
206	C9	DYY	0.29528	0.00000	0.11471	0.00000	0.00000
207	C9	DZZ	-0.04343	0.00000	0.04259	0.00000	0.00000
208	C9	DXY	-0.15204	0.00000	-0.10600	0.00000	0.00000
209	C9	DXZ	0.00000	0.03697	0.00000	0.00857	0.05574
210	C9	DYZ	0.00000	0.01229	0.00000	-0.02264	0.04609
211	H3	S	-0.19344	0.00000	-0.04263	0.00000	0.00000
212	H3	S	0.01556	0.00000	0.08985	0.00000	0.00000
213	H3	PX	-0.19985	0.00000	-0.07625	0.00000	0.00000
214	H3	PY	-0.16480	0.00000	-0.08351	0.00000	0.00000
215	H3	PZ	0.00000	0.03309	0.00000	-0.05598	0.15545
216	H5	S	0.19872	0.00828	0.02556	0.03507	-0.04690
217	H5	S	0.01156	-0.03278	0.02097	0.01084	-0.06438
218	H5	PX	0.05879	0.08230	-0.01623	0.00290	0.07258
219	H5	PY	0.06176	0.04914	-0.01132	0.01160	0.00930
220	H5	PZ	-0.02333	0.02661	-0.01770	-0.03492	0.08202
221	H7	S	0.19872	-0.00828	0.02556	-0.03507	0.04690
222	H7	S	0.01156	0.03278	0.02097	-0.01084	0.06438
223	H7	PX	0.05879	-0.08230	-0.01623	-0.00290	-0.07258
224	H7	PY	0.06176	-0.04914	-0.01132	-0.01160	-0.00930
225	H7	PZ	0.02333	0.02661	0.01770	-0.03492	0.08202

MO:	166	167	168	169	170
Eigenvalues:	2.63875	2.64334	2.68250	2.68802	2.72102
(ev):	71.80413	71.92893	72.99470	73.14466	74.04273

		A	A	A	A	A	
1	H1	S	-0.14924	0.00000	0.13262	0.00000	0.08486
2	H1	S	0.17018	0.00000	-0.17897	0.00000	-0.03949
3	H1	PX	-0.22235	0.00000	0.07119	0.00000	-0.05745
4	H1	PY	0.10714	0.00000	0.09716	0.00000	0.12680
5	H1	PZ	0.00000	0.30492	0.00000	-0.20333	0.00000
6	C1	S	-0.05104	0.00000	0.01956	0.00000	0.01887
7	C1	S	-0.32063	0.00000	-0.05381	0.00000	0.26443
8	C1	PX	-0.07723	0.00000	0.20744	0.00000	-0.03397
9	C1	PY	-0.07012	0.00000	-0.05720	0.00000	-0.02389
10	C1	PZ	0.00000	-0.02799	0.00000	0.06528	0.00000
11	C1	S	2.23251	0.00000	-0.25222	0.00000	-2.07409
12	C1	PX	-0.41051	0.00000	0.21248	0.00000	0.32965
13	C1	PY	-1.13182	0.00000	-0.11854	0.00000	0.41615
14	C1	PZ	0.00000	-0.07293	0.00000	0.09315	0.00000
15	C1	DXX	0.11500	0.00000	-0.18753	0.00000	0.03457
16	C1	DYY	0.23038	0.00000	-0.03232	0.00000	-0.15114
17	C1	DZZ	-0.48682	0.00000	0.23781	0.00000	0.08642
18	C1	DXY	0.19343	0.00000	-0.04993	0.00000	-0.16300
19	C1	DXZ	0.00000	-0.06832	0.00000	-0.08473	0.00000
20	C1	DYZ	0.00000	-0.22905	0.00000	0.40437	0.00000
21	C2	S	-0.02761	0.00000	-0.00403	0.00000	0.01439
22	C2	S	-0.47040	0.00000	-0.04239	0.00000	0.20073
23	C2	PX	-0.02065	0.00000	-0.01392	0.00000	-0.05085
24	C2	PY	-0.12064	0.00000	-0.04710	0.00000	-0.00999
25	C2	PZ	0.00000	-0.08702	0.00000	-0.08332	0.00000
26	C2	S	2.87479	0.00000	-0.18298	0.00000	-0.28693
27	C2	PX	1.81558	0.00000	0.22120	0.00000	-0.82916
28	C2	PY	0.09791	0.00000	-1.06185	0.00000	0.20218
29	C2	PZ	0.00000	-0.03660	0.00000	-0.08153	0.00000
30	C2	DXX	0.22666	0.00000	0.02224	0.00000	-0.13828
31	C2	DYY	-0.12347	0.00000	0.02439	0.00000	0.05089
32	C2	DZZ	-0.06869	0.00000	-0.05921	0.00000	0.16050
33	C2	DXY	-0.03014	0.00000	-0.19854	0.00000	-0.02590
34	C2	DXZ	0.00000	0.11545	0.00000	0.11734	0.00000
35	C2	DYZ	0.00000	-0.16367	0.00000	0.25426	0.00000
36	C3	S	0.00604	0.00000	0.01822	0.00000	0.03949
37	C3	S	-0.07608	0.00000	-0.01198	0.00000	0.25846
38	C3	PX	0.15784	0.00000	-0.06463	0.00000	0.03302
39	C3	PY	-0.26264	0.00000	0.25896	0.00000	0.00405
40	C3	PZ	0.00000	-0.01566	0.00000	0.04704	0.00000
41	C3	S	0.76007	0.00000	-1.06009	0.00000	-1.36385
42	C3	PX	-0.40299	0.00000	-0.95095	0.00000	0.63969
43	C3	PY	-2.26361	0.00000	0.65178	0.00000	1.79494
44	C3	PZ	0.00000	0.11125	0.00000	-0.04323	0.00000
45	C3	DXX	0.10363	0.00000	-0.17813	0.00000	-0.17806
46	C3	DYY	-0.05430	0.00000	-0.02132	0.00000	-0.06800
47	C3	DZZ	-0.00619	0.00000	0.09975	0.00000	0.33377
48	C3	DXY	-0.04476	0.00000	0.08159	0.00000	0.06575

49	C3	DXZ	0.00000	-0.03936	0.00000	-0.12205	0.00000
50	C3	DYZ	0.00000	-0.23928	0.00000	0.18733	0.00000
51	C4	S	0.00142	0.00000	-0.01332	0.00000	0.02317
52	C4	S	0.03633	0.00000	0.12678	0.00000	-0.04243
53	C4	PX	0.03573	0.00000	0.04412	0.00000	0.06990
54	C4	PY	0.18418	0.00000	-0.11876	0.00000	0.17040
55	C4	PZ	0.00000	-0.05000	0.00000	-0.03134	0.00000
56	C4	S	0.64653	0.00000	0.42131	0.00000	-0.47972
57	C4	PX	-0.44929	0.00000	0.09368	0.00000	1.20172
58	C4	PY	-0.02893	0.00000	0.28271	0.00000	-0.23529
59	C4	PZ	0.00000	-0.04868	0.00000	-0.00704	0.00000
60	C4	DXX	0.01234	0.00000	0.02515	0.00000	-0.25754
61	C4	DYY	-0.08401	0.00000	0.10946	0.00000	0.11950
62	C4	DZZ	0.11043	0.00000	-0.16939	0.00000	0.14605
63	C4	DXY	-0.04195	0.00000	-0.24880	0.00000	-0.13697
64	C4	DXZ	0.00000	-0.12393	0.00000	-0.35484	0.00000
65	C4	DYZ	0.00000	-0.53306	0.00000	0.24893	0.00000
66	C5	S	-0.00460	0.00000	-0.01163	0.00000	-0.02598
67	C5	S	0.28918	0.00000	-0.06498	0.00000	-0.05358
68	C5	PX	0.04655	0.00000	0.03314	0.00000	0.15723
69	C5	PY	-0.10567	0.00000	-0.02859	0.00000	-0.00918
70	C5	PZ	0.00000	-0.01345	0.00000	-0.08504	0.00000
71	C5	S	-1.60770	0.00000	0.96497	0.00000	1.13819
72	C5	PX	-0.82156	0.00000	-0.25632	0.00000	0.88849
73	C5	PY	0.78574	0.00000	-0.62294	0.00000	0.52199
74	C5	PZ	0.00000	-0.03629	0.00000	-0.02757	0.00000
75	C5	DXX	0.05608	0.00000	-0.06824	0.00000	0.28108
76	C5	DYY	0.00490	0.00000	0.16053	0.00000	-0.09308
77	C5	DZZ	-0.14136	0.00000	-0.06919	0.00000	-0.21549
78	C5	DXY	0.09306	0.00000	-0.10830	0.00000	0.05134
79	C5	DXZ	0.00000	-0.12295	0.00000	-0.00584	0.00000
80	C5	DYZ	0.00000	-0.33174	0.00000	-0.08729	0.00000
81	C6	S	-0.01313	0.00000	0.04470	0.00000	-0.04961
82	C6	S	0.05998	0.00000	0.33639	0.00000	-0.40267
83	C6	PX	-0.11010	0.00000	0.14018	0.00000	0.02945
84	C6	PY	-0.00566	0.00000	-0.13534	0.00000	0.22317
85	C6	PZ	0.00000	-0.02941	0.00000	-0.07389	0.00000
86	C6	S	-1.28132	0.00000	-1.04821	0.00000	1.57637
87	C6	PX	0.76188	0.00000	0.27191	0.00000	0.69872
88	C6	PY	-1.99094	0.00000	-0.26928	0.00000	0.63275
89	C6	PZ	0.00000	-0.08734	0.00000	-0.07413	0.00000
90	C6	DXX	-0.02752	0.00000	0.10272	0.00000	0.05399
91	C6	DYY	0.16585	0.00000	-0.28534	0.00000	0.13785
92	C6	DZZ	-0.29431	0.00000	0.22338	0.00000	-0.23484
93	C6	DXY	0.12397	0.00000	-0.02418	0.00000	0.07684
94	C6	DXZ	0.00000	-0.10512	0.00000	-0.20947	0.00000
95	C6	DYZ	0.00000	0.02227	0.00000	0.39000	0.00000
96	C7	S	0.07218	0.00000	0.00282	0.00000	0.04096
97	C7	S	0.57880	0.00000	0.05584	0.00000	0.17731
98	C7	PX	0.08099	0.00000	0.04343	0.00000	-0.04673
99	C7	PY	-0.08561	0.00000	0.23815	0.00000	0.27367
100	C7	PZ	0.00000	-0.04156	0.00000	0.04052	0.00000
101	C7	S	-3.42213	0.00000	-0.40277	0.00000	-0.15602
102	C7	PX	2.12006	0.00000	0.49660	0.00000	-0.25673

103	C7	PY	-0.06384	0.00000	1.67289	0.00000	0.76357
104	C7	PZ	0.00000	-0.07668	0.00000	0.09778	0.00000
105	C7	DXX	-0.37362	0.00000	-0.14035	0.00000	0.07530
106	C7	DYY	-0.13943	0.00000	0.16140	0.00000	-0.32310
107	C7	DZZ	0.63637	0.00000	-0.03972	0.00000	0.33386
108	C7	DXY	0.07297	0.00000	-0.43325	0.00000	-0.28744
109	C7	DXZ	0.00000	-0.04702	0.00000	0.11665	0.00000
110	C7	DYZ	0.00000	-0.10114	0.00000	0.18194	0.00000
111	O1	S	0.00396	0.00000	-0.01348	0.00000	0.00579
112	O1	S	0.21801	0.00000	-0.14725	0.00000	0.01844
113	O1	PX	-0.05255	0.00000	0.01676	0.00000	0.00782
114	O1	PY	-0.09748	0.00000	0.03256	0.00000	0.01979
115	O1	PZ	0.00000	-0.06755	0.00000	0.01081	0.00000
116	O1	S	-0.51523	0.00000	0.37501	0.00000	0.05813
117	O1	PX	0.12886	0.00000	0.25967	0.00000	-0.11999
118	O1	PY	0.29666	0.00000	0.25591	0.00000	0.11032
119	O1	PZ	0.00000	0.34653	0.00000	-0.13926	0.00000
120	O1	DXX	0.05416	0.00000	0.04834	0.00000	-0.09045
121	O1	DYY	-0.10359	0.00000	-0.01593	0.00000	-0.03865
122	O1	DZZ	0.11162	0.00000	-0.13310	0.00000	0.14483
123	O1	DXY	-0.06049	0.00000	0.09171	0.00000	0.06246
124	O1	DXZ	0.00000	0.17925	0.00000	-0.03752	0.00000
125	O1	DYZ	0.00000	-0.44969	0.00000	0.08086	0.00000
126	H4	S	-0.06487	0.00000	-0.09955	0.00000	-0.06343
127	H4	S	-0.29381	0.00000	0.11972	0.00000	0.01699
128	H4	PX	0.01704	0.00000	0.00199	0.00000	-0.00181
129	H4	PY	0.01877	0.00000	-0.04552	0.00000	-0.07542
130	H4	PZ	0.00000	0.28218	0.00000	0.20202	0.00000
131	N1	S	0.00589	0.00000	0.01500	0.00000	-0.03705
132	N1	S	0.13653	0.00000	0.42682	0.00000	-0.73216
133	N1	PX	0.04752	0.00000	0.00079	0.00000	-0.04921
134	N1	PY	-0.19050	0.00000	0.19563	0.00000	-0.10502
135	N1	PZ	0.00000	-0.00703	0.00000	0.00311	0.00000
136	N1	S	-1.05454	0.00000	-0.86186	0.00000	2.10120
137	N1	PX	-0.24644	0.00000	-0.39964	0.00000	0.61177
138	N1	PY	-0.41703	0.00000	-0.55387	0.00000	0.31358
139	N1	PZ	0.00000	0.11633	0.00000	0.24790	0.00000
140	N1	DXX	-0.13591	0.00000	-0.16483	0.00000	0.20405
141	N1	DYY	0.01071	0.00000	-0.04649	0.00000	0.18596
142	N1	DZZ	0.07763	0.00000	0.28965	0.00000	-0.47124
143	N1	DXY	-0.10138	0.00000	-0.20238	0.00000	-0.04406
144	N1	DXZ	0.00000	0.25405	0.00000	0.32234	0.00000
145	N1	DYZ	0.00000	-0.00142	0.00000	0.31278	0.00000
146	H6	S	-0.00405	0.00000	0.02674	0.00000	-0.02424
147	H6	S	0.49142	0.00000	-0.09020	0.00000	-0.27315
148	H6	PX	0.04529	0.00000	-0.11073	0.00000	-0.09522
149	H6	PY	0.03635	0.00000	0.25240	0.00000	-0.23252
150	H6	PZ	0.00000	0.23316	0.00000	0.42850	0.00000
151	C8	S	0.00858	0.00000	-0.02703	0.00000	-0.03281
152	C8	S	0.12079	0.00000	-0.15774	0.00000	-0.20266
153	C8	PX	-0.04929	0.00000	-0.01855	0.00000	0.33230
154	C8	PY	0.40261	0.00000	0.33305	0.00000	-0.09032
155	C8	PZ	0.00000	-0.05137	0.00000	-0.02677	0.00000
156	C8	S	0.39122	0.00000	0.25739	0.00000	0.74548

157	C8	PX	0.81962	0.00000	0.56298	0.00000	1.30470
158	C8	PY	0.81077	0.00000	2.45866	0.00000	-0.09003
159	C8	PZ	0.00000	-0.00452	0.00000	-0.09585	0.00000
160	C8	DXX	-0.12315	0.00000	0.12931	0.00000	0.13222
161	C8	DYY	-0.05151	0.00000	-0.07099	0.00000	0.16934
162	C8	DZZ	0.13088	0.00000	-0.15431	0.00000	-0.27216
163	C8	DXY	0.07945	0.00000	0.19001	0.00000	0.17152
164	C8	DXZ	0.00000	0.18136	0.00000	0.22077	0.00000
165	C8	DYZ	0.00000	-0.14356	0.00000	-0.00165	0.00000
166	H8	S	0.14771	0.00000	0.03308	0.00000	0.03559
167	H8	S	-0.71610	0.00000	-0.14237	0.00000	0.15455
168	H8	PX	0.20623	0.00000	-0.01919	0.00000	-0.04950
169	H8	PY	0.03466	0.00000	-0.37573	0.00000	-0.12159
170	H8	PZ	0.00000	0.17238	0.00000	-0.25378	0.00000
171	C10	S	-0.02802	0.00000	-0.04380	0.00000	0.01857
172	C10	S	-0.11720	0.00000	-0.15524	0.00000	0.05194
173	C10	PX	-0.03146	0.00000	-0.08944	0.00000	-0.05822
174	C10	PY	0.11568	0.00000	0.16529	0.00000	-0.15787
175	C10	PZ	0.00000	-0.06960	0.00000	-0.02820	0.00000
176	C10	S	0.80880	0.00000	2.20445	0.00000	-0.75442
177	C10	PX	-0.59340	0.00000	-0.54738	0.00000	-0.50763
178	C10	PY	0.39465	0.00000	1.12096	0.00000	-0.39679
179	C10	PZ	0.00000	-0.09301	0.00000	-0.02490	0.00000
180	C10	DXX	0.00529	0.00000	0.04142	0.00000	0.12211
181	C10	DYY	0.27170	0.00000	0.29455	0.00000	-0.25661
182	C10	DZZ	-0.34811	0.00000	-0.40138	0.00000	0.21332
183	C10	DXY	-0.16105	0.00000	-0.24052	0.00000	-0.14825
184	C10	DXZ	0.00000	0.02258	0.00000	0.07614	0.00000
185	C10	DYZ	0.00000	0.09388	0.00000	0.12312	0.00000
186	H16	S	-0.03304	0.00000	-0.16636	0.00000	0.01308
187	H16	S	0.25606	0.00000	0.33085	0.00000	0.31130
188	H16	PX	-0.09317	0.00000	-0.08921	0.00000	-0.00020
189	H16	PY	-0.01373	0.00000	0.01663	0.00000	0.14474
190	H16	PZ	0.00000	0.19526	0.00000	0.02656	0.00000
191	H18	S	-0.08098	0.00000	-0.05353	0.00000	0.03902
192	H18	S	-0.15393	0.00000	-0.06006	0.00000	-0.25063
193	H18	PX	0.10042	0.00000	0.13297	0.00000	-0.04485
194	H18	PY	-0.08774	0.00000	-0.19724	0.00000	-0.20917
195	H18	PZ	0.00000	0.29512	0.00000	0.25053	0.00000
196	C9	S	-0.01290	0.00000	0.01252	0.00000	0.00826
197	C9	S	-0.10022	0.00000	-0.02069	0.00000	0.10009
198	C9	PX	0.00534	0.00000	0.13067	0.00000	-0.00014
199	C9	PY	-0.01116	0.00000	0.06253	0.00000	-0.06443
200	C9	PZ	0.00000	0.01156	0.00000	0.00540	0.00000
201	C9	S	0.22477	0.00000	-0.46360	0.00000	-0.20327
202	C9	PX	0.02014	0.00000	0.32143	0.00000	0.06986
203	C9	PY	-0.23749	0.00000	-0.04788	0.00000	0.01571
204	C9	PZ	0.00000	-0.31913	0.00000	0.20859	0.00000
205	C9	DXX	-0.06720	0.00000	-0.16421	0.00000	-0.07310
206	C9	DYY	0.06906	0.00000	0.12307	0.00000	0.15025
207	C9	DZZ	-0.00813	0.00000	0.01978	0.00000	-0.06202
208	C9	DXY	0.07929	0.00000	-0.03301	0.00000	0.06600
209	C9	DXZ	0.00000	0.10823	0.00000	-0.13639	0.00000
210	C9	DYZ	0.00000	0.04881	0.00000	-0.03752	0.00000

211	H3	S	-0.01024	0.00000	0.00237	0.00000	-0.03275
212	H3	S	0.10631	0.00000	0.15298	0.00000	0.07882
213	H3	PX	-0.04606	0.00000	-0.19498	0.00000	-0.14386
214	H3	PY	-0.05582	0.00000	-0.06695	0.00000	-0.07490
215	H3	PZ	0.00000	0.20456	0.00000	-0.12716	0.00000
216	H5	S	-0.01327	-0.03353	0.00953	-0.01144	0.04356
217	H5	S	-0.06640	-0.11710	-0.01830	0.11902	-0.03369
218	H5	PX	0.04654	0.09335	-0.04326	-0.12657	0.03215
219	H5	PY	0.01741	-0.00093	0.07069	-0.03100	0.12317
220	H5	PZ	-0.00678	0.09797	-0.04663	-0.05415	-0.05403
221	H7	S	-0.01327	0.03353	0.00953	0.01144	0.04356
222	H7	S	-0.06640	0.11710	-0.01830	-0.11902	-0.03369
223	H7	PX	0.04654	-0.09335	-0.04326	0.12657	0.03215
224	H7	PY	0.01741	0.00093	0.07069	0.03100	0.12317
225	H7	PZ	0.00678	0.09797	0.04663	-0.05415	0.05403

MO:	171	172	173	174	175
Eigenvalues:	2.72457	2.73628	2.76280	2.80715	2.83712
(ev):	74.13948	74.45804	75.17970	76.38635	77.20205

		A	A	A	A	A	
1	H1	S	0.00000	-0.03202	0.02954	0.00000	-0.06280
2	H1	S	0.00000	0.00156	-0.50945	0.00000	0.20956
3	H1	PX	0.00000	0.04783	0.18170	0.00000	0.10954
4	H1	PY	0.00000	-0.15424	0.08144	0.00000	-0.48909
5	H1	PZ	0.24424	0.00000	0.00000	-0.18170	0.00000
6	C1	S	0.00000	-0.02350	-0.00929	0.00000	-0.01151
7	C1	S	0.00000	0.05420	0.18563	0.00000	-0.00423
8	C1	PX	0.00000	-0.14773	-0.00240	0.00000	-0.19002
9	C1	PY	0.00000	0.13470	0.08873	0.00000	0.30004
10	C1	PZ	0.00212	0.00000	0.00000	0.03895	0.00000
11	C1	S	0.00000	0.64513	0.55446	0.00000	0.85161
12	C1	PX	0.00000	-0.34011	0.71822	0.00000	-1.32114
13	C1	PY	0.00000	0.53171	0.28769	0.00000	2.79786
14	C1	PZ	-0.02864	0.00000	0.00000	0.05610	0.00000
15	C1	DXX	0.00000	0.10425	-0.14461	0.00000	0.33545
16	C1	DYY	0.00000	0.09540	0.25361	0.00000	-0.15321
17	C1	DZZ	0.00000	-0.24859	-0.05703	0.00000	-0.16911
18	C1	DXY	0.00000	-0.25706	-0.26850	0.00000	-0.39002
19	C1	DXZ	-0.21870	0.00000	0.00000	0.10843	0.00000
20	C1	DYZ	0.10417	0.00000	0.00000	0.00306	0.00000
21	C2	S	0.00000	0.02475	0.04131	0.00000	-0.01124
22	C2	S	0.00000	0.10944	0.07456	0.00000	-0.04604
23	C2	PX	0.00000	-0.10023	-0.07243	0.00000	0.07203
24	C2	PY	0.00000	-0.17426	-0.08908	0.00000	0.26546
25	C2	PZ	0.03235	0.00000	0.00000	-0.03412	0.00000
26	C2	S	0.00000	-1.20562	-1.54977	0.00000	0.70880
27	C2	PX	0.00000	0.23264	0.34094	0.00000	0.14700
28	C2	PY	0.00000	-0.91993	-0.41933	0.00000	1.11788
29	C2	PZ	0.06577	0.00000	0.00000	-0.04511	0.00000
30	C2	DXX	0.00000	-0.07528	-0.03956	0.00000	0.07450
31	C2	DYY	0.00000	-0.05156	-0.24349	0.00000	0.09753
32	C2	DZZ	0.00000	0.25390	0.36729	0.00000	-0.15119
33	C2	DXY	0.00000	-0.29742	-0.11310	0.00000	0.13241

34	C2	DXZ	-0.33076	0.00000	0.00000	0.06561	0.00000
35	C2	DYZ	-0.07171	0.00000	0.00000	-0.30907	0.00000
36	C3	S	0.00000	-0.02727	-0.01412	0.00000	-0.02697
37	C3	S	0.00000	-0.13934	-0.11295	0.00000	-0.21103
38	C3	PX	0.00000	-0.04052	-0.14851	0.00000	-0.06715
39	C3	PY	0.00000	-0.10936	0.05140	0.00000	0.16808
40	C3	PZ	-0.01167	0.00000	0.00000	0.05351	0.00000
41	C3	S	0.00000	-0.08358	1.90074	0.00000	1.85916
42	C3	PX	0.00000	-0.74275	-0.88551	0.00000	0.62386
43	C3	PY	0.00000	1.32344	-1.38554	0.00000	1.75498
44	C3	PZ	0.05074	0.00000	0.00000	-0.05292	0.00000
45	C3	DXX	0.00000	0.15657	0.09400	0.00000	-0.13141
46	C3	DYY	0.00000	0.00171	-0.04847	0.00000	0.23210
47	C3	DZZ	0.00000	-0.20623	-0.03054	0.00000	-0.14773
48	C3	DXY	0.00000	-0.11912	0.18635	0.00000	0.15537
49	C3	DXZ	-0.20842	0.00000	0.00000	-0.05943	0.00000
50	C3	DYZ	0.07498	0.00000	0.00000	-0.13482	0.00000
51	C4	S	0.00000	0.03290	-0.06013	0.00000	0.03631
52	C4	S	0.00000	0.33217	-0.60384	0.00000	0.08527
53	C4	PX	0.00000	-0.08737	-0.22642	0.00000	-0.21497
54	C4	PY	0.00000	0.38036	-0.03241	0.00000	0.23324
55	C4	PZ	-0.03100	0.00000	0.00000	0.01577	0.00000
56	C4	S	0.00000	-0.65901	2.92770	0.00000	-2.49233
57	C4	PX	0.00000	-0.50097	-2.04873	0.00000	-2.09860
58	C4	PY	0.00000	1.45941	-1.31032	0.00000	0.92642
59	C4	PZ	-0.01860	0.00000	0.00000	-0.01428	0.00000
60	C4	DXX	0.00000	-0.20028	0.02468	0.00000	-0.19133
61	C4	DYY	0.00000	-0.06990	0.21427	0.00000	-0.12260
62	C4	DZZ	0.00000	0.24094	-0.31603	0.00000	0.24312
63	C4	DXY	0.00000	0.03252	0.30431	0.00000	0.30642
64	C4	DXZ	-0.25491	0.00000	0.00000	-0.11961	0.00000
65	C4	DYZ	-0.03726	0.00000	0.00000	-0.07193	0.00000
66	C5	S	0.00000	-0.04030	0.04521	0.00000	0.03638
67	C5	S	0.00000	-0.21084	0.44754	0.00000	0.05789
68	C5	PX	0.00000	0.18071	-0.12854	0.00000	0.01961
69	C5	PY	0.00000	-0.17213	-0.21789	0.00000	0.14492
70	C5	PZ	0.04837	0.00000	0.00000	0.01247	0.00000
71	C5	S	0.00000	1.66548	-2.15379	0.00000	-2.10645
72	C5	PX	0.00000	-0.19692	-2.37672	0.00000	0.03375
73	C5	PY	0.00000	-1.35065	-0.87733	0.00000	0.28860
74	C5	PZ	0.04675	0.00000	0.00000	0.01067	0.00000
75	C5	DXX	0.00000	0.20904	-0.33938	0.00000	0.12127
76	C5	DYY	0.00000	0.10368	0.16261	0.00000	-0.34335
77	C5	DZZ	0.00000	-0.39440	0.25975	0.00000	0.26792
78	C5	DXY	0.00000	-0.20324	0.01946	0.00000	-0.08202
79	C5	DXZ	-0.34307	0.00000	0.00000	-0.08070	0.00000
80	C5	DYZ	0.12565	0.00000	0.00000	-0.34428	0.00000
81	C6	S	0.00000	0.02008	-0.00420	0.00000	0.00389
82	C6	S	0.00000	0.15749	-0.07795	0.00000	0.20742
83	C6	PX	0.00000	0.01939	-0.09810	0.00000	0.05354
84	C6	PY	0.00000	0.02363	0.05134	0.00000	-0.16354
85	C6	PZ	0.03512	0.00000	0.00000	0.00964	0.00000
86	C6	S	0.00000	-0.57155	-1.58051	0.00000	1.21707
87	C6	PX	0.00000	0.05705	-1.13788	0.00000	-0.51592

88	C6	PY	0.00000	-1.08016	0.55522	0.00000	-0.58361
89	C6	PZ	-0.07549	0.00000	0.00000	0.07183	0.00000
90	C6	DXX	0.00000	-0.18783	-0.31250	0.00000	0.14708
91	C6	DYY	0.00000	-0.00439	0.25373	0.00000	-0.06903
92	C6	DZZ	0.00000	0.12517	-0.07025	0.00000	-0.04002
93	C6	DXY	0.00000	-0.07515	-0.08929	0.00000	-0.12556
94	C6	DXZ	-0.23129	0.00000	0.00000	0.01485	0.00000
95	C6	DYZ	-0.02476	0.00000	0.00000	-0.33984	0.00000
96	C7	S	0.00000	-0.03493	0.02605	0.00000	-0.00262
97	C7	S	0.00000	-0.32525	0.27435	0.00000	0.06847
98	C7	PX	0.00000	0.02287	0.02441	0.00000	-0.04470
99	C7	PY	0.00000	-0.10532	0.06999	0.00000	0.04618
100	C7	PZ	0.01379	0.00000	0.00000	0.03920	0.00000
101	C7	S	0.00000	2.42661	-2.23153	0.00000	-0.48934
102	C7	PX	0.00000	-0.98616	1.40206	0.00000	0.13872
103	C7	PY	0.00000	0.12036	0.56375	0.00000	0.48171
104	C7	PZ	0.00697	0.00000	0.00000	0.08760	0.00000
105	C7	DXX	0.00000	0.07689	-0.11770	0.00000	-0.00924
106	C7	DYY	0.00000	0.06790	0.03921	0.00000	0.01752
107	C7	DZZ	0.00000	-0.21937	0.13702	0.00000	-0.05130
108	C7	DXY	0.00000	0.02817	-0.14487	0.00000	-0.24400
109	C7	DXZ	0.05669	0.00000	0.00000	0.34468	0.00000
110	C7	DYZ	0.24457	0.00000	0.00000	-0.07137	0.00000
111	O1	S	0.00000	0.02194	0.01727	0.00000	0.02824
112	O1	S	0.00000	0.53565	-0.17446	0.00000	0.30646
113	O1	PX	0.00000	-0.00918	0.06776	0.00000	-0.04668
114	O1	PY	0.00000	-0.10849	0.20512	0.00000	-0.02736
115	O1	PZ	-0.01000	0.00000	0.00000	-0.00850	0.00000
116	O1	S	0.00000	-1.64641	0.03466	0.00000	-0.98345
117	O1	PX	0.00000	-0.13464	-0.31818	0.00000	0.00884
118	O1	PY	0.00000	0.65495	-0.61625	0.00000	-0.11573
119	O1	PZ	0.01555	0.00000	0.00000	0.03009	0.00000
120	O1	DXX	0.00000	0.01535	-0.08720	0.00000	-0.09386
121	O1	DYY	0.00000	-0.17977	0.15051	0.00000	0.06142
122	O1	DZZ	0.00000	0.29923	-0.03710	0.00000	0.23449
123	O1	DXY	0.00000	-0.01022	-0.20107	0.00000	-0.23117
124	O1	DXZ	0.03725	0.00000	0.00000	0.01318	0.00000
125	O1	DYZ	-0.09501	0.00000	0.00000	-0.06104	0.00000
126	H4	S	0.00000	-0.15612	0.07252	0.00000	0.12674
127	H4	S	0.00000	0.32338	-0.30393	0.00000	0.01548
128	H4	PX	0.00000	0.43042	0.31976	0.00000	-0.01369
129	H4	PY	0.00000	0.05129	0.39808	0.00000	0.00158
130	H4	PZ	-0.50457	0.00000	0.00000	0.19821	0.00000
131	N1	S	0.00000	0.01698	-0.00843	0.00000	0.00922
132	N1	S	0.00000	0.27490	-0.31756	0.00000	0.22652
133	N1	PX	0.00000	-0.01719	-0.08036	0.00000	-0.00578
134	N1	PY	0.00000	-0.00268	-0.10145	0.00000	0.05430
135	N1	PZ	-0.00959	0.00000	0.00000	-0.02926	0.00000
136	N1	S	0.00000	-1.24880	1.03299	0.00000	-1.09906
137	N1	PX	0.00000	-0.27271	0.25991	0.00000	-0.00936
138	N1	PY	0.00000	-0.00376	0.27651	0.00000	-0.78233
139	N1	PZ	0.09513	0.00000	0.00000	-0.04251	0.00000
140	N1	DXX	0.00000	-0.18542	-0.19045	0.00000	0.13931
141	N1	DYY	0.00000	0.06451	0.19745	0.00000	-0.22378

142	N1	DZZ	0.00000	0.12701	-0.07207	0.00000	0.07601
143	N1	DXY	0.00000	0.10064	0.08085	0.00000	-0.17101
144	N1	DXZ	0.28997	0.00000	0.00000	0.09874	0.00000
145	N1	DYZ	-0.15797	0.00000	0.00000	-0.30169	0.00000
146	H6	S	0.00000	0.21095	0.21626	0.00000	-0.03527
147	H6	S	0.00000	-0.07820	0.04532	0.00000	0.19728
148	H6	PX	0.00000	-0.19877	-0.02737	0.00000	0.20792
149	H6	PY	0.00000	-0.01722	-0.08329	0.00000	-0.27043
150	H6	PZ	-0.51345	0.00000	0.00000	0.01502	0.00000
151	C8	S	0.00000	0.00245	-0.01772	0.00000	0.00119
152	C8	S	0.00000	0.19185	-0.11092	0.00000	-0.10254
153	C8	PX	0.00000	-0.18030	-0.02694	0.00000	0.09590
154	C8	PY	0.00000	0.02456	0.13345	0.00000	0.14770
155	C8	PZ	-0.02905	0.00000	0.00000	0.10048	0.00000
156	C8	S	0.00000	-0.46244	0.74863	0.00000	-0.34664
157	C8	PX	0.00000	-0.75020	0.73479	0.00000	0.24877
158	C8	PY	0.00000	-0.81819	1.26521	0.00000	1.61516
159	C8	PZ	-0.03917	0.00000	0.00000	-0.06547	0.00000
160	C8	DXX	0.00000	0.01337	0.12576	0.00000	0.07557
161	C8	DYY	0.00000	-0.01155	-0.01824	0.00000	-0.18858
162	C8	DZZ	0.00000	-0.01892	-0.06384	0.00000	0.08841
163	C8	DXY	0.00000	-0.06900	0.06215	0.00000	0.04859
164	C8	DXZ	0.30450	0.00000	0.00000	0.14943	0.00000
165	C8	DYZ	0.04007	0.00000	0.00000	-0.25336	0.00000
166	H8	S	0.00000	-0.07509	-0.01228	0.00000	-0.01123
167	H8	S	0.00000	0.24994	-0.37649	0.00000	0.03851
168	H8	PX	0.00000	-0.04238	0.08156	0.00000	-0.02931
169	H8	PY	0.00000	0.07120	-0.12719	0.00000	-0.02987
170	H8	PZ	-0.06342	0.00000	0.00000	-0.47328	0.00000
171	C10	S	0.00000	0.00036	-0.01271	0.00000	-0.01931
172	C10	S	0.00000	-0.02156	-0.03107	0.00000	0.00048
173	C10	PX	0.00000	0.05292	-0.02012	0.00000	-0.13213
174	C10	PY	0.00000	-0.01909	0.04483	0.00000	0.18096
175	C10	PZ	-0.01094	0.00000	0.00000	0.01985	0.00000
176	C10	S	0.00000	-0.31807	0.73668	0.00000	1.42042
177	C10	PX	0.00000	0.48475	-0.45814	0.00000	-0.39820
178	C10	PY	0.00000	-0.02156	0.35818	0.00000	0.61832
179	C10	PZ	-0.01261	0.00000	0.00000	0.08908	0.00000
180	C10	DXX	0.00000	-0.05351	0.02764	0.00000	0.05042
181	C10	DYY	0.00000	0.04764	0.07859	0.00000	0.10524
182	C10	DZZ	0.00000	0.00040	-0.11467	0.00000	-0.16841
183	C10	DXY	0.00000	0.13499	-0.02990	0.00000	-0.21872
184	C10	DXZ	0.17443	0.00000	0.00000	0.26941	0.00000
185	C10	DYZ	0.09094	0.00000	0.00000	-0.45213	0.00000
186	H16	S	0.00000	-0.00075	-0.00281	0.00000	-0.08574
187	H16	S	0.00000	-0.22007	0.19860	0.00000	0.23790
188	H16	PX	0.00000	0.03880	-0.03448	0.00000	-0.09834
189	H16	PY	0.00000	-0.09341	-0.07611	0.00000	0.09259
190	H16	PZ	-0.13607	0.00000	0.00000	-0.52364	0.00000
191	H18	S	0.00000	0.00658	-0.08708	0.00000	-0.00261
192	H18	S	0.00000	0.21246	-0.03441	0.00000	-0.14344
193	H18	PX	0.00000	-0.01621	0.01370	0.00000	0.09386
194	H18	PY	0.00000	0.12296	-0.02730	0.00000	-0.20708
195	H18	PZ	0.26500	0.00000	0.00000	-0.20233	0.00000

196	C9	S	0.00000	-0.00768	-0.02227	0.00000	-0.00958
197	C9	S	0.00000	0.01786	-0.00116	0.00000	0.06611
198	C9	PX	0.00000	-0.08499	-0.17147	0.00000	-0.18290
199	C9	PY	0.00000	-0.08806	-0.04673	0.00000	-0.11051
200	C9	PZ	-0.00073	0.00000	0.00000	0.00962	0.00000
201	C9	S	0.00000	0.26034	0.66881	0.00000	0.36019
202	C9	PX	0.00000	0.06704	-0.36853	0.00000	-0.38834
203	C9	PY	0.00000	-0.23356	-0.25567	0.00000	0.11448
204	C9	PZ	0.04538	0.00000	0.00000	-0.00709	0.00000
205	C9	DXX	0.00000	-0.08850	0.09436	0.00000	0.09518
206	C9	DYY	0.00000	0.14769	-0.07600	0.00000	-0.03265
207	C9	DZZ	0.00000	-0.04460	-0.02221	0.00000	0.00915
208	C9	DXY	0.00000	0.22744	-0.03312	0.00000	0.08010
209	C9	DXZ	-0.04949	0.00000	0.00000	-0.01121	0.00000
210	C9	DYZ	-0.02296	0.00000	0.00000	-0.00181	0.00000
211	H3	S	0.00000	-0.01827	-0.01078	0.00000	-0.03929
212	H3	S	0.00000	0.11701	-0.00932	0.00000	-0.15812
213	H3	PX	0.00000	-0.22010	0.21450	0.00000	0.15526
214	H3	PY	0.00000	-0.09291	0.06590	0.00000	0.06620
215	H3	PZ	-0.00803	0.00000	0.00000	-0.00125	0.00000
216	H5	S	-0.01467	0.00961	-0.05795	-0.00200	0.03291
217	H5	S	0.04232	-0.14947	0.04045	0.00283	-0.00550
218	H5	PX	-0.05009	0.06828	0.06834	-0.01717	0.14691
219	H5	PY	-0.02396	0.12915	0.01359	-0.00771	0.06521
220	H5	PZ	-0.00787	-0.03281	0.04439	0.00440	0.07029
221	H7	S	0.01467	0.00961	-0.05795	0.00200	0.03291
222	H7	S	-0.04232	-0.14947	0.04045	-0.00283	-0.00550
223	H7	PX	0.05009	0.06828	0.06834	0.01717	0.14691
224	H7	PY	0.02396	0.12915	0.01359	0.00771	0.06521
225	H7	PZ	-0.00787	0.03281	-0.04439	0.00440	-0.07029

MO:	176	177	178	179	180
Eigenvalues:	2.85185	2.85480	2.88036	2.90289	2.92225
(ev):	77.60292	77.68298	78.37870	78.99170	79.51862

		A	A	A	A	A	
1	H1	S	0.00000	-0.02579	0.00000	-0.05860	0.00125
2	H1	S	0.00000	0.20113	0.00000	0.06948	-0.01798
3	H1	PX	0.00000	-0.06758	0.00000	0.05083	-0.15170
4	H1	PY	0.00000	-0.12370	0.00000	-0.24263	0.08485
5	H1	PZ	-0.19835	0.00000	-0.47410	0.00000	0.00000
6	C1	S	0.00000	-0.00680	0.00000	0.01547	-0.02752
7	C1	S	0.00000	0.01509	0.00000	0.10653	-0.11683
8	C1	PX	0.00000	-0.11314	0.00000	-0.05382	-0.10914
9	C1	PY	0.00000	-0.06232	0.00000	0.08007	-0.05751
10	C1	PZ	0.02689	0.00000	0.02666	0.00000	0.00000
11	C1	S	0.00000	0.12138	0.00000	-1.19992	1.19608
12	C1	PX	0.00000	-0.85678	0.00000	-0.38895	0.19202
13	C1	PY	0.00000	1.74582	0.00000	2.55666	-1.51334
14	C1	PZ	0.09791	0.00000	0.07670	0.00000	0.00000
15	C1	DXX	0.00000	0.18366	0.00000	0.10111	0.04452
16	C1	DYY	0.00000	-0.12211	0.00000	-0.17908	0.09590
17	C1	DZZ	0.00000	-0.07680	0.00000	0.05458	-0.18541
18	C1	DXY	0.00000	-0.05263	0.00000	-0.07906	-0.02486

19	C1	DXZ	0.07471	0.00000	0.42482	0.00000	0.00000
20	C1	DYZ	0.14738	0.00000	-0.02643	0.00000	0.00000
21	C2	S	0.00000	-0.00472	0.00000	0.02982	-0.00031
22	C2	S	0.00000	-0.15250	0.00000	0.08110	-0.08028
23	C2	PX	0.00000	-0.03039	0.00000	-0.24491	0.03306
24	C2	PY	0.00000	-0.31259	0.00000	0.03415	0.17049
25	C2	PZ	-0.01230	0.00000	0.01059	0.00000	0.00000
26	C2	S	0.00000	-0.24168	0.00000	-0.34662	0.69318
27	C2	PX	0.00000	0.76218	0.00000	-0.95677	0.02939
28	C2	PY	0.00000	-3.16160	0.00000	0.13005	1.71444
29	C2	PZ	-0.05736	0.00000	0.01326	0.00000	0.00000
30	C2	DXX	0.00000	0.08494	0.00000	-0.25674	-0.04756
31	C2	DYY	0.00000	-0.19275	0.00000	0.06477	0.10443
32	C2	DZZ	0.00000	0.02553	0.00000	0.22614	-0.02895
33	C2	DXY	0.00000	-0.18388	0.00000	0.06696	0.25564
34	C2	DXZ	-0.00886	0.00000	-0.18071	0.00000	0.00000
35	C2	DYZ	-0.15624	0.00000	0.17096	0.00000	0.00000
36	C3	S	0.00000	0.03151	0.00000	-0.00332	0.03834
37	C3	S	0.00000	0.16185	0.00000	0.10813	0.14918
38	C3	PX	0.00000	0.08206	0.00000	0.02564	0.01485
39	C3	PY	0.00000	-0.06881	0.00000	-0.06122	-0.04287
40	C3	PZ	0.05072	0.00000	0.01453	0.00000	0.00000
41	C3	S	0.00000	-1.81454	0.00000	0.26316	-1.60599
42	C3	PX	0.00000	1.39810	0.00000	1.79603	-2.49757
43	C3	PY	0.00000	2.50947	0.00000	2.54958	-0.57723
44	C3	PZ	-0.04661	0.00000	-0.01754	0.00000	0.00000
45	C3	DXX	0.00000	-0.00636	0.00000	-0.14836	0.08086
46	C3	DYY	0.00000	-0.10407	0.00000	0.24121	-0.29761
47	C3	DZZ	0.00000	0.17753	0.00000	-0.04973	0.28449
48	C3	DXY	0.00000	-0.10077	0.00000	0.02757	0.29818
49	C3	DXZ	0.28833	0.00000	-0.20606	0.00000	0.00000
50	C3	DYZ	-0.09280	0.00000	-0.00504	0.00000	0.00000
51	C4	S	0.00000	0.00774	0.00000	0.05329	0.00386
52	C4	S	0.00000	0.08323	0.00000	-0.14079	0.25524
53	C4	PX	0.00000	-0.12082	0.00000	-0.08141	-0.04034
54	C4	PY	0.00000	0.01951	0.00000	-0.24859	0.21070
55	C4	PZ	0.00180	0.00000	0.08020	0.00000	0.00000
56	C4	S	0.00000	-0.80589	0.00000	-3.04476	0.19176
57	C4	PX	0.00000	-1.58567	0.00000	-0.63164	0.87690
58	C4	PY	0.00000	0.82713	0.00000	-0.47023	0.66033
59	C4	PZ	-0.12398	0.00000	-0.10878	0.00000	0.00000
60	C4	DXX	0.00000	0.22015	0.00000	-0.02251	-0.02138
61	C4	DYY	0.00000	-0.25727	0.00000	-0.27077	0.01359
62	C4	DZZ	0.00000	0.06337	0.00000	0.45339	-0.04567
63	C4	DXY	0.00000	0.08759	0.00000	-0.11411	0.07607
64	C4	DXZ	-0.28439	0.00000	0.14881	0.00000	0.00000
65	C4	DYZ	-0.26463	0.00000	-0.10240	0.00000	0.00000
66	C5	S	0.00000	-0.02906	0.00000	-0.02243	0.01889
67	C5	S	0.00000	-0.14838	0.00000	-0.08370	-0.00208
68	C5	PX	0.00000	-0.10594	0.00000	0.10687	0.00075
69	C5	PY	0.00000	-0.24912	0.00000	-0.07433	0.11854
70	C5	PZ	0.02823	0.00000	-0.02361	0.00000	0.00000
71	C5	S	0.00000	2.09808	0.00000	0.54125	-1.04411

72	C5	PX	0.00000	-1.26176	0.00000	0.78153	0.77038
73	C5	PY	0.00000	-2.09985	0.00000	0.09142	1.13619
74	C5	PZ	0.10768	0.00000	0.02439	0.00000	0.00000
75	C5	DXX	0.00000	-0.23223	0.00000	-0.09613	0.05486
76	C5	DYY	0.00000	0.44134	0.00000	0.13033	-0.18988
77	C5	DZZ	0.00000	-0.25170	0.00000	-0.15249	0.13105
78	C5	DXY	0.00000	0.02540	0.00000	-0.09769	-0.00667
79	C5	DXZ	-0.42214	0.00000	0.13305	0.00000	0.00000
80	C5	DYZ	0.02937	0.00000	0.09933	0.00000	0.00000
81	C6	S	0.00000	0.01189	0.00000	-0.06770	0.00919
82	C6	S	0.00000	0.00791	0.00000	-0.23606	0.12819
83	C6	PX	0.00000	0.02382	0.00000	-0.05915	-0.06712
84	C6	PY	0.00000	0.05413	0.00000	0.23845	0.10244
85	C6	PZ	-0.09556	0.00000	-0.01332	0.00000	0.00000
86	C6	S	0.00000	-0.20785	0.00000	2.85803	-0.59950
87	C6	PX	0.00000	3.20606	0.00000	1.22411	-1.76411
88	C6	PY	0.00000	-0.93276	0.00000	0.19443	-0.30772
89	C6	PZ	-0.03202	0.00000	-0.02224	0.00000	0.00000
90	C6	DXX	0.00000	0.12322	0.00000	0.07860	0.04800
91	C6	DYY	0.00000	-0.18870	0.00000	0.13715	-0.13982
92	C6	DZZ	0.00000	0.11491	0.00000	-0.40052	0.01064
93	C6	DXY	0.00000	0.15783	0.00000	-0.31926	-0.16323
94	C6	DXZ	0.23132	0.00000	-0.21717	0.00000	0.00000
95	C6	DYZ	0.43108	0.00000	0.13161	0.00000	0.00000
96	C7	S	0.00000	0.01913	0.00000	0.02368	0.00038
97	C7	S	0.00000	-0.00004	0.00000	0.01128	-0.00585
98	C7	PX	0.00000	-0.06660	0.00000	0.05158	-0.00226
99	C7	PY	0.00000	0.06327	0.00000	0.03130	0.30030
100	C7	PZ	-0.00919	0.00000	0.02365	0.00000	0.00000
101	C7	S	0.00000	0.86443	0.00000	0.32220	0.45703
102	C7	PX	0.00000	-0.80378	0.00000	-0.42867	0.55457
103	C7	PY	0.00000	0.33971	0.00000	-0.24302	1.77010
104	C7	PZ	0.03857	0.00000	0.01786	0.00000	0.00000
105	C7	DXX	0.00000	0.12226	0.00000	0.01614	0.01442
106	C7	DYY	0.00000	-0.24694	0.00000	-0.15747	0.11877
107	C7	DZZ	0.00000	0.15212	0.00000	0.18602	-0.04140
108	C7	DXY	0.00000	-0.09453	0.00000	0.01232	0.03234
109	C7	DXZ	0.20226	0.00000	0.04633	0.00000	0.00000
110	C7	DYZ	-0.22922	0.00000	0.08859	0.00000	0.00000
111	O1	S	0.00000	0.01548	0.00000	-0.04827	0.02877
112	O1	S	0.00000	0.26894	0.00000	-0.71403	0.53133
113	O1	PX	0.00000	0.00860	0.00000	-0.09597	-0.00538
114	O1	PY	0.00000	-0.06634	0.00000	-0.05995	-0.03172
115	O1	PZ	-0.03179	0.00000	-0.04117	0.00000	0.00000
116	O1	S	0.00000	-0.86704	0.00000	2.63501	-1.68810
117	O1	PX	0.00000	-0.14093	0.00000	0.75024	-0.27792
118	O1	PY	0.00000	-0.22522	0.00000	-0.64965	0.36923
119	O1	PZ	0.19369	0.00000	0.31405	0.00000	0.00000
120	O1	DXX	0.00000	0.10080	0.00000	0.11190	-0.03159
121	O1	DYY	0.00000	-0.01447	0.00000	0.13596	-0.09270
122	O1	DZZ	0.00000	0.09355	0.00000	-0.43195	0.28637
123	O1	DXY	0.00000	-0.33207	0.00000	-0.05288	-0.10348
124	O1	DXZ	0.14239	0.00000	0.33118	0.00000	0.00000
125	O1	DYZ	-0.17908	0.00000	0.19515	0.00000	0.00000

126	H4	S	0.00000	-0.08765	0.00000	-0.02581	0.04896
127	H4	S	0.00000	0.14752	0.00000	0.24942	-0.09222
128	H4	PX	0.00000	0.10868	0.00000	-0.07627	-0.15890
129	H4	PY	0.00000	-0.00322	0.00000	-0.32601	-0.11797
130	H4	PZ	-0.41136	0.00000	0.01925	0.00000	0.00000
131	N1	S	0.00000	-0.01167	0.00000	0.00255	0.02173
132	N1	S	0.00000	-0.08332	0.00000	0.13816	0.28309
133	N1	PX	0.00000	-0.03709	0.00000	0.00601	-0.01347
134	N1	PY	0.00000	0.08219	0.00000	-0.09597	0.12345
135	N1	PZ	0.03790	0.00000	0.00368	0.00000	0.00000
136	N1	S	0.00000	0.43242	0.00000	-0.97303	-1.10556
137	N1	PX	0.00000	-0.00468	0.00000	-0.73782	-0.28494
138	N1	PY	0.00000	-0.08063	0.00000	0.35219	-0.09713
139	N1	PZ	0.13188	0.00000	0.03398	0.00000	0.00000
140	N1	DXX	0.00000	0.09306	0.00000	-0.31642	-0.27747
141	N1	DYY	0.00000	0.02000	0.00000	0.20984	0.15442
142	N1	DZZ	0.00000	-0.09881	0.00000	0.02560	0.19200
143	N1	DXY	0.00000	-0.11645	0.00000	0.04102	0.22865
144	N1	DXZ	-0.02947	0.00000	0.05004	0.00000	0.00000
145	N1	DYZ	0.44553	0.00000	0.08683	0.00000	0.00000
146	H6	S	0.00000	-0.03500	0.00000	-0.01376	0.02275
147	H6	S	0.00000	-0.06557	0.00000	-0.42093	0.20389
148	H6	PX	0.00000	-0.17666	0.00000	-0.16988	0.12695
149	H6	PY	0.00000	0.54267	0.00000	-0.12683	-0.05779
150	H6	PZ	-0.01816	0.00000	-0.13574	0.00000	0.00000
151	C8	S	0.00000	-0.01593	0.00000	-0.00331	-0.06101
152	C8	S	0.00000	-0.02317	0.00000	0.16367	-0.17235
153	C8	PX	0.00000	0.13841	0.00000	-0.20059	-0.23946
154	C8	PY	0.00000	-0.11064	0.00000	0.22780	-0.09399
155	C8	PZ	0.03273	0.00000	-0.01532	0.00000	0.00000
156	C8	S	0.00000	0.34599	0.00000	-0.22664	2.53045
157	C8	PX	0.00000	0.65437	0.00000	-0.65600	0.40921
158	C8	PY	0.00000	-0.84105	0.00000	0.55991	0.60363
159	C8	PZ	-0.04393	0.00000	0.00015	0.00000	0.00000
160	C8	DXX	0.00000	0.00726	0.00000	0.17188	0.12753
161	C8	DYY	0.00000	0.15957	0.00000	-0.15573	0.31115
162	C8	DZZ	0.00000	-0.18499	0.00000	-0.01046	-0.45550
163	C8	DXY	0.00000	-0.00021	0.00000	0.20108	0.13517
164	C8	DXZ	-0.05983	0.00000	-0.01884	0.00000	0.00000
165	C8	DYZ	-0.06489	0.00000	0.07087	0.00000	0.00000
166	H8	S	0.00000	0.01615	0.00000	0.02424	-0.08909
167	H8	S	0.00000	0.30616	0.00000	0.13578	-0.20063
168	H8	PX	0.00000	-0.09163	0.00000	0.01386	-0.00566
169	H8	PY	0.00000	-0.05040	0.00000	-0.11165	-0.60407
170	H8	PZ	-0.24322	0.00000	-0.06633	0.00000	0.00000
171	C10	S	0.00000	0.01719	0.00000	-0.01296	0.00832
172	C10	S	0.00000	0.00250	0.00000	-0.00825	-0.07556
173	C10	PX	0.00000	-0.02770	0.00000	0.06885	0.18009
174	C10	PY	0.00000	-0.17444	0.00000	0.16980	-0.23307
175	C10	PZ	0.00253	0.00000	0.00365	0.00000	0.00000
176	C10	S	0.00000	-0.98273	0.00000	0.70710	-0.40717
177	C10	PX	0.00000	-0.14467	0.00000	0.08062	0.18263
178	C10	PY	0.00000	-0.52170	0.00000	0.50451	-0.08822
179	C10	PZ	0.02411	0.00000	-0.01079	0.00000	0.00000

180	C10	DXX	0.00000	0.05819	0.00000	-0.00836	-0.00548
181	C10	DYY	0.00000	-0.18231	0.00000	0.16861	-0.04494
182	C10	DZZ	0.00000	0.16546	0.00000	-0.13394	0.07352
183	C10	DXY	0.00000	-0.05554	0.00000	0.11776	0.23428
184	C10	DXZ	-0.28846	0.00000	0.17649	0.00000	0.00000
185	C10	DYZ	-0.15242	0.00000	0.12978	0.00000	0.00000
186	H16	S	0.00000	0.03040	0.00000	-0.01714	-0.00880
187	H16	S	0.00000	0.10064	0.00000	-0.04934	-0.09540
188	H16	PX	0.00000	0.01553	0.00000	-0.00038	0.16219
189	H16	PY	0.00000	0.12005	0.00000	-0.22690	-0.17551
190	H16	PZ	0.20861	0.00000	-0.11466	0.00000	0.00000
191	H18	S	0.00000	0.03873	0.00000	-0.06947	-0.03686
192	H18	S	0.00000	-0.17559	0.00000	0.21521	0.22852
193	H18	PX	0.00000	-0.06679	0.00000	0.09349	-0.09500
194	H18	PY	0.00000	-0.08355	0.00000	0.05695	0.22646
195	H18	PZ	-0.34460	0.00000	0.22244	0.00000	0.00000
196	C9	S	0.00000	-0.00856	0.00000	0.03176	-0.01661
197	C9	S	0.00000	0.10304	0.00000	0.00529	0.01416
198	C9	PX	0.00000	-0.21416	0.00000	0.24970	-0.18086
199	C9	PY	0.00000	-0.05340	0.00000	0.15194	-0.07672
200	C9	PZ	-0.01763	0.00000	-0.12769	0.00000	0.00000
201	C9	S	0.00000	0.31421	0.00000	-0.99123	0.45246
202	C9	PX	0.00000	-0.48354	0.00000	0.09080	-0.18902
203	C9	PY	0.00000	0.33737	0.00000	0.80396	-0.26390
204	C9	PZ	-0.17863	0.00000	-0.61639	0.00000	0.00000
205	C9	DXX	0.00000	0.14559	0.00000	0.13381	-0.02907
206	C9	DYY	0.00000	-0.25297	0.00000	-0.14398	-0.00911
207	C9	DZZ	0.00000	0.10042	0.00000	0.05981	0.03014
208	C9	DXY	0.00000	-0.08153	0.00000	-0.23536	0.08737
209	C9	DXZ	0.08762	0.00000	0.43439	0.00000	0.00000
210	C9	DYZ	-0.01716	0.00000	0.04108	0.00000	0.00000
211	H3	S	0.00000	-0.01234	0.00000	-0.00332	0.00218
212	H3	S	0.00000	-0.32981	0.00000	-0.30375	0.04931
213	H3	PX	0.00000	0.34019	0.00000	0.08002	0.07913
214	H3	PY	0.00000	0.13009	0.00000	0.11529	-0.01017
215	H3	PZ	0.12983	0.00000	0.38622	0.00000	0.00000
216	H5	S	0.00108	0.01314	0.03572	0.09777	-0.04116
217	H5	S	-0.08791	0.11899	-0.39100	0.19745	-0.03571
218	H5	PX	0.04817	0.13321	0.34104	-0.11942	0.13245
219	H5	PY	-0.03449	-0.10875	-0.01789	-0.18716	0.06037
220	H5	PZ	0.03520	0.18423	0.07121	0.01686	0.06999
221	H7	S	-0.00108	0.01314	-0.03572	0.09777	-0.04116
222	H7	S	0.08791	0.11899	0.39100	0.19745	-0.03571
223	H7	PX	-0.04817	0.13321	-0.34104	-0.11942	0.13245
224	H7	PY	0.03449	-0.10875	0.01789	-0.18716	0.06037
225	H7	PZ	0.03520	-0.18423	0.07121	-0.01686	-0.06999

M0:	181	182	183	184	185
Eigenvalues:	2.94553	2.94938	2.97878	3.01727	3.01793
(ev):	80.15209	80.25685	81.05685	82.10424	82.12217

		A	A	A	A	A	
1	H1	S	0.00000	-0.10624	0.00000	-0.09706	0.00000
2	H1	S	0.00000	0.05306	0.00000	-0.16669	0.00000

3	H1	PX	0.00000	-0.04889	0.00000	-0.15534	0.00000
4	H1	PY	0.00000	-0.14138	0.00000	0.37878	0.00000
5	H1	PZ	-0.30449	0.00000	-0.06437	0.00000	0.12034
6	C1	S	0.00000	-0.02180	0.00000	-0.04293	0.00000
7	C1	S	0.00000	-0.06441	0.00000	-0.01568	0.00000
8	C1	PX	0.00000	-0.13272	0.00000	-0.11929	0.00000
9	C1	PY	0.00000	-0.07582	0.00000	0.15184	0.00000
10	C1	PZ	0.00010	0.00000	-0.01609	0.00000	0.04020
11	C1	S	0.00000	1.09094	0.00000	0.97688	0.00000
12	C1	PX	0.00000	-0.46340	0.00000	0.98631	0.00000
13	C1	PY	0.00000	1.49613	0.00000	-1.88169	0.00000
14	C1	PZ	0.04819	0.00000	0.03091	0.00000	0.03282
15	C1	DXX	0.00000	0.12368	0.00000	0.10072	0.00000
16	C1	DYY	0.00000	0.03088	0.00000	0.07453	0.00000
17	C1	DZZ	0.00000	-0.17930	0.00000	-0.32900	0.00000
18	C1	DXY	0.00000	-0.05096	0.00000	-0.34579	0.00000
19	C1	DXZ	0.25809	0.00000	0.06739	0.00000	-0.27956
20	C1	DYZ	0.19486	0.00000	0.02565	0.00000	0.24097
21	C2	S	0.00000	0.00451	0.00000	-0.00986	0.00000
22	C2	S	0.00000	0.01171	0.00000	-0.06691	0.00000
23	C2	PX	0.00000	0.05798	0.00000	0.13268	0.00000
24	C2	PY	0.00000	0.06098	0.00000	-0.17526	0.00000
25	C2	PZ	-0.02602	0.00000	0.00966	0.00000	-0.00254
26	C2	S	0.00000	-0.34159	0.00000	0.74961	0.00000
27	C2	PX	0.00000	0.37661	0.00000	0.43237	0.00000
28	C2	PY	0.00000	-0.29825	0.00000	2.05918	0.00000
29	C2	PZ	0.04543	0.00000	-0.01976	0.00000	-0.08845
30	C2	DXX	0.00000	0.13370	0.00000	0.13494	0.00000
31	C2	DYY	0.00000	-0.09548	0.00000	-0.04420	0.00000
32	C2	DZZ	0.00000	0.00634	0.00000	-0.03559	0.00000
33	C2	DXY	0.00000	-0.11161	0.00000	-0.06360	0.00000
34	C2	DXZ	-0.28885	0.00000	0.08565	0.00000	0.38337
35	C2	DYZ	-0.41836	0.00000	-0.08317	0.00000	-0.17567
36	C3	S	0.00000	0.01521	0.00000	-0.05194	0.00000
37	C3	S	0.00000	-0.01264	0.00000	-0.38858	0.00000
38	C3	PX	0.00000	-0.00982	0.00000	-0.16624	0.00000
39	C3	PY	0.00000	-0.02702	0.00000	0.14373	0.00000
40	C3	PZ	0.00744	0.00000	0.02435	0.00000	0.01254
41	C3	S	0.00000	0.20949	0.00000	3.16397	0.00000
42	C3	PX	0.00000	-0.14282	0.00000	-3.93545	0.00000
43	C3	PY	0.00000	0.87176	0.00000	-2.62850	0.00000
44	C3	PZ	-0.05597	0.00000	-0.03368	0.00000	-0.05289
45	C3	DXX	0.00000	0.07350	0.00000	0.32230	0.00000
46	C3	DYY	0.00000	-0.15395	0.00000	-0.14792	0.00000
47	C3	DZZ	0.00000	0.14051	0.00000	-0.21449	0.00000
48	C3	DXY	0.00000	0.13006	0.00000	0.30821	0.00000
49	C3	DXZ	-0.03047	0.00000	0.21142	0.00000	0.06732
50	C3	DYZ	0.23334	0.00000	-0.02828	0.00000	0.15617
51	C4	S	0.00000	-0.00546	0.00000	0.06604	0.00000
52	C4	S	0.00000	0.00829	0.00000	-0.37607	0.00000
53	C4	PX	0.00000	-0.07542	0.00000	-0.09390	0.00000
54	C4	PY	0.00000	0.21648	0.00000	-0.06018	0.00000
55	C4	PZ	-0.01098	0.00000	-0.01363	0.00000	0.01775
56	C4	S	0.00000	0.01155	0.00000	-1.26053	0.00000

57	C4	PX	0.00000	-1.91096	0.00000	1.92200	0.00000
58	C4	PY	0.00000	0.53877	0.00000	-0.71607	0.00000
59	C4	PZ	-0.00781	0.00000	-0.03016	0.00000	-0.04189
60	C4	DXX	0.00000	0.06459	0.00000	-0.34138	0.00000
61	C4	DYY	0.00000	0.02657	0.00000	-0.13310	0.00000
62	C4	DZZ	0.00000	-0.04280	0.00000	0.55948	0.00000
63	C4	DXY	0.00000	0.17933	0.00000	-0.22992	0.00000
64	C4	DXZ	-0.08518	0.00000	-0.03129	0.00000	-0.34299
65	C4	DYZ	-0.15302	0.00000	-0.18367	0.00000	0.28841
66	C5	S	0.00000	0.02613	0.00000	-0.04418	0.00000
67	C5	S	0.00000	0.14533	0.00000	-0.01070	0.00000
68	C5	PX	0.00000	-0.04711	0.00000	0.15678	0.00000
69	C5	PY	0.00000	-0.05078	0.00000	0.09530	0.00000
70	C5	PZ	0.03885	0.00000	0.01496	0.00000	-0.00745
71	C5	S	0.00000	-1.19461	0.00000	0.09875	0.00000
72	C5	PX	0.00000	-1.03628	0.00000	1.43417	0.00000
73	C5	PY	0.00000	-0.66594	0.00000	1.46117	0.00000
74	C5	PZ	-0.04287	0.00000	0.02749	0.00000	0.06639
75	C5	DXX	0.00000	0.01063	0.00000	0.36470	0.00000
76	C5	DYY	0.00000	-0.11086	0.00000	-0.09003	0.00000
77	C5	DZZ	0.00000	0.15563	0.00000	-0.30433	0.00000
78	C5	DXY	0.00000	-0.09357	0.00000	0.21223	0.00000
79	C5	DXZ	0.05174	0.00000	-0.13095	0.00000	-0.26832
80	C5	DYZ	-0.47691	0.00000	0.03148	0.00000	-0.06755
81	C6	S	0.00000	0.01507	0.00000	0.09406	0.00000
82	C6	S	0.00000	0.02100	0.00000	0.53378	0.00000
83	C6	PX	0.00000	0.03549	0.00000	-0.04604	0.00000
84	C6	PY	0.00000	-0.11026	0.00000	-0.04343	0.00000
85	C6	PZ	0.03510	0.00000	-0.02517	0.00000	0.04503
86	C6	S	0.00000	-0.07221	0.00000	-3.87472	0.00000
87	C6	PX	0.00000	-0.04491	0.00000	-4.06144	0.00000
88	C6	PY	0.00000	-0.27124	0.00000	-1.30567	0.00000
89	C6	PZ	0.01778	0.00000	0.03615	0.00000	0.15046
90	C6	DXX	0.00000	0.03998	0.00000	-0.42004	0.00000
91	C6	DYY	0.00000	-0.08354	0.00000	-0.08734	0.00000
92	C6	DZZ	0.00000	0.07095	0.00000	0.50689	0.00000
93	C6	DXY	0.00000	0.01459	0.00000	0.05397	0.00000
94	C6	DXZ	0.14014	0.00000	0.22960	0.00000	0.19998
95	C6	DYZ	-0.09177	0.00000	0.07953	0.00000	-0.48265
96	C7	S	0.00000	0.00770	0.00000	-0.02306	0.00000
97	C7	S	0.00000	0.09074	0.00000	0.12381	0.00000
98	C7	PX	0.00000	-0.07908	0.00000	-0.02505	0.00000
99	C7	PY	0.00000	0.09637	0.00000	0.08347	0.00000
100	C7	PZ	0.01581	0.00000	0.00946	0.00000	0.00631
101	C7	S	0.00000	-0.34322	0.00000	-0.93374	0.00000
102	C7	PX	0.00000	0.15941	0.00000	1.47968	0.00000
103	C7	PY	0.00000	0.81974	0.00000	0.91055	0.00000
104	C7	PZ	0.00715	0.00000	-0.00084	0.00000	-0.00805
105	C7	DXX	0.00000	0.06292	0.00000	-0.07925	0.00000
106	C7	DYY	0.00000	-0.04187	0.00000	0.22083	0.00000
107	C7	DZZ	0.00000	0.01274	0.00000	-0.19546	0.00000
108	C7	DXY	0.00000	-0.03035	0.00000	-0.20135	0.00000
109	C7	DXZ	0.08545	0.00000	0.02060	0.00000	0.08527
110	C7	DYZ	0.21302	0.00000	-0.23470	0.00000	0.09122

111	O1	S	0.00000	-0.01636	0.00000	-0.01922	0.00000
112	O1	S	0.00000	-0.26086	0.00000	-0.47104	0.00000
113	O1	PX	0.00000	-0.12488	0.00000	-0.05475	0.00000
114	O1	PY	0.00000	-0.05306	0.00000	0.03378	0.00000
115	O1	PZ	-0.00183	0.00000	0.00443	0.00000	-0.02918
116	O1	S	0.00000	0.77164	0.00000	1.49566	0.00000
117	O1	PX	0.00000	0.78434	0.00000	0.09720	0.00000
118	O1	PY	0.00000	0.44875	0.00000	-0.76020	0.00000
119	O1	PZ	-0.00286	0.00000	-0.00590	0.00000	0.08473
120	O1	DXX	0.00000	0.29414	0.00000	-0.01142	0.00000
121	O1	DYY	0.00000	-0.37513	0.00000	0.24418	0.00000
122	O1	DZZ	0.00000	-0.10961	0.00000	-0.27604	0.00000
123	O1	DXY	0.00000	0.05906	0.00000	-0.19973	0.00000
124	O1	DXZ	-0.08683	0.00000	-0.08852	0.00000	0.23157
125	O1	DYZ	-0.18102	0.00000	-0.19829	0.00000	0.29123
126	H4	S	0.00000	0.02681	0.00000	-0.02515	0.00000
127	H4	S	0.00000	-0.00689	0.00000	-0.01673	0.00000
128	H4	PX	0.00000	0.23279	0.00000	-0.11097	0.00000
129	H4	PY	0.00000	0.24320	0.00000	-0.04395	0.00000
130	H4	PZ	0.35248	0.00000	-0.12281	0.00000	-0.14693
131	N1	S	0.00000	-0.00133	0.00000	0.01148	0.00000
132	N1	S	0.00000	-0.05055	0.00000	0.15339	0.00000
133	N1	PX	0.00000	-0.02529	0.00000	-0.07559	0.00000
134	N1	PY	0.00000	0.06200	0.00000	0.12618	0.00000
135	N1	PZ	0.00200	0.00000	-0.00503	0.00000	-0.03656
136	N1	S	0.00000	0.16185	0.00000	-0.72554	0.00000
137	N1	PX	0.00000	0.25376	0.00000	0.55895	0.00000
138	N1	PY	0.00000	-0.40143	0.00000	-0.51888	0.00000
139	N1	PZ	-0.08700	0.00000	-0.10471	0.00000	-0.21285
140	N1	DXX	0.00000	0.10064	0.00000	-0.03995	0.00000
141	N1	DYY	0.00000	-0.04845	0.00000	0.01406	0.00000
142	N1	DZZ	0.00000	-0.02268	0.00000	0.01759	0.00000
143	N1	DXY	0.00000	-0.10262	0.00000	0.19492	0.00000
144	N1	DXZ	-0.16035	0.00000	-0.37171	0.00000	-0.22486
145	N1	DYZ	-0.10318	0.00000	0.20450	0.00000	-0.37625
146	H6	S	0.00000	0.04632	0.00000	0.08616	0.00000
147	H6	S	0.00000	0.14018	0.00000	0.35422	0.00000
148	H6	PX	0.00000	0.10782	0.00000	0.06740	0.00000
149	H6	PY	0.00000	-0.12798	0.00000	-0.07620	0.00000
150	H6	PZ	-0.38872	0.00000	0.05253	0.00000	0.30712
151	C8	S	0.00000	-0.02164	0.00000	-0.02474	0.00000
152	C8	S	0.00000	-0.21555	0.00000	-0.11740	0.00000
153	C8	PX	0.00000	0.07314	0.00000	0.02169	0.00000
154	C8	PY	0.00000	-0.12389	0.00000	-0.01814	0.00000
155	C8	PZ	-0.04610	0.00000	-0.00050	0.00000	-0.01931
156	C8	S	0.00000	0.90457	0.00000	1.09164	0.00000
157	C8	PX	0.00000	0.87397	0.00000	0.41679	0.00000
158	C8	PY	0.00000	0.45515	0.00000	0.92350	0.00000
159	C8	PZ	0.04816	0.00000	0.05782	0.00000	0.04928
160	C8	DXX	0.00000	-0.02914	0.00000	0.07594	0.00000
161	C8	DYY	0.00000	0.15935	0.00000	0.04647	0.00000
162	C8	DZZ	0.00000	-0.14042	0.00000	-0.11470	0.00000
163	C8	DXY	0.00000	-0.03134	0.00000	-0.15164	0.00000
164	C8	DXZ	-0.02039	0.00000	-0.51511	0.00000	-0.07251

165	C8	DYZ	0.41800	0.00000	0.11580	0.00000	0.31202
166	H8	S	0.00000	-0.01623	0.00000	-0.12815	0.00000
167	H8	S	0.00000	0.02811	0.00000	-0.46917	0.00000
168	H8	PX	0.00000	-0.04862	0.00000	0.04954	0.00000
169	H8	PY	0.00000	-0.22640	0.00000	0.04697	0.00000
170	H8	PZ	-0.07447	0.00000	-0.04301	0.00000	-0.06336
171	C10	S	0.00000	0.00519	0.00000	-0.00074	0.00000
172	C10	S	0.00000	-0.01553	0.00000	0.01076	0.00000
173	C10	PX	0.00000	-0.02835	0.00000	-0.07265	0.00000
174	C10	PY	0.00000	-0.13020	0.00000	-0.08254	0.00000
175	C10	PZ	0.03590	0.00000	0.01700	0.00000	0.03257
176	C10	S	0.00000	-0.12554	0.00000	0.28854	0.00000
177	C10	PX	0.00000	-0.28942	0.00000	-0.11912	0.00000
178	C10	PY	0.00000	-0.17827	0.00000	0.04894	0.00000
179	C10	PZ	-0.02839	0.00000	-0.02068	0.00000	-0.01013
180	C10	DXX	0.00000	0.02319	0.00000	0.01361	0.00000
181	C10	DYY	0.00000	-0.09123	0.00000	-0.04103	0.00000
182	C10	DZZ	0.00000	0.05988	0.00000	0.01021	0.00000
183	C10	DXY	0.00000	-0.04223	0.00000	-0.07777	0.00000
184	C10	DXZ	-0.25251	0.00000	0.57136	0.00000	-0.07934
185	C10	DYZ	0.36318	0.00000	0.31106	0.00000	0.26569
186	H16	S	0.00000	0.01623	0.00000	-0.02735	0.00000
187	H16	S	0.00000	0.12995	0.00000	0.08198	0.00000
188	H16	PX	0.00000	0.01338	0.00000	0.00248	0.00000
189	H16	PY	0.00000	0.08642	0.00000	0.10939	0.00000
190	H16	PZ	0.32310	0.00000	-0.38499	0.00000	0.12365
191	H18	S	0.00000	-0.00825	0.00000	0.00264	0.00000
192	H18	S	0.00000	-0.15139	0.00000	-0.07729	0.00000
193	H18	PX	0.00000	-0.07553	0.00000	-0.07565	0.00000
194	H18	PY	0.00000	-0.02156	0.00000	-0.05673	0.00000
195	H18	PZ	0.05405	0.00000	0.56250	0.00000	0.09414
196	C9	S	0.00000	0.00945	0.00000	0.01074	0.00000
197	C9	S	0.00000	0.01743	0.00000	-0.02689	0.00000
198	C9	PX	0.00000	0.28896	0.00000	0.02222	0.00000
199	C9	PY	0.00000	0.06940	0.00000	0.10882	0.00000
200	C9	PZ	0.06743	0.00000	0.06276	0.00000	-0.14409
201	C9	S	0.00000	-0.64212	0.00000	-0.23756	0.00000
202	C9	PX	0.00000	0.48525	0.00000	-0.07699	0.00000
203	C9	PY	0.00000	0.75740	0.00000	0.25224	0.00000
204	C9	PZ	0.12664	0.00000	0.14650	0.00000	-0.33854
205	C9	DXX	0.00000	0.13297	0.00000	0.21363	0.00000
206	C9	DYY	0.00000	-0.17627	0.00000	-0.07714	0.00000
207	C9	DZZ	0.00000	-0.02910	0.00000	-0.06668	0.00000
208	C9	DXY	0.00000	0.19488	0.00000	-0.19524	0.00000
209	C9	DXZ	-0.10720	0.00000	-0.10646	0.00000	0.17919
210	C9	DYZ	0.00579	0.00000	-0.00121	0.00000	-0.09657
211	H3	S	0.00000	0.04195	0.00000	-0.02805	0.00000
212	H3	S	0.00000	-0.31088	0.00000	-0.11035	0.00000
213	H3	PX	0.00000	-0.37549	0.00000	0.11509	0.00000
214	H3	PY	0.00000	-0.06509	0.00000	0.10662	0.00000
215	H3	PZ	-0.10582	0.00000	-0.10356	0.00000	0.30184
216	H5	S	-0.00499	0.10071	-0.00252	0.02830	-0.00733
217	H5	S	0.09514	-0.00706	0.10458	0.11632	-0.22112
218	H5	PX	-0.10242	-0.27172	-0.10129	-0.07685	0.17630

219	H5	PY	0.01457	-0.46724	0.01417	-0.05640	-0.10423
220	H5	PZ	0.00390	-0.06996	0.00290	-0.00132	-0.00312
221	H7	S	0.00499	0.10071	0.00252	0.02830	0.00733
222	H7	S	-0.09514	-0.00706	-0.10458	0.11632	0.22112
223	H7	PX	0.10242	-0.27172	0.10129	-0.07685	-0.17630
224	H7	PY	-0.01457	-0.46724	-0.01417	-0.05640	0.10423
225	H7	PZ	0.00390	0.06996	0.00290	0.00132	-0.00312

MO:	186	187	188	189	190
Eigenvalues:	3.04983	3.05511	3.06524	3.07307	3.11348
(ev):	82.99007	83.13370	83.40947	83.62244	84.72227

			A	A	A	A	A
1	H1	S	0.02461	-0.05763	0.02825	0.00000	0.00000
2	H1	S	-0.06801	-0.16967	0.04274	0.00000	0.00000
3	H1	PX	-0.16996	-0.04958	-0.01648	0.00000	0.00000
4	H1	PY	0.37088	-0.22089	-0.00725	0.00000	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.06853	-0.37760
6	C1	S	0.02807	0.02481	-0.02903	0.00000	0.00000
7	C1	S	0.01190	0.05975	-0.15517	0.00000	0.00000
8	C1	PX	0.08451	-0.00285	0.04147	0.00000	0.00000
9	C1	PY	-0.11395	-0.03502	-0.12089	0.00000	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	-0.00103	-0.06246
11	C1	S	-1.66109	-0.99646	1.37446	0.00000	0.00000
12	C1	PX	1.13983	0.67624	-0.60776	0.00000	0.00000
13	C1	PY	-1.64554	0.47776	0.25580	0.00000	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.01674	0.09695
15	C1	DXX	0.00777	-0.05501	-0.12569	0.00000	0.00000
16	C1	DYY	-0.24396	-0.15170	0.19792	0.00000	0.00000
17	C1	DZZ	0.19377	0.15923	-0.15077	0.00000	0.00000
18	C1	DXY	0.02343	0.21949	0.06493	0.00000	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.02759	0.46115
20	C1	DYZ	0.00000	0.00000	0.00000	-0.37364	0.11814
21	C2	S	0.03214	0.04401	-0.00581	0.00000	0.00000
22	C2	S	0.20701	0.10292	0.06712	0.00000	0.00000
23	C2	PX	-0.05991	0.01529	-0.03664	0.00000	0.00000
24	C2	PY	0.01354	-0.16179	0.16649	0.00000	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.02534	0.04513
26	C2	S	-1.74125	-1.98168	0.66335	0.00000	0.00000
27	C2	PX	-1.39518	-0.66688	0.16521	0.00000	0.00000
28	C2	PY	0.82608	-0.52744	0.33885	0.00000	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	-0.02425	-0.08025
30	C2	DXX	0.02081	0.21234	0.06205	0.00000	0.00000
31	C2	DYY	-0.18808	-0.50465	0.13564	0.00000	0.00000
32	C2	DZZ	0.17191	0.28298	-0.07834	0.00000	0.00000
33	C2	DXY	-0.01117	-0.14704	-0.18412	0.00000	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.09946	0.35805
35	C2	DYZ	0.00000	0.00000	0.00000	0.25939	0.16783
36	C3	S	-0.00248	-0.00351	0.03346	0.00000	0.00000
37	C3	S	0.04305	0.00525	0.07911	0.00000	0.00000
38	C3	PX	-0.02884	0.07070	0.02066	0.00000	0.00000
39	C3	PY	0.14112	-0.10573	-0.04357	0.00000	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.06528	-0.00518
41	C3	S	-1.15054	-0.06232	-1.13603	0.00000	0.00000

42	C3	PX	-1.60069	-1.22803	1.10340	0.00000	0.00000
43	C3	PY	0.28963	1.43577	-0.30214	0.00000	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	-0.02165	-0.10886
45	C3	DXX	0.08556	0.05003	-0.14114	0.00000	0.00000
46	C3	DYY	-0.08105	0.05493	-0.06650	0.00000	0.00000
47	C3	DZZ	-0.01357	-0.03626	0.19326	0.00000	0.00000
48	C3	DXY	0.13323	0.15912	-0.18308	0.00000	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	-0.08793	-0.21080
50	C3	DYZ	0.00000	0.00000	0.00000	-0.48933	0.33871
51	C4	S	-0.02370	0.03154	0.00012	0.00000	0.00000
52	C4	S	0.30033	-0.03043	-0.10749	0.00000	0.00000
53	C4	PX	0.09470	0.20865	-0.00775	0.00000	0.00000
54	C4	PY	0.22918	-0.31733	-0.06606	0.00000	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.01245	0.02027
56	C4	S	1.34063	-0.43817	-0.33023	0.00000	0.00000
57	C4	PX	2.47524	-0.11155	-1.15733	0.00000	0.00000
58	C4	PY	0.56022	-0.25486	-0.25557	0.00000	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	-0.00104	-0.13115
60	C4	DXX	-0.00802	0.21527	0.07480	0.00000	0.00000
61	C4	DYY	0.20927	-0.33006	-0.04783	0.00000	0.00000
62	C4	DZZ	-0.26419	0.23290	0.05161	0.00000	0.00000
63	C4	DXY	-0.32086	-0.17033	-0.17252	0.00000	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.23896	0.06414
65	C4	DYZ	0.00000	0.00000	0.00000	-0.11369	-0.47366
66	C5	S	-0.01414	-0.01792	0.02990	0.00000	0.00000
67	C5	S	-0.14468	0.01344	0.14441	0.00000	0.00000
68	C5	PX	0.02340	-0.09066	0.10475	0.00000	0.00000
69	C5	PY	-0.13987	-0.26888	0.01418	0.00000	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	-0.01844	-0.02997
71	C5	S	1.61399	1.28942	-1.63740	0.00000	0.00000
72	C5	PX	1.47683	0.06075	-0.41987	0.00000	0.00000
73	C5	PY	0.25788	-0.92087	0.23124	0.00000	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.01581	0.08693
75	C5	DXX	0.16883	0.10172	0.04185	0.00000	0.00000
76	C5	DYY	-0.00445	0.18131	-0.23411	0.00000	0.00000
77	C5	DZZ	-0.07381	-0.16138	0.20290	0.00000	0.00000
78	C5	DXY	-0.01662	0.11678	-0.26150	0.00000	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.06570	-0.19574
80	C5	DYZ	0.00000	0.00000	0.00000	0.27606	0.33410
81	C6	S	0.00206	0.02740	-0.03400	0.00000	0.00000
82	C6	S	-0.21595	-0.17599	0.09616	0.00000	0.00000
83	C6	PX	-0.05536	-0.02014	0.16063	0.00000	0.00000
84	C6	PY	0.05830	0.17198	-0.35123	0.00000	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00722	0.01910
86	C6	S	0.23245	-0.41966	2.24589	0.00000	0.00000
87	C6	PX	-1.72500	-0.77896	0.75456	0.00000	0.00000
88	C6	PY	1.09928	0.09430	-0.39517	0.00000	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.05113	0.12980
90	C6	DXX	0.03295	0.15193	0.06915	0.00000	0.00000
91	C6	DYY	-0.00623	-0.27397	0.18647	0.00000	0.00000
92	C6	DZZ	0.05372	0.24359	-0.29637	0.00000	0.00000
93	C6	DXY	-0.22948	-0.20080	0.14168	0.00000	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	-0.20846	-0.02731
95	C6	DYZ	0.00000	0.00000	0.00000	-0.10152	-0.36184

96	C7	S	-0.04790	-0.00728	0.00321	0.00000	0.00000
97	C7	S	-0.22038	-0.04888	0.00320	0.00000	0.00000
98	C7	PX	-0.13216	0.03676	0.04192	0.00000	0.00000
99	C7	PY	0.05248	-0.02441	-0.00730	0.00000	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	-0.04450	0.04515
101	C7	S	2.47411	1.21218	-0.31117	0.00000	0.00000
102	C7	PX	-1.09525	-0.61773	-0.03725	0.00000	0.00000
103	C7	PY	0.39425	1.17450	-0.36658	0.00000	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.01284	0.03302
105	C7	DXX	0.02377	0.03127	-0.01691	0.00000	0.00000
106	C7	DYY	0.17668	0.10485	0.01641	0.00000	0.00000
107	C7	DZZ	-0.24629	-0.02930	-0.00290	0.00000	0.00000
108	C7	DXY	0.02474	0.26707	-0.04477	0.00000	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.63885	-0.24954
110	C7	DYZ	0.00000	0.00000	0.00000	-0.06660	0.25577
111	O1	S	0.01172	-0.03303	-0.03840	0.00000	0.00000
112	O1	S	0.33916	-0.23000	-0.43793	0.00000	0.00000
113	O1	PX	0.01398	0.04074	-0.00709	0.00000	0.00000
114	O1	PY	0.02300	-0.09240	0.01231	0.00000	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.01683	0.00340
116	O1	S	-1.08795	0.99106	1.48115	0.00000	0.00000
117	O1	PX	0.05752	0.04177	0.89276	0.00000	0.00000
118	O1	PY	0.72743	-0.30972	0.07079	0.00000	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	-0.03607	0.09853
120	O1	DXX	0.35148	-0.06230	0.39229	0.00000	0.00000
121	O1	DYY	-0.40844	0.23941	-0.04378	0.00000	0.00000
122	O1	DZZ	0.09456	-0.25540	-0.44027	0.00000	0.00000
123	O1	DXY	-0.02159	0.14689	0.22658	0.00000	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	-0.07896	-0.07438
125	O1	DYZ	0.00000	0.00000	0.00000	-0.09081	-0.35774
126	H4	S	0.00217	0.01961	-0.01157	0.00000	0.00000
127	H4	S	0.24148	0.17228	0.06761	0.00000	0.00000
128	H4	PX	0.05666	0.16967	0.18728	0.00000	0.00000
129	H4	PY	-0.03329	0.17368	0.03567	0.00000	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	-0.12174	-0.31742
131	N1	S	-0.02287	-0.04662	0.04143	0.00000	0.00000
132	N1	S	-0.31827	-0.33974	0.39955	0.00000	0.00000
133	N1	PX	0.03899	0.07379	-0.00515	0.00000	0.00000
134	N1	PY	0.02596	0.17500	-0.13874	0.00000	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	-0.01430	-0.02621
136	N1	S	1.68648	2.23953	-2.24460	0.00000	0.00000
137	N1	PX	0.82885	1.19929	-0.74519	0.00000	0.00000
138	N1	PY	0.08233	-0.38114	-0.47734	0.00000	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	-0.06192	-0.10480
140	N1	DXX	0.23408	0.28413	-0.06230	0.00000	0.00000
141	N1	DYY	0.03386	0.17584	-0.32902	0.00000	0.00000
142	N1	DZZ	-0.19472	-0.37005	0.34430	0.00000	0.00000
143	N1	DXY	-0.08055	-0.33816	-0.07540	0.00000	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	-0.04851	0.03269
145	N1	DYZ	0.00000	0.00000	0.00000	-0.14489	-0.29961
146	H6	S	-0.05917	-0.02137	0.01090	0.00000	0.00000
147	H6	S	-0.25836	-0.08523	-0.02263	0.00000	0.00000
148	H6	PX	0.03664	0.13473	-0.02563	0.00000	0.00000
149	H6	PY	-0.25357	-0.15982	-0.29716	0.00000	0.00000

150	H6	PZ	0.00000	0.00000	0.00000	0.14144	0.31971
151	C8	S	0.06846	0.03396	-0.05097	0.00000	0.00000
152	C8	S	-0.05560	-0.36532	0.09592	0.00000	0.00000
153	C8	PX	0.08569	0.14607	-0.07326	0.00000	0.00000
154	C8	PY	0.00204	-0.17143	-0.00001	0.00000	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	-0.01565	-0.00518
156	C8	S	-2.91273	-0.94441	1.98405	0.00000	0.00000
157	C8	PX	-0.01211	1.62555	-0.45817	0.00000	0.00000
158	C8	PY	0.11526	-0.21848	-0.81615	0.00000	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	-0.01442	0.01630
160	C8	DXX	-0.05445	-0.40432	-0.07811	0.00000	0.00000
161	C8	DYY	-0.29640	0.18325	0.24622	0.00000	0.00000
162	C8	DZZ	0.48744	0.29165	-0.37200	0.00000	0.00000
163	C8	DXY	0.11011	0.04530	-0.19987	0.00000	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.03313	0.11228
165	C8	DYZ	0.00000	0.00000	0.00000	0.45204	-0.04023
166	H8	S	0.03727	0.02876	0.00501	0.00000	0.00000
167	H8	S	0.24040	0.11051	0.03140	0.00000	0.00000
168	H8	PX	-0.10473	0.09970	0.03579	0.00000	0.00000
169	H8	PY	-0.00670	-0.37004	0.08641	0.00000	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	-0.50780	0.17888
171	C10	S	-0.02080	-0.01092	0.01616	0.00000	0.00000
172	C10	S	-0.04683	-0.01498	0.07040	0.00000	0.00000
173	C10	PX	-0.06770	-0.00780	0.03950	0.00000	0.00000
174	C10	PY	0.30477	-0.02708	-0.27800	0.00000	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.05310	-0.00780
176	C10	S	1.14471	-0.03790	-1.26441	0.00000	0.00000
177	C10	PX	-0.01293	-0.34999	0.36164	0.00000	0.00000
178	C10	PY	0.74790	-0.12700	-0.79892	0.00000	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.01121	-0.00570
180	C10	DXX	0.00735	-0.10477	-0.08644	0.00000	0.00000
181	C10	DYY	0.14041	0.05286	-0.06911	0.00000	0.00000
182	C10	DZZ	-0.16306	-0.06008	0.13172	0.00000	0.00000
183	C10	DXY	-0.00634	-0.01294	-0.04917	0.00000	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	-0.18740	-0.06045
185	C10	DYZ	0.00000	0.00000	0.00000	0.32647	-0.06093
186	H16	S	-0.04883	0.04509	0.01668	0.00000	0.00000
187	H16	S	0.03600	0.08121	-0.18026	0.00000	0.00000
188	H16	PX	-0.14986	-0.00179	0.16521	0.00000	0.00000
189	H16	PY	-0.16523	0.03198	0.25704	0.00000	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.20033	0.03315
191	H18	S	-0.02203	-0.02373	0.09250	0.00000	0.00000
192	H18	S	0.17531	-0.10743	-0.13803	0.00000	0.00000
193	H18	PX	0.19158	-0.07516	-0.21730	0.00000	0.00000
194	H18	PY	-0.03771	0.14229	0.06485	0.00000	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.03943	-0.06020
196	C9	S	0.01651	0.01599	0.03379	0.00000	0.00000
197	C9	S	0.01946	-0.09438	-0.36275	0.00000	0.00000
198	C9	PX	-0.02835	0.08498	0.34259	0.00000	0.00000
199	C9	PY	0.03935	0.06692	0.21129	0.00000	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.05065	0.10837
201	C9	S	-0.44751	-0.23999	-0.87462	0.00000	0.00000
202	C9	PX	-0.06127	0.06635	0.10983	0.00000	0.00000
203	C9	PY	0.44322	-0.21460	0.05813	0.00000	0.00000

204	C9	PZ	0.00000	0.00000	0.00000	0.14492	0.13979
205	C9	DXX	-0.26155	-0.01188	-0.41210	0.00000	0.00000
206	C9	DYY	-0.16181	0.13726	0.07421	0.00000	0.00000
207	C9	DZZ	0.33374	-0.05633	0.37831	0.00000	0.00000
208	C9	DXY	0.01530	-0.26328	-0.35548	0.00000	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	-0.04265	-0.05065
210	C9	DYZ	0.00000	0.00000	0.00000	0.08725	0.07175
211	H3	S	0.03040	-0.01525	0.01902	0.00000	0.00000
212	H3	S	-0.22456	0.18883	0.11626	0.00000	0.00000
213	H3	PX	0.04827	0.14965	0.19920	0.00000	0.00000
214	H3	PY	-0.02709	0.04293	-0.00967	0.00000	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	-0.15009	-0.15462
216	H5	S	0.04124	-0.01249	0.00129	0.00484	0.01741
217	H5	S	0.15965	0.00315	0.17074	0.09152	0.11078
218	H5	PX	0.20780	-0.05310	0.16102	-0.04907	-0.10140
219	H5	PY	-0.18707	0.23856	0.06481	0.06950	0.06901
220	H5	PZ	0.31495	-0.08472	0.17628	-0.00137	0.03463
221	H7	S	0.04124	-0.01249	0.00129	-0.00484	-0.01741
222	H7	S	0.15965	0.00315	0.17074	-0.09152	-0.11078
223	H7	PX	0.20780	-0.05310	0.16102	0.04907	0.10140
224	H7	PY	-0.18707	0.23856	0.06481	-0.06950	-0.06901
225	H7	PZ	-0.31495	0.08472	-0.17628	-0.00137	0.03463

MO:	191	192	193	194	195
Eigenvalues:	3.13185	3.15634	3.19293	3.20217	3.25015
(ev):	85.22204	85.88837	86.88420	87.13548	88.44107

			A	A	A	A	A
1	H1	S	-0.00388	0.03913	0.04692	0.00000	0.03307
2	H1	S	0.00207	0.00954	0.25529	0.00000	0.06769
3	H1	PX	-0.14110	-0.18187	-0.03400	0.00000	0.01418
4	H1	PY	0.15532	0.19337	0.17907	0.00000	-0.34834
5	H1	PZ	0.00000	0.00000	0.00000	-0.05135	0.00000
6	C1	S	-0.03690	0.03761	-0.08698	0.00000	-0.00627
7	C1	S	-0.03078	0.10998	-0.34813	0.00000	-0.13811
8	C1	PX	-0.10937	0.01718	-0.06223	0.00000	-0.06394
9	C1	PY	-0.15204	-0.06112	-0.01923	0.00000	0.06334
10	C1	PZ	0.00000	0.00000	0.00000	-0.03358	0.00000
11	C1	S	1.51080	-2.73604	3.31032	0.00000	-0.00980
12	C1	PX	-0.10765	1.01229	-1.54630	0.00000	-0.31360
13	C1	PY	-0.75837	-0.84329	-0.58870	0.00000	0.54341
14	C1	PZ	0.00000	0.00000	0.00000	0.01530	0.00000
15	C1	DXX	0.02943	0.05594	-0.01489	0.00000	-0.20744
16	C1	DYY	0.11487	-0.32986	0.44296	0.00000	0.23484
17	C1	DZZ	-0.19326	0.23169	-0.47632	0.00000	-0.04132
18	C1	DXY	-0.03671	0.03988	-0.24940	0.00000	0.23042
19	C1	DXZ	0.00000	0.00000	0.00000	0.10725	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	-0.08920	0.00000
21	C2	S	0.00039	0.09448	-0.03057	0.00000	0.02582
22	C2	S	-0.08404	0.22033	-0.02988	0.00000	0.23508
23	C2	PX	0.05929	-0.13713	-0.10814	0.00000	-0.01324
24	C2	PY	0.15395	-0.09499	0.01294	0.00000	-0.26541
25	C2	PZ	0.00000	0.00000	0.00000	0.00840	0.00000
26	C2	S	0.43055	-3.39969	1.24342	0.00000	-1.61824

27	C2	PX	0.76053	-1.97480	0.18487	0.00000	-0.77992
28	C2	PY	0.33434	0.49419	-1.51763	0.00000	-0.89103
29	C2	PZ	0.00000	0.00000	0.00000	0.01577	0.00000
30	C2	DXX	0.05898	0.02255	0.03626	0.00000	0.08559
31	C2	DYY	0.03955	-0.55076	0.13760	0.00000	-0.20730
32	C2	DZZ	-0.00915	0.55711	-0.19932	0.00000	0.14242
33	C2	DXY	0.00790	0.15546	-0.15383	0.00000	-0.02237
34	C2	DXZ	0.00000	0.00000	0.00000	-0.00083	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.06571	0.00000
36	C3	S	0.02291	0.01438	0.13139	0.00000	0.05019
37	C3	S	0.04951	0.08924	0.57733	0.00000	0.13397
38	C3	PX	0.09938	0.00940	-0.11402	0.00000	-0.05314
39	C3	PY	-0.08171	0.20705	0.05184	0.00000	-0.11192
40	C3	PZ	0.00000	0.00000	0.00000	0.00640	0.00000
41	C3	S	-0.11655	-1.29324	-8.82005	0.00000	-3.21012
42	C3	PX	-0.60884	-0.07866	1.31677	0.00000	0.05385
43	C3	PY	-1.37014	1.12372	1.68518	0.00000	2.57296
44	C3	PZ	0.00000	0.00000	0.00000	-0.02917	0.00000
45	C3	DXX	0.32958	-0.09774	-0.34130	0.00000	-0.21488
46	C3	DYY	-0.33329	0.01131	-0.35561	0.00000	-0.05214
47	C3	DZZ	0.11216	0.08977	0.67138	0.00000	0.26043
48	C3	DXY	-0.24497	0.13861	-0.11819	0.00000	0.39007
49	C3	DXZ	0.00000	0.00000	0.00000	-0.04004	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	-0.03523	0.00000
51	C4	S	-0.00432	-0.01886	0.00668	0.00000	0.05101
52	C4	S	-0.19448	-0.06421	0.01032	0.00000	0.05557
53	C4	PX	-0.05319	0.09037	-0.27980	0.00000	0.14857
54	C4	PY	-0.04126	0.01487	0.00573	0.00000	-0.15596
55	C4	PZ	0.00000	0.00000	0.00000	-0.00523	0.00000
56	C4	S	0.61891	0.72569	-1.42566	0.00000	-1.83065
57	C4	PX	-0.78105	2.18853	-1.11977	0.00000	0.07674
58	C4	PY	-0.45863	-0.59287	0.85108	0.00000	0.64301
59	C4	PZ	0.00000	0.00000	0.00000	0.04221	0.00000
60	C4	DXX	0.27679	0.20268	-0.05528	0.00000	-0.24118
61	C4	DYY	-0.31740	-0.07163	-0.15893	0.00000	0.16551
62	C4	DZZ	0.04690	-0.16499	0.08201	0.00000	0.27032
63	C4	DXY	0.10265	-0.13637	0.06686	0.00000	-0.07143
64	C4	DXZ	0.00000	0.00000	0.00000	0.15623	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	-0.08699	0.00000
66	C5	S	0.02907	-0.03246	0.02410	0.00000	-0.05224
67	C5	S	0.04984	-0.17407	0.09967	0.00000	-0.00223
68	C5	PX	-0.03317	-0.15093	0.10367	0.00000	0.00614
69	C5	PY	0.01704	-0.36263	-0.03067	0.00000	-0.02788
70	C5	PZ	0.00000	0.00000	0.00000	0.01009	0.00000
71	C5	S	-1.48760	2.51261	0.05863	0.00000	2.38702
72	C5	PX	-0.77748	1.34061	-0.63073	0.00000	0.49051
73	C5	PY	0.13589	-0.36389	-0.46177	0.00000	-0.99937
74	C5	PZ	0.00000	0.00000	0.00000	-0.03072	0.00000
75	C5	DXX	0.01863	-0.02972	-0.17731	0.00000	0.07783
76	C5	DYY	-0.18583	0.31373	0.02350	0.00000	0.19577
77	C5	DZZ	0.16150	-0.21156	0.16846	0.00000	-0.28651
78	C5	DXY	-0.12683	0.19478	-0.12767	0.00000	0.20624
79	C5	DXZ	0.00000	0.00000	0.00000	0.05420	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.07234	0.00000

81	C6	S	0.01117	-0.07728	-0.04558	0.00000	-0.02570
82	C6	S	0.23309	0.29062	-0.43326	0.00000	0.12204
83	C6	PX	-0.03910	-0.11605	0.16041	0.00000	-0.05751
84	C6	PY	-0.18803	-0.40532	0.01757	0.00000	-0.27679
85	C6	PZ	0.00000	0.00000	0.00000	0.00040	0.00000
86	C6	S	-0.42369	4.74689	2.08432	0.00000	2.48750
87	C6	PX	-0.66173	-1.02418	3.65630	0.00000	0.74553
88	C6	PY	-0.73060	-0.02007	0.17558	0.00000	-0.68726
89	C6	PZ	0.00000	0.00000	0.00000	0.00378	0.00000
90	C6	DXX	0.03247	0.10177	0.21641	0.00000	-0.15013
91	C6	DYY	-0.00304	0.37714	0.11261	0.00000	0.39838
92	C6	DZZ	-0.04767	-0.60063	-0.19257	0.00000	-0.21683
93	C6	DXY	0.04089	-0.27754	0.16924	0.00000	0.39661
94	C6	DXZ	0.00000	0.00000	0.00000	-0.03782	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	-0.00046	0.00000
96	C7	S	0.01344	-0.03386	-0.07912	0.00000	-0.05479
97	C7	S	-0.07392	-0.09889	-0.57189	0.00000	-0.21680
98	C7	PX	-0.21171	-0.09583	-0.17138	0.00000	-0.10761
99	C7	PY	-0.02236	0.13480	0.09364	0.00000	0.10887
100	C7	PZ	0.00000	0.00000	0.00000	-0.00189	0.00000
101	C7	S	-1.03979	2.12009	5.92529	0.00000	4.00236
102	C7	PX	0.66763	-1.14026	-3.37981	0.00000	-1.97237
103	C7	PY	0.10793	-0.24080	0.47090	0.00000	0.49776
104	C7	PZ	0.00000	0.00000	0.00000	0.01420	0.00000
105	C7	DXX	0.06324	0.00636	-0.00870	0.00000	0.07493
106	C7	DYY	-0.31107	0.15053	0.47244	0.00000	0.35446
107	C7	DZZ	0.10165	-0.17200	-0.41696	0.00000	-0.30193
108	C7	DXY	0.04772	-0.08302	-0.02145	0.00000	0.19249
109	C7	DXZ	0.00000	0.00000	0.00000	0.02202	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.01265	0.00000
111	O1	S	-0.02014	0.02504	0.01349	0.00000	-0.01607
112	O1	S	-0.19444	0.20171	0.07105	0.00000	-0.14971
113	O1	PX	-0.00072	0.04992	-0.03710	0.00000	0.02115
114	O1	PY	-0.07576	-0.02794	-0.00015	0.00000	0.05375
115	O1	PZ	0.00000	0.00000	0.00000	-0.01339	0.00000
116	O1	S	0.69308	-0.59793	-0.50529	0.00000	0.45838
117	O1	PX	0.22000	-0.75861	-0.10516	0.00000	0.02097
118	O1	PY	-0.12767	-0.21932	-0.36132	0.00000	-0.13902
119	O1	PZ	0.00000	0.00000	0.00000	-0.08233	0.00000
120	O1	DXX	0.07799	-0.18502	-0.16952	0.00000	-0.05687
121	O1	DYY	0.09928	0.03027	0.19700	0.00000	0.08571
122	O1	DZZ	-0.18761	0.29772	0.04886	0.00000	-0.15509
123	O1	DXY	0.15011	-0.17585	-0.31991	0.00000	0.09372
124	O1	DXZ	0.00000	0.00000	0.00000	-0.36682	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	-0.09993	0.00000
126	H4	S	0.00003	0.06310	-0.00101	0.00000	-0.01962
127	H4	S	-0.08620	0.23816	-0.01676	0.00000	0.12695
128	H4	PX	0.19380	0.04529	-0.02061	0.00000	-0.10347
129	H4	PY	0.10958	-0.04540	-0.13727	0.00000	0.10915
130	H4	PZ	0.00000	0.00000	0.00000	-0.00075	0.00000
131	N1	S	0.02647	0.05978	-0.02313	0.00000	0.02624
132	N1	S	0.21536	0.65613	-0.35731	0.00000	0.12988
133	N1	PX	-0.06485	-0.08086	0.16027	0.00000	-0.05073
134	N1	PY	0.01290	-0.16659	-0.19146	0.00000	-0.24117

135	N1	PZ	0.00000	0.00000	0.00000	-0.00038	0.00000
136	N1	S	-1.21382	-3.41394	1.61447	0.00000	-1.46792
137	N1	PX	-0.04434	-0.47269	0.14307	0.00000	0.01162
138	N1	PY	-0.51652	-1.12161	0.38847	0.00000	-0.60494
139	N1	PZ	0.00000	0.00000	0.00000	0.00095	0.00000
140	N1	DXX	0.10840	-0.00002	0.33792	0.00000	0.15432
141	N1	DYY	-0.28201	-0.62860	-0.09450	0.00000	-0.47617
142	N1	DZZ	0.18736	0.50604	-0.15834	0.00000	0.19281
143	N1	DXY	0.18928	-0.01198	-0.30195	0.00000	0.21248
144	N1	DXZ	0.00000	0.00000	0.00000	0.01398	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	-0.00843	0.00000
146	H6	S	0.09882	-0.02019	-0.17662	0.00000	-0.09417
147	H6	S	0.30894	-0.36644	-0.23144	0.00000	-0.28122
148	H6	PX	0.10378	0.06821	-0.17022	0.00000	-0.16864
149	H6	PY	-0.00769	-0.13464	-0.05876	0.00000	0.06477
150	H6	PZ	0.00000	0.00000	0.00000	0.00457	0.00000
151	C8	S	0.01112	-0.02310	0.07735	0.00000	0.01954
152	C8	S	0.09353	0.19628	0.14078	0.00000	0.21059
153	C8	PX	0.00807	-0.13640	0.04943	0.00000	-0.10708
154	C8	PY	-0.10461	0.11813	0.00398	0.00000	-0.26582
155	C8	PZ	0.00000	0.00000	0.00000	-0.00082	0.00000
156	C8	S	-0.32107	0.28527	-3.17514	0.00000	-1.51075
157	C8	PX	-0.04975	-1.14106	-0.20840	0.00000	-0.64014
158	C8	PY	1.04011	-0.63971	-3.22424	0.00000	-0.95155
159	C8	PZ	0.00000	0.00000	0.00000	-0.00328	0.00000
160	C8	DXX	0.34673	0.06214	-0.37615	0.00000	0.03160
161	C8	DYY	-0.21324	-0.09579	-0.05376	0.00000	-0.04831
162	C8	DZZ	-0.00232	-0.15514	0.41551	0.00000	0.01611
163	C8	DXY	0.14793	-0.21015	0.09009	0.00000	-0.31103
164	C8	DXZ	0.00000	0.00000	0.00000	0.01337	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.01166	0.00000
166	H8	S	0.02317	0.04480	0.12877	0.00000	0.01333
167	H8	S	-0.00488	0.28066	0.80107	0.00000	0.40070
168	H8	PX	-0.40454	-0.03691	-0.09520	0.00000	0.06158
169	H8	PY	-0.03334	0.10753	-0.03937	0.00000	-0.23238
170	H8	PZ	0.00000	0.00000	0.00000	-0.02035	0.00000
171	C10	S	0.01860	0.00537	-0.01077	0.00000	0.02502
172	C10	S	-0.15630	0.11758	-0.07112	0.00000	-0.27346
173	C10	PX	-0.02506	-0.05028	0.07016	0.00000	-0.10632
174	C10	PY	0.15404	-0.04757	0.08356	0.00000	-0.03439
175	C10	PZ	0.00000	0.00000	0.00000	0.00174	0.00000
176	C10	S	0.72460	-0.45702	-1.17341	0.00000	-0.33979
177	C10	PX	-0.16899	0.65601	0.61569	0.00000	0.37600
178	C10	PY	0.60939	-0.29012	-0.23568	0.00000	0.24106
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.29446	-0.08228	-0.13380	0.00000	0.21412
181	C10	DYY	-0.20485	0.06348	0.15532	0.00000	-0.29450
182	C10	DZZ	0.10283	0.02909	-0.08242	0.00000	0.17155
183	C10	DXY	0.12593	-0.09586	-0.02024	0.00000	0.06424
184	C10	DXZ	0.00000	0.00000	0.00000	-0.01012	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00471	0.00000
186	H16	S	-0.02791	-0.06094	-0.03952	0.00000	-0.03339
187	H16	S	0.17602	-0.26715	-0.22025	0.00000	0.08126
188	H16	PX	-0.20784	0.09827	0.01306	0.00000	-0.28214

189	H16	PY	-0.32952	0.19265	-0.01276	0.00000	-0.10340
190	H16	PZ	0.00000	0.00000	0.00000	0.00747	0.00000
191	H18	S	-0.03835	0.12136	0.12650	0.00000	0.08769
192	H18	S	0.15722	0.00653	0.22834	0.00000	0.21988
193	H18	PX	0.33126	-0.12211	0.07962	0.00000	0.28985
194	H18	PY	-0.21829	-0.01891	0.16399	0.00000	-0.18881
195	H18	PZ	0.00000	0.00000	0.00000	-0.00352	0.00000
196	C9	S	0.00367	-0.01685	-0.02792	0.00000	0.01080
197	C9	S	-0.21206	0.25981	0.03818	0.00000	-0.00810
198	C9	PX	0.15378	-0.23977	-0.14782	0.00000	0.02904
199	C9	PY	0.06568	-0.10711	-0.02266	0.00000	0.04226
200	C9	PZ	0.00000	0.00000	0.00000	0.03652	0.00000
201	C9	S	-0.03907	0.51227	0.59341	0.00000	-0.20527
202	C9	PX	0.12141	-0.13933	-0.12283	0.00000	0.00868
203	C9	PY	-0.39551	-0.03387	-0.25037	0.00000	0.13856
204	C9	PZ	0.00000	0.00000	0.00000	-0.10230	0.00000
205	C9	DXX	0.04112	0.31198	0.27027	0.00000	-0.17441
206	C9	DYY	0.09637	-0.07767	-0.03450	0.00000	0.05604
207	C9	DZZ	-0.09674	-0.27815	-0.21334	0.00000	0.14414
208	C9	DXY	-0.29270	0.03157	0.01970	0.00000	0.10429
209	C9	DXZ	0.00000	0.00000	0.00000	-0.31192	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	-0.85972	0.00000
211	H3	S	0.00911	-0.02821	-0.03098	0.00000	-0.00946
212	H3	S	0.26715	-0.06933	0.03629	0.00000	-0.05052
213	H3	PX	0.17211	0.02645	0.03489	0.00000	-0.11202
214	H3	PY	-0.01206	0.04859	0.06990	0.00000	0.01002
215	H3	PZ	0.00000	0.00000	0.00000	0.59188	0.00000
216	H5	S	-0.04433	-0.00687	-0.03944	0.02484	0.01649
217	H5	S	-0.04201	-0.06439	-0.08057	-0.06015	0.04392
218	H5	PX	-0.10663	-0.11940	-0.07851	-0.19444	0.08970
219	H5	PY	0.18667	0.02605	0.01488	-0.46070	-0.04081
220	H5	PZ	-0.14138	-0.11652	-0.11325	0.05273	0.09787
221	H7	S	-0.04433	-0.00687	-0.03944	-0.02484	0.01649
222	H7	S	-0.04201	-0.06439	-0.08057	0.06015	0.04392
223	H7	PX	-0.10663	-0.11940	-0.07851	0.19444	0.08970
224	H7	PY	0.18667	0.02605	0.01488	0.46070	-0.04081
225	H7	PZ	0.14138	0.11652	0.11325	0.05273	-0.09787

MO:	196	197	198	199	200
Eigenvalues:	3.30396	3.34005	3.35844	3.43095	3.45749
(ev):	89.90539	90.88745	91.38780	93.36103	94.08322

			A	A	A	A	A
1	H1	S	-0.14225	0.01944	-0.01062	-0.10608	0.18676
2	H1	S	-0.50753	0.06258	0.03420	-0.18966	0.31540
3	H1	PX	0.38430	-0.11079	-0.06560	0.13371	-0.40927
4	H1	PY	0.07788	-0.07082	0.11540	0.18505	-0.06589
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02773	-0.00881	0.02010	-0.00407	0.02745
7	C1	S	0.20121	-0.11992	-0.05674	0.05459	-0.37374
8	C1	PX	0.28877	-0.14105	0.09197	0.10689	-0.01752
9	C1	PY	-0.10761	-0.05109	-0.02154	0.21541	-0.19185
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.12890	1.34093	-0.28940	0.40862	-0.34332

12	C1	PX	1.02338	-0.00813	0.28880	0.27916	-0.18930
13	C1	PY	-0.90841	-1.15185	-0.49948	-0.12334	0.00489
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.18470	-0.04583	0.08182	0.18464	-0.11945
16	C1	DYY	0.29562	0.13361	-0.22364	-0.20375	-0.15669
17	C1	DZZ	-0.17172	-0.01385	0.13106	-0.03684	0.22409
18	C1	DXY	0.13677	0.13499	-0.03839	-0.27078	0.03780
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.00170	-0.03718	-0.03117	-0.02120	-0.02427
22	C2	S	-0.23685	-0.05394	0.06836	0.15211	0.30111
23	C2	PX	-0.04356	-0.18634	-0.10003	-0.00618	0.02783
24	C2	PY	-0.10570	-0.05462	0.03790	0.04770	0.13781
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.75069	1.07542	0.76943	0.18703	0.20713
27	C2	PX	0.37277	0.25950	-0.03966	0.55460	0.08805
28	C2	PY	1.86914	0.72854	1.04182	0.07907	-0.30036
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.10726	-0.10728	-0.01841	-0.08759	0.03912
31	C2	DYY	-0.18845	0.21793	0.14567	0.20653	0.18447
32	C2	DZZ	0.05041	-0.21365	-0.20098	-0.13041	-0.19307
33	C2	DXY	-0.19490	-0.03231	-0.12217	0.24147	0.02063
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03998	-0.00779	-0.03910	-0.06488	-0.01843
37	C3	S	-0.18788	0.04899	0.04783	0.14006	0.08412
38	C3	PX	0.13665	-0.08421	0.03495	0.17867	0.10363
39	C3	PY	-0.34531	-0.11065	0.00862	-0.13058	0.00395
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	3.84317	-0.19678	2.17177	2.31791	0.75772
42	C3	PX	-2.09938	-1.56112	-0.50079	-1.40423	0.60200
43	C3	PY	-2.37624	-1.30951	-1.48753	-0.88078	-0.76650
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.40259	0.39535	-0.09072	-0.23542	-0.18650
46	C3	DYY	-0.07540	-0.27453	0.23118	0.48306	0.24019
47	C3	DZZ	-0.19458	-0.04863	-0.17685	-0.33436	-0.12472
48	C3	DXY	-0.49737	0.24052	-0.02058	-0.17331	0.03000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00076	-0.01380	-0.05249	-0.01283	-0.03765
52	C4	S	-0.19111	0.35641	0.20510	0.09964	-0.36328
53	C4	PX	-0.00458	-0.05070	-0.05801	-0.01243	0.05982
54	C4	PY	-0.26900	0.08817	0.09456	0.30209	-0.45878
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.14686	0.32343	1.10964	0.58890	0.39663
57	C4	PX	1.07922	0.12446	0.35017	-0.09675	-0.20206
58	C4	PY	-1.10239	0.47571	-0.21797	0.33418	-0.85339
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.08772	0.04977	0.14780	-0.23092	0.44433
61	C4	DYY	0.06112	-0.01409	-0.08835	0.17056	-0.49713
62	C4	DZZ	0.06992	-0.11451	-0.32104	-0.09202	-0.14197
63	C4	DXY	-0.22263	0.19950	-0.12087	0.01268	-0.40521
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

66	C5	S	-0.01102	0.02132	0.04749	-0.01827	0.06359
67	C5	S	0.09847	-0.06215	-0.11729	-0.13099	-0.26710
68	C5	PX	0.04204	0.05648	0.07656	0.06925	0.09649
69	C5	PY	-0.12501	0.00035	-0.09609	0.19325	0.01433
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-1.05358	-1.00513	-1.51959	0.00323	-0.75147
72	C5	PX	0.80413	0.23339	0.29055	-0.10974	-0.43686
73	C5	PY	1.17786	0.45802	0.69141	-0.18168	-0.15754
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.13818	-0.30561	-0.13026	0.20736	0.24954
76	C5	DYY	0.22899	0.11599	-0.03890	-0.24648	-0.35128
77	C5	DZZ	-0.09387	0.14395	0.28086	-0.06575	0.37886
78	C5	DXY	0.05375	-0.08961	-0.15754	0.01798	-0.15030
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.02665	0.02650	0.02485	0.01157	0.01666
82	C6	S	0.56473	-0.00678	0.09544	0.65635	-0.09658
83	C6	PX	0.04813	-0.09744	0.15041	-0.04508	0.01665
84	C6	PY	-0.31262	-0.03882	-0.07241	-0.37335	0.04125
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-1.00395	-1.67050	-0.95616	-0.81205	-0.54640
87	C6	PX	-3.02262	-1.06017	-1.26323	-1.34403	0.24054
88	C6	PY	-1.59435	-0.23783	0.33223	-1.67518	0.33891
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.18825	-0.46403	-0.15809	-0.37133	0.00600
91	C6	DYY	0.08908	0.30564	0.04678	0.51037	0.00619
92	C6	DZZ	-0.00456	0.12975	0.14065	-0.09865	0.10945
93	C6	DXY	-0.26598	-0.22087	-0.08222	0.19708	0.35888
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.05182	-0.01986	0.00281	0.02755	0.00994
97	C7	S	0.12463	-0.00281	0.31039	0.08279	0.03832
98	C7	PX	0.04330	-0.29204	0.35662	0.33553	0.05447
99	C7	PY	-0.26300	-0.07779	-0.16427	-0.19040	-0.07745
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-3.74140	0.22525	-2.01191	-1.81835	-1.02117
102	C7	PX	2.16096	0.15012	1.47045	1.24057	0.42871
103	C7	PY	0.62249	0.45881	-0.15446	0.76519	-0.47846
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.00557	0.05286	0.10108	0.08966	0.02133
106	C7	DYY	-0.41204	0.04847	-0.02134	-0.24872	-0.07117
107	C7	DZZ	0.28602	-0.09853	-0.03721	0.13024	0.04906
108	C7	DXY	0.36409	0.34899	0.16735	0.45275	0.23066
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00467	-0.01136	0.02154	0.01988	0.01281
112	O1	S	-0.06431	0.17978	0.22771	0.05013	-0.09109
113	O1	PX	0.02891	-0.03610	-0.02140	-0.03189	0.08591
114	O1	PY	0.06739	-0.04745	-0.03898	0.01618	0.00107
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.33518	-0.45389	-0.74357	-0.47011	0.26255
117	O1	PX	-0.43854	0.15477	-0.08514	0.21665	-0.51868
118	O1	PY	-0.65054	0.45029	0.16038	0.42949	-1.02059
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

120	O1	DXX	-0.37439	0.09341	0.02369	0.29053	-0.43735
121	O1	DYY	0.36160	-0.23211	-0.11547	-0.29832	0.71567
122	O1	DZZ	0.04205	-0.00299	0.21253	0.09377	0.00432
123	O1	DXY	-0.22500	0.12455	-0.21309	-0.03371	-0.26249
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.03829	0.08122	0.11529	-0.00592	0.09736
127	H4	S	0.02520	0.08082	0.14739	0.02129	0.14045
128	H4	PX	-0.15363	-0.06094	0.10583	0.09296	0.36068
129	H4	PY	-0.23953	-0.28938	-0.27538	0.10281	-0.00029
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.01412	0.01067	-0.00343	0.00386	0.00579
132	N1	S	0.21860	-0.27698	0.09305	-0.06108	-0.09196
133	N1	PX	-0.06909	-0.14820	-0.01722	-0.02370	-0.01201
134	N1	PY	0.02361	-0.05620	0.00796	-0.19440	0.01243
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-1.23713	0.49140	-0.10836	-0.43587	0.23862
137	N1	PX	0.63897	0.16554	-0.16017	0.96664	-0.07708
138	N1	PY	-1.53342	0.13652	-0.04786	-1.53177	0.32685
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.23447	-0.11770	-0.22724	0.58220	0.00065
141	N1	DYY	-0.38450	0.09802	0.10468	-0.75496	0.02637
142	N1	DZZ	0.09331	0.00673	0.02549	0.06188	0.00781
143	N1	DXY	-0.28568	-0.03255	-0.23615	-0.10810	0.31465
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.09856	-0.03690	-0.03229	-0.02236	-0.08378
147	H6	S	0.29640	-0.05682	-0.07999	0.14768	-0.10163
148	H6	PX	0.14122	-0.21527	-0.11777	-0.22407	-0.19369
149	H6	PY	-0.22825	-0.06671	-0.20585	0.20690	-0.01339
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.01405	0.03382	-0.03601	0.03132	0.01564
152	C8	S	-0.32214	-0.28164	0.15152	-0.46027	-0.13565
153	C8	PX	0.09876	-0.15801	0.05044	0.10698	-0.09819
154	C8	PY	-0.14035	0.15572	-0.39700	-0.03459	0.08911
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	1.71287	-0.13974	1.30611	0.35530	0.00696
157	C8	PX	1.66252	0.31957	0.17777	1.71494	-0.24931
158	C8	PY	1.47201	-0.21700	1.04683	0.57322	0.19427
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.03972	0.34668	-0.27227	-0.00067	0.27022
161	C8	DYY	0.14215	-0.46003	0.49473	-0.04611	-0.26923
162	C8	DZZ	-0.05071	0.23190	-0.25018	0.22160	0.09791
163	C8	DXY	0.04430	-0.38832	-0.42191	0.31492	0.02732
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00496	0.03702	-0.24166	-0.14641	-0.00489
167	H8	S	-0.40924	0.02926	-0.62598	-0.38421	-0.11544
168	H8	PX	-0.20407	-0.24100	0.51682	0.21453	0.01470
169	H8	PY	-0.20877	-0.21891	-0.08099	-0.37454	-0.09836
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.01320	-0.02624	0.04174	-0.00580	-0.01662
172	C10	S	0.01090	0.19869	-0.39494	0.17076	0.17558
173	C10	PX	-0.03756	-0.41575	-0.11225	0.12495	-0.04118

174	C10	PY	-0.06801	0.04571	-0.24172	0.07250	0.06869
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.17891	0.11352	-0.08847	0.10802	0.33219
177	C10	PX	-0.64817	-0.34974	-0.36179	-0.40534	-0.04308
178	C10	PY	-0.18907	-0.12738	0.11358	-0.20966	0.03565
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	0.04980	-0.15264	0.19982	0.00035	-0.01112
181	C10	DYY	-0.09340	0.33590	-0.58190	0.13538	0.18362
182	C10	DZZ	0.08443	-0.20954	0.34097	-0.07820	-0.14181
183	C10	DXY	0.02330	-0.13884	0.19604	-0.09258	-0.04132
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.08350	0.10957	0.16308	-0.06085	-0.03735
187	H16	S	0.19825	0.19488	0.37533	0.00103	-0.05032
188	H16	PX	-0.02666	-0.12658	-0.45191	0.24326	0.11521
189	H16	PY	-0.00481	0.33087	-0.05649	-0.05803	0.02789
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.06296	-0.17090	0.00395	-0.00774	-0.08627
192	H18	S	-0.28037	-0.35519	0.00809	-0.20626	-0.08941
193	H18	PX	-0.04828	-0.36107	0.28043	-0.06969	-0.14749
194	H18	PY	-0.03474	-0.26136	-0.13139	0.08430	-0.07711
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.02681	0.00281	-0.01217	0.01844	-0.04368
197	C9	S	0.22951	-0.16023	0.06812	-0.16036	0.37647
198	C9	PX	-0.18115	0.06271	-0.10934	0.01594	-0.17839
199	C9	PY	-0.00685	0.01309	-0.03163	0.00467	0.03265
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.50918	-0.07527	0.23325	-0.29584	0.92058
202	C9	PX	-0.21703	0.14154	-0.04753	0.07719	-0.30348
203	C9	PY	-0.00386	-0.29267	-0.05751	-0.00126	0.13734
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.05128	0.01938	0.21356	0.14736	-0.09106
206	C9	DYY	0.00531	0.01308	-0.06867	-0.06072	0.11426
207	C9	DZZ	0.04471	-0.01819	-0.16402	-0.08021	-0.02192
208	C9	DXY	0.27644	-0.09911	-0.07007	-0.14351	0.19287
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.06556	0.05540	-0.01385	0.05993	-0.22580
212	H3	S	-0.13643	0.19656	-0.01174	0.07286	-0.29099
213	H3	PX	-0.19091	0.08719	0.09661	0.13654	-0.20600
214	H3	PY	0.13289	-0.06882	0.03588	-0.09709	0.32954
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.05527	-0.02720	-0.00106	0.05259	-0.06167
217	H5	S	0.02908	-0.04699	-0.04288	0.03421	-0.08369
218	H5	PX	0.13535	-0.04767	-0.07912	-0.11949	0.15549
219	H5	PY	-0.13516	0.09337	0.03126	0.05955	-0.12571
220	H5	PZ	0.04483	-0.04346	-0.06851	0.02485	-0.05603
221	H7	S	-0.05527	-0.02720	-0.00106	0.05259	-0.06167
222	H7	S	0.02908	-0.04699	-0.04288	0.03421	-0.08369
223	H7	PX	0.13535	-0.04767	-0.07912	-0.11949	0.15549
224	H7	PY	-0.13516	0.09337	0.03126	0.05955	-0.12571
225	H7	PZ	-0.04483	0.04346	0.06851	-0.02485	0.05603

MO:

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Eigenvalues:	3.52337	3.56160	3.57691	3.66981	3.72630
(ev):	95.87591	96.91612	97.33263	99.86077	101.39790

		A	A	A	A	A	
1	H1	S	-0.04330	0.22972	-0.12081	0.07766	0.01208
2	H1	S	-0.04892	0.17382	0.06527	0.04686	-0.02133
3	H1	PX	0.03345	-0.48068	0.17057	-0.11620	0.02010
4	H1	PY	0.28089	-0.03319	0.05683	-0.01976	-0.18129
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.02783	0.01993	-0.00250	-0.00094	0.00516
7	C1	S	0.12237	-0.01099	0.07455	-0.02621	-0.10345
8	C1	PX	-0.06844	-0.43907	0.08044	-0.04071	0.10548
9	C1	PY	0.10772	-0.02461	0.07589	-0.06373	-0.12162
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	0.21798	-0.28041	-0.00538	-0.05516	0.18004
12	C1	PX	-0.19315	0.34797	-0.12836	-0.00760	-0.03680
13	C1	PY	0.10923	-0.64942	0.07576	-0.01609	0.34903
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.21334	-0.01351	0.12247	-0.07204	-0.20603
16	C1	DYY	-0.09252	-0.01939	-0.04721	0.00402	0.12190
17	C1	DZZ	-0.16691	0.11194	-0.04326	0.01162	0.05378
18	C1	DXY	-0.34679	-0.25386	0.01800	-0.05104	0.24815
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	0.03757	-0.01840	0.00687	-0.02469	-0.00260
22	C2	S	0.00708	0.05198	-0.02142	0.31002	0.02111
23	C2	PX	0.09138	-0.19026	-0.00157	-0.53312	0.02921
24	C2	PY	0.31312	-0.05451	0.00696	-0.02880	0.18859
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.82855	0.00948	-0.29814	0.46780	0.19785
27	C2	PX	-0.22269	0.09300	-0.05542	-0.18562	0.32766
28	C2	PY	-1.33167	0.55636	-0.26845	0.12978	-0.05588
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.37435	-0.09137	-0.02114	0.48035	-0.17527
31	C2	DYY	0.22956	0.04339	0.02069	-0.18586	0.24494
32	C2	DZZ	0.18962	-0.11140	0.03559	-0.19847	-0.02977
33	C2	DXY	0.46416	0.14964	0.06521	0.36348	0.24760
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.04138	-0.03755	0.00318	-0.02117	-0.02119
37	C3	S	0.49682	-0.17578	0.04073	-0.03274	-0.15879
38	C3	PX	0.07199	-0.21220	0.01623	0.01842	-0.13103
39	C3	PY	-0.05722	0.14774	-0.02031	-0.03902	-0.04589
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	-3.93029	2.12391	-0.78744	0.93063	1.15737
42	C3	PX	1.01872	-1.71149	-0.06786	-0.17098	-0.22691
43	C3	PY	1.60404	-1.24683	0.80794	-0.35110	-0.24459
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.18164	0.34661	-0.03317	0.06061	0.15575
46	C3	DYY	0.07402	-0.25248	0.01874	-0.02194	-0.10610
47	C3	DZZ	0.14634	-0.12148	0.00992	-0.10152	-0.08814
48	C3	DXY	-0.31001	0.29485	0.00411	-0.12906	0.17675
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

51	C4	S	0.04210	0.02001	0.00824	-0.01580	-0.02340
52	C4	S	-0.47560	-0.39648	0.21990	0.06096	0.21246
53	C4	PX	-0.08959	-0.15226	0.01045	-0.05688	0.19821
54	C4	PY	-0.10540	-0.16898	0.23514	-0.02474	0.01191
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-0.76218	0.07911	0.12966	0.29282	0.35252
57	C4	PX	-0.05911	0.55566	0.10248	-0.08438	-0.53524
58	C4	PY	0.00715	-0.56913	1.02540	-0.13796	0.15796
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	0.08397	0.27424	-0.17810	0.07595	-0.15672
61	C4	DYY	-0.22739	-0.26249	0.24361	-0.11232	0.13295
62	C4	DZZ	0.30375	0.16929	-0.01684	-0.05713	-0.15891
63	C4	DXY	0.22416	0.46639	0.02809	-0.05668	-0.36013
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.02493	0.00871	-0.02843	-0.02934	0.00694
67	C5	S	-0.12959	-0.17323	0.07780	0.38183	-0.09475
68	C5	PX	-0.00287	-0.06244	-0.00917	-0.46541	0.16997
69	C5	PY	0.23847	0.00958	0.09251	0.42146	0.12011
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	1.64690	-0.11980	0.71506	-0.01255	-0.52998
72	C5	PX	-0.36408	0.19356	0.11338	-0.34813	-0.27857
73	C5	PY	-0.74542	0.16376	-0.34142	0.44268	-0.13798
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	0.22826	-0.25146	0.05380	0.19384	0.26588
76	C5	DYY	-0.32672	0.15302	-0.03769	0.08071	-0.35964
77	C5	DZZ	-0.08849	0.07307	-0.14448	-0.23430	0.06613
78	C5	DXY	0.05602	0.04203	-0.02114	-0.63341	0.06324
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	-0.06717	0.03664	-0.00936	0.00213	0.00724
82	C6	S	-0.06331	0.45840	-0.01763	0.10348	0.11921
83	C6	PX	-0.04213	-0.13794	-0.01701	-0.04036	-0.12819
84	C6	PY	0.28394	-0.34399	0.03413	0.07136	-0.03186
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	1.67318	-1.16995	0.25425	-0.26772	-0.61482
87	C6	PX	2.32562	-1.99389	0.35934	-0.33953	-0.20961
88	C6	PY	0.36907	-0.93803	-0.04974	-0.02825	-0.32726
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.18889	-0.49842	0.02654	0.08225	-0.21428
91	C6	DYY	-0.09350	0.48283	-0.01191	-0.14066	0.18624
92	C6	DZZ	-0.25724	0.06403	-0.03760	0.02771	0.00424
93	C6	DXY	-0.46909	-0.33222	-0.04701	-0.18543	-0.17918
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	-0.03317	0.01105	-0.01032	0.01652	0.05935
97	C7	S	-0.26032	0.23308	-0.07486	0.01827	-0.12055
98	C7	PX	0.02184	0.06698	-0.00593	-0.03744	-0.25661
99	C7	PY	-0.17920	0.17567	0.00385	-0.04819	0.11060
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	2.99782	-1.54857	1.09591	-0.92887	-1.42964
102	C7	PX	-1.68849	1.11861	-0.53213	0.48753	0.35177
103	C7	PY	-0.05911	0.69608	0.13648	-0.00696	0.33282
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

105	C7	DXX	0.09461	0.02385	0.01901	-0.06640	-0.21728
106	C7	DYY	0.06197	-0.00965	0.03464	-0.04205	0.17075
107	C7	DZZ	-0.10835	-0.00472	-0.03611	0.09314	0.29821
108	C7	DXY	0.35948	-0.40767	0.03382	0.03402	-0.10839
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.02087	-0.03397	-0.00930	0.01001	0.03029
112	O1	S	-0.22877	-0.18839	0.25334	0.06897	0.05540
113	O1	PX	0.03799	0.05226	0.09661	-0.00299	-0.00773
114	O1	PY	0.01042	-0.00155	0.03900	-0.03608	0.01767
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.75921	0.91385	-0.65507	-0.22716	-0.50142
117	O1	PX	-0.15213	-0.20550	0.32177	-0.05606	0.12727
118	O1	PY	-0.45387	-0.37647	0.74708	-0.02298	0.12663
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.16382	-0.18159	0.38862	-0.04282	0.11972
121	O1	DYY	0.34434	0.29402	-0.40886	0.05924	-0.06391
122	O1	DZZ	-0.22499	-0.23688	-0.03124	0.06777	0.15228
123	O1	DXY	0.23075	0.40851	0.11948	-0.10724	-0.22264
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	-0.05327	0.07282	-0.06516	-0.66170	0.09229
127	H4	S	-0.10378	0.04702	0.00659	-0.52909	0.05767
128	H4	PX	0.12152	0.00427	-0.07847	-0.67502	0.21443
129	H4	PY	0.22825	-0.13826	0.11849	0.77471	0.00415
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.00554	-0.01430	-0.00009	-0.00733	0.01633
132	N1	S	0.05886	-0.02327	-0.01197	0.15799	-0.13916
133	N1	PX	-0.04687	-0.00887	-0.00354	-0.01653	-0.04352
134	N1	PY	0.03635	-0.16052	-0.00094	0.09070	-0.04052
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	0.20124	-0.01286	0.03132	-0.20249	0.00393
137	N1	PX	-0.52594	0.80459	-0.02538	-0.08928	0.13212
138	N1	PY	0.48560	-1.15778	0.06273	-0.07989	-0.15471
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	-0.29822	0.35953	-0.01556	-0.12279	0.12554
141	N1	DYY	0.22896	-0.49884	0.02583	0.04630	-0.02287
142	N1	DZZ	0.01283	-0.02196	-0.00099	-0.01281	0.05035
143	N1	DXY	-0.26914	-0.42790	-0.01697	-0.04627	-0.11714
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.09616	-0.05448	-0.00051	-0.54816	0.04483
147	H6	S	-0.05241	-0.02089	-0.00256	-0.36532	0.09953
148	H6	PX	0.15231	-0.22623	0.00157	-0.83240	-0.02283
149	H6	PY	0.40813	0.04393	0.05207	-0.30872	0.17700
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.01591	-0.00818	0.00426	-0.01745	-0.05743
152	C8	S	0.18458	-0.11796	0.02822	0.00926	-0.13032
153	C8	PX	-0.17195	0.29686	-0.02368	-0.02587	0.02702
154	C8	PY	-0.01400	-0.05992	0.00031	-0.00079	0.16730
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	-0.71764	0.43475	-0.32034	0.60693	1.61330
157	C8	PX	-0.50617	1.31217	-0.10968	0.12368	0.69720
158	C8	PY	-1.73495	0.76284	-0.35358	0.40581	-0.21013

159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.06496	-0.30181	-0.00941	-0.01876	-0.07688
161	C8	DYY	-0.05225	0.31352	-0.01803	0.03678	-0.03658
162	C8	DZZ	0.04092	0.00037	0.01458	-0.08174	-0.25933
163	C8	DXY	-0.40112	0.27148	-0.04179	-0.03044	0.11192
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.01393	-0.11391	0.00234	0.05100	0.28861
167	H8	S	0.35156	-0.33190	0.11356	-0.08210	0.12656
168	H8	PX	0.06404	0.15573	0.01094	-0.10225	-0.40664
169	H8	PY	-0.13781	0.10698	-0.02612	0.00982	0.05165
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.01404	0.01150	0.00117	0.00795	0.09051
172	C10	S	-0.13216	-0.05780	-0.02370	-0.04316	-0.50768
173	C10	PX	-0.32827	0.25320	-0.03935	-0.05511	0.02391
174	C10	PY	-0.06217	0.02034	0.00092	-0.00381	0.43752
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	-1.08140	0.09360	-0.15098	0.01850	-1.52800
177	C10	PX	0.15496	-0.21926	0.07397	-0.12325	-0.09125
178	C10	PY	-0.30492	-0.03788	-0.01248	-0.01434	-0.28136
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.15078	0.03255	-0.02480	-0.04691	-0.58250
181	C10	DYY	0.02528	-0.15359	0.01632	-0.00159	0.27791
182	C10	DZZ	0.09754	0.09839	0.00853	0.05495	0.55602
183	C10	DXY	0.11620	-0.11116	0.01072	0.04084	-0.31767
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.22888	-0.07290	0.01925	0.07883	0.41186
187	H16	S	0.14295	0.00278	0.00464	0.07424	0.30491
188	H16	PX	-0.39604	0.14283	-0.04816	-0.09689	-0.49024
189	H16	PY	0.20695	-0.10658	0.02377	0.03975	0.35215
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.03187	0.15554	0.00569	-0.01224	0.50952
192	H18	S	-0.02822	0.00979	0.02620	-0.03704	0.27717
193	H18	PX	-0.07806	0.19885	-0.00318	-0.00928	0.45334
194	H18	PY	-0.12108	0.22346	-0.00765	0.00743	0.66980
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.01042	-0.00752	-0.09889	-0.00163	-0.00135
197	C9	S	-0.02925	0.06745	0.76442	-0.00249	0.00138
198	C9	PX	0.03747	0.18516	0.55603	-0.09595	-0.13456
199	C9	PY	-0.02325	-0.03751	0.16306	0.00664	0.16491
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.05268	0.14581	0.55897	0.10142	0.03702
202	C9	PX	-0.04814	0.04195	0.40811	-0.06858	-0.07105
203	C9	PY	0.07221	-0.02163	0.21225	-0.01767	0.11522
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.19540	-0.31544	-0.42529	0.05183	0.06903
206	C9	DYY	0.07056	0.05824	-0.12481	0.03014	0.16963
207	C9	DZZ	0.12344	0.24658	0.33190	-0.08737	-0.21190
208	C9	DXY	0.15352	0.08758	-0.58926	0.04786	-0.06405
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.01256	-0.00159	-0.26969	-0.02369	-0.16659
212	H3	S	-0.01871	-0.00113	-0.30931	-0.01801	-0.11839

213	H3	PX	-0.12717	-0.14497	0.01125	0.00095	0.01594
214	H3	PY	-0.06379	-0.01722	0.57637	0.02743	0.23671
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.01601	-0.08832	-0.37629	0.03258	0.08354
217	H5	S	0.04728	-0.06395	-0.37822	0.01138	0.04182
218	H5	PX	0.07257	0.17062	0.38718	-0.03792	-0.09289
219	H5	PY	-0.04884	-0.06392	-0.16235	0.01463	0.03369
220	H5	PZ	0.09180	-0.06026	-0.64438	0.04193	0.06972
221	H7	S	0.01601	-0.08832	-0.37629	0.03258	0.08354
222	H7	S	0.04728	-0.06395	-0.37822	0.01138	0.04182
223	H7	PX	0.07257	0.17062	0.38718	-0.03792	-0.09289
224	H7	PY	-0.04884	-0.06392	-0.16235	0.01463	0.03369
225	H7	PZ	-0.09180	0.06026	0.64438	-0.04193	-0.06972

MO:	206	207	208	209	210
Eigenvalues:	3.78192	3.79244	3.84127	3.87761	3.98970
(ev):	102.91138	103.19748	104.52633	105.51517	108.56519

		A	A	A	A	A	
1	H1	S	0.04729	0.00000	-0.02568	0.75223	0.03842
2	H1	S	-0.04375	0.00000	-0.09396	0.56436	-0.07560
3	H1	PX	-0.11510	0.00000	0.09291	-0.93001	-0.09735
4	H1	PY	0.17433	0.00000	-0.12664	-0.36155	0.09844
5	H1	PZ	0.00000	-0.02276	0.00000	0.00000	0.00000
6	C1	S	0.01696	0.00000	0.00546	0.07856	0.03767
7	C1	S	0.02584	0.00000	-0.11078	-0.43974	-0.06232
8	C1	PX	-0.13033	0.00000	0.16523	-0.52787	-0.08681
9	C1	PY	0.17030	0.00000	-0.10709	-0.18431	0.19475
10	C1	PZ	0.00000	0.00379	0.00000	0.00000	0.00000
11	C1	S	-0.33049	0.00000	0.02727	-1.12745	-0.84565
12	C1	PX	0.36053	0.00000	0.05360	-0.40697	0.45924
13	C1	PY	-0.66705	0.00000	-0.09691	0.09465	-0.01387
14	C1	PZ	0.00000	-0.04473	0.00000	0.00000	0.00000
15	C1	DXX	0.20063	0.00000	-0.13141	-0.69217	0.16165
16	C1	DYY	-0.16759	0.00000	0.10680	0.54936	-0.11371
17	C1	DZZ	0.06140	0.00000	0.04931	0.46015	0.14254
18	C1	DXY	-0.34421	0.00000	0.27869	-0.48140	-0.29480
19	C1	DXZ	0.00000	0.04292	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	-0.01082	0.00000	0.00000	0.00000
21	C2	S	-0.00684	0.00000	-0.00633	0.05563	-0.02176
22	C2	S	-0.04420	0.00000	0.12274	-0.28990	0.07525
23	C2	PX	0.03191	0.00000	-0.07862	0.32636	-0.06188
24	C2	PY	-0.26505	0.00000	0.13592	0.14317	-0.10915
25	C2	PZ	0.00000	0.00026	0.00000	0.00000	0.00000
26	C2	S	0.14879	0.00000	-0.00216	-0.56304	0.20857
27	C2	PX	-0.00750	0.00000	-0.05279	0.10474	-0.04568
28	C2	PY	0.61787	0.00000	-0.24098	0.09170	0.39210
29	C2	PZ	0.00000	0.01353	0.00000	0.00000	0.00000
30	C2	DXX	0.23746	0.00000	-0.03464	-0.36873	0.09393
31	C2	DYY	-0.27822	0.00000	0.09376	0.33859	-0.15664
32	C2	DZZ	-0.00211	0.00000	-0.06809	0.32257	-0.09577
33	C2	DXY	-0.37756	0.00000	0.30035	-0.31467	0.02762
34	C2	DXZ	0.00000	0.00306	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00694	0.00000	0.00000	0.00000

36	C3	S	-0.03406	0.00000	0.00829	-0.03121	-0.08786
37	C3	S	0.09045	0.00000	-0.05516	0.03048	0.17810
38	C3	PX	0.21555	0.00000	-0.10083	-0.00635	0.02063
39	C3	PY	0.04336	0.00000	-0.03453	-0.18246	-0.00068
40	C3	PZ	0.00000	-0.00444	0.00000	0.00000	0.00000
41	C3	S	1.16356	0.00000	-0.37156	0.64553	2.49330
42	C3	PX	-0.63667	0.00000	0.01213	0.24956	-0.29754
43	C3	PY	-1.04549	0.00000	0.16556	0.27177	-0.71765
44	C3	PZ	0.00000	0.03084	0.00000	0.00000	0.00000
45	C3	DXX	-0.31491	0.00000	0.13479	-0.09564	-0.51703
46	C3	DYY	0.32801	0.00000	-0.14464	0.04557	0.37045
47	C3	DZZ	-0.16996	0.00000	0.03772	-0.16649	-0.39417
48	C3	DXY	-0.16663	0.00000	0.10350	-0.28506	0.02189
49	C3	DXZ	0.00000	-0.00544	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00605	0.00000	0.00000	0.00000
51	C4	S	0.01782	0.00000	0.01042	-0.03835	-0.00276
52	C4	S	-0.29156	0.00000	-0.06824	0.25686	-0.13951
53	C4	PX	-0.22311	0.00000	0.16722	-0.11911	-0.08903
54	C4	PY	-0.01447	0.00000	-0.15586	0.08441	0.09410
55	C4	PZ	0.00000	-0.02358	0.00000	0.00000	0.00000
56	C4	S	0.13151	0.00000	0.09312	0.23315	0.56294
57	C4	PX	0.78630	0.00000	-0.11947	0.23658	0.38576
58	C4	PY	-0.47668	0.00000	0.01132	0.34802	-0.34398
59	C4	PZ	0.00000	0.01585	0.00000	0.00000	0.00000
60	C4	DXX	0.16049	0.00000	0.00462	-0.38714	-0.05322
61	C4	DYY	-0.10402	0.00000	0.08647	0.21303	0.04442
62	C4	DZZ	0.13309	0.00000	0.02062	-0.21133	0.00865
63	C4	DXY	0.33953	0.00000	-0.42773	-0.11679	0.20640
64	C4	DXZ	0.00000	0.03387	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	-0.09218	0.00000	0.00000	0.00000
66	C5	S	0.00353	0.00000	0.01350	-0.05711	0.01481
67	C5	S	0.06969	0.00000	-0.13683	0.26443	-0.05527
68	C5	PX	-0.14079	0.00000	0.13612	-0.05548	0.02111
69	C5	PY	-0.18424	0.00000	0.07632	0.21217	-0.12053
70	C5	PZ	0.00000	0.00408	0.00000	0.00000	0.00000
71	C5	S	-0.08536	0.00000	-0.00694	0.57427	-0.38136
72	C5	PX	0.36684	0.00000	-0.06941	0.04931	0.16441
73	C5	PY	0.47101	0.00000	-0.21495	0.09315	0.28421
74	C5	PZ	0.00000	-0.01602	0.00000	0.00000	0.00000
75	C5	DXX	-0.29463	0.00000	0.29226	-0.03921	-0.08136
76	C5	DYY	0.40371	0.00000	-0.29712	0.00568	0.08390
77	C5	DZZ	-0.02178	0.00000	0.09410	-0.30115	0.07367
78	C5	DXY	-0.01983	0.00000	0.08344	-0.31659	0.19302
79	C5	DXZ	0.00000	0.00036	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.01242	0.00000	0.00000	0.00000
81	C6	S	0.01174	0.00000	0.00114	-0.01667	0.00679
82	C6	S	-0.03211	0.00000	0.03766	0.06404	0.11738
83	C6	PX	0.14618	0.00000	-0.09801	0.08441	0.07618
84	C6	PY	0.03218	0.00000	0.00842	-0.04223	0.07304
85	C6	PZ	0.00000	0.00129	0.00000	0.00000	0.00000
86	C6	S	-0.57866	0.00000	-0.03019	0.37994	-0.90544
87	C6	PX	-0.95566	0.00000	0.22587	-0.04892	-0.83661
88	C6	PY	-0.13015	0.00000	0.02429	-0.09758	0.15435
89	C6	PZ	0.00000	-0.01617	0.00000	0.00000	0.00000

90	C6	DXX	0.16254	0.00000	-0.06380	-0.08622	0.01576
91	C6	DYY	-0.20778	0.00000	0.08405	0.04323	-0.09684
92	C6	DZZ	0.05468	0.00000	0.00455	-0.08785	0.03439
93	C6	DXY	0.42157	0.00000	-0.21106	-0.02602	0.06040
94	C6	DXZ	0.00000	-0.00416	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	-0.00143	0.00000	0.00000	0.00000
96	C7	S	0.01627	0.00000	0.01213	0.01764	0.12393
97	C7	S	-0.05967	0.00000	-0.05777	-0.18601	-0.52593
98	C7	PX	0.10101	0.00000	-0.14480	0.04996	-0.50752
99	C7	PY	-0.09597	0.00000	0.05669	-0.12849	-0.09881
100	C7	PZ	0.00000	0.00098	0.00000	0.00000	0.00000
101	C7	S	-1.01012	0.00000	0.10279	-0.23357	-2.54037
102	C7	PX	0.64453	0.00000	-0.19334	-0.01940	0.65015
103	C7	PY	0.08204	0.00000	0.03575	-0.09894	-0.08237
104	C7	PZ	0.00000	-0.00900	0.00000	0.00000	0.00000
105	C7	DXX	-0.00673	0.00000	-0.11605	-0.00446	-0.73029
106	C7	DYY	-0.08285	0.00000	0.14599	0.00188	0.76712
107	C7	DZZ	0.08711	0.00000	0.06831	0.10202	0.65335
108	C7	DXY	0.24648	0.00000	-0.08236	0.14791	0.40053
109	C7	DXZ	0.00000	-0.00042	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00065	0.00000	0.00000	0.00000
111	O1	S	-0.02174	0.00000	0.03003	0.05677	-0.00424
112	O1	S	-0.06448	0.00000	0.01854	0.04798	-0.03224
113	O1	PX	0.00361	0.00000	-0.00308	-0.00381	0.00440
114	O1	PY	-0.00608	0.00000	0.02153	0.05499	0.01552
115	O1	PZ	0.00000	-0.01481	0.00000	0.00000	0.00000
116	O1	S	0.46037	0.00000	-0.41479	-0.81581	0.16300
117	O1	PX	-0.19866	0.00000	-0.15781	0.06650	-0.01149
118	O1	PY	-0.17270	0.00000	-0.18847	0.23186	0.06597
119	O1	PZ	0.00000	0.06877	0.00000	0.00000	0.00000
120	O1	DXX	-0.11208	0.00000	-0.01397	0.25300	0.03996
121	O1	DYY	0.09899	0.00000	0.18524	-0.03604	-0.05822
122	O1	DZZ	-0.13145	0.00000	0.05067	0.21649	-0.01375
123	O1	DXY	0.17386	0.00000	-0.32174	-0.17195	0.13234
124	O1	DXZ	0.00000	-0.05729	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	-0.14977	0.00000	0.00000	0.00000
126	H4	S	-0.03565	0.00000	0.09228	-0.28875	0.13253
127	H4	S	-0.02751	0.00000	0.08881	-0.17269	0.04526
128	H4	PX	-0.17361	0.00000	0.20173	-0.31169	0.08410
129	H4	PY	-0.09448	0.00000	0.01729	0.21885	-0.15207
130	H4	PZ	0.00000	-0.00199	0.00000	0.00000	0.00000
131	N1	S	0.03613	0.00000	-0.01552	0.00697	0.00294
132	N1	S	-0.02891	0.00000	0.02441	-0.06368	0.00404
133	N1	PX	-0.00442	0.00000	-0.00504	0.00495	-0.02371
134	N1	PY	0.09936	0.00000	-0.02682	-0.04401	0.05013
135	N1	PZ	0.00000	-0.00040	0.00000	0.00000	0.00000
136	N1	S	-0.45477	0.00000	0.21232	-0.03638	0.06202
137	N1	PX	0.06841	0.00000	-0.00279	0.07758	0.00096
138	N1	PY	0.05631	0.00000	-0.04246	-0.12230	-0.05502
139	N1	PZ	0.00000	0.00420	0.00000	0.00000	0.00000
140	N1	DXX	0.07134	0.00000	-0.04745	0.08152	-0.16173
141	N1	DYY	0.11243	0.00000	-0.03556	-0.01497	0.18733
142	N1	DZZ	0.11176	0.00000	-0.04451	0.01490	0.01002
143	N1	DXY	0.38257	0.00000	-0.16928	-0.09427	-0.08285

144	N1	DXZ	0.00000	0.00090	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00052	0.00000	0.00000	0.00000
146	H6	S	0.00939	0.00000	-0.10995	0.43963	-0.08729
147	H6	S	0.05698	0.00000	-0.08930	0.27649	-0.04669
148	H6	PX	0.06245	0.00000	-0.17682	0.57221	-0.11630
149	H6	PY	-0.21893	0.00000	0.08216	0.15956	-0.06658
150	H6	PZ	0.00000	-0.00093	0.00000	0.00000	0.00000
151	C8	S	-0.02899	0.00000	0.00185	0.00975	-0.02446
152	C8	S	-0.20518	0.00000	0.08719	-0.03861	0.05164
153	C8	PX	-0.12877	0.00000	0.04285	0.00961	-0.03294
154	C8	PY	0.17401	0.00000	-0.06634	-0.06549	-0.21778
155	C8	PZ	0.00000	0.00006	0.00000	0.00000	0.00000
156	C8	S	1.26456	0.00000	-0.25488	-0.13479	0.81944
157	C8	PX	0.11475	0.00000	0.05854	0.15057	0.22129
158	C8	PY	-0.04178	0.00000	-0.01010	0.02830	0.80860
159	C8	PZ	0.00000	0.00053	0.00000	0.00000	0.00000
160	C8	DXX	0.24312	0.00000	-0.13852	-0.07676	-0.27063
161	C8	DYY	-0.28171	0.00000	0.13652	0.09150	0.28297
162	C8	DZZ	-0.12210	0.00000	0.00125	0.03945	-0.13307
163	C8	DXY	0.08833	0.00000	-0.05437	0.00635	-0.42037
164	C8	DXZ	0.00000	0.00168	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	-0.00035	0.00000	0.00000	0.00000
166	H8	S	0.00072	0.00000	0.12414	0.05181	0.73192
167	H8	S	-0.17716	0.00000	0.12712	0.02112	0.24212
168	H8	PX	-0.02342	0.00000	-0.16475	-0.05007	-0.95600
169	H8	PY	-0.13100	0.00000	0.06528	-0.03212	-0.00717
170	H8	PZ	0.00000	0.00216	0.00000	0.00000	0.00000
171	C10	S	0.06815	0.00000	-0.01885	-0.00686	-0.02857
172	C10	S	-0.31628	0.00000	0.06674	0.02482	0.02399
173	C10	PX	-0.08883	0.00000	0.03634	-0.08219	0.32525
174	C10	PY	0.40527	0.00000	-0.14451	-0.08390	-0.25392
175	C10	PZ	0.00000	-0.00032	0.00000	0.00000	0.00000
176	C10	S	-1.00652	0.00000	0.22597	0.09216	0.56594
177	C10	PX	-0.02733	0.00000	0.00653	-0.12838	0.02184
178	C10	PY	-0.12520	0.00000	0.00518	-0.03403	0.08364
179	C10	PZ	0.00000	0.00037	0.00000	0.00000	0.00000
180	C10	DXX	-0.47623	0.00000	0.14443	0.01262	0.38577
181	C10	DYY	0.38702	0.00000	-0.15028	-0.01738	-0.47863
182	C10	DZZ	0.37661	0.00000	-0.09496	-0.03491	-0.12158
183	C10	DXY	-0.20115	0.00000	0.06051	0.15413	-0.27076
184	C10	DXZ	0.00000	0.00018	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	-0.00032	0.00000	0.00000	0.00000
186	H16	S	0.34076	0.00000	-0.09643	0.05304	-0.34964
187	H16	S	0.24068	0.00000	-0.07155	0.03543	-0.17729
188	H16	PX	-0.40442	0.00000	0.11145	-0.05872	0.41377
189	H16	PY	0.30485	0.00000	-0.09193	-0.01547	-0.18972
190	H16	PZ	0.00000	-0.00013	0.00000	0.00000	0.00000
191	H18	S	0.31086	0.00000	-0.07886	-0.12254	0.09833
192	H18	S	0.20822	0.00000	-0.05820	-0.09852	0.00097
193	H18	PX	0.23677	0.00000	-0.05342	-0.10821	0.18093
194	H18	PY	0.42954	0.00000	-0.11291	-0.10738	-0.00558
195	H18	PZ	0.00000	-0.00020	0.00000	0.00000	0.00000
196	C9	S	0.00446	0.00000	0.00489	0.00023	0.00156
197	C9	S	-0.05035	0.00000	-0.11121	0.01756	0.02525

198	C9	PX	0.22494	0.00000	0.22789	0.02425	0.02421
199	C9	PY	-0.39396	0.00000	-0.72340	-0.05344	0.06142
200	C9	PZ	0.00000	-0.93616	0.00000	0.00000	0.00000
201	C9	S	0.01718	0.00000	0.20625	0.05685	-0.07997
202	C9	PX	0.11032	0.00000	0.09555	-0.01239	0.01638
203	C9	PY	-0.32189	0.00000	-0.62238	0.07837	0.10418
204	C9	PZ	0.00000	-0.55713	0.00000	0.00000	0.00000
205	C9	DXX	0.06524	0.00000	0.46152	0.10463	-0.09004
206	C9	DYY	-0.48476	0.00000	-1.01742	-0.11797	0.09306
207	C9	DZZ	0.42974	0.00000	0.65516	0.02691	-0.03130
208	C9	DXY	0.08953	0.00000	0.10217	-0.07092	-0.02453
209	C9	DXZ	0.00000	-1.10350	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.49943	0.00000	0.00000	0.00000
211	H3	S	0.40557	0.00000	0.74563	0.02812	-0.06534
212	H3	S	0.29232	0.00000	0.52271	-0.03563	-0.06350
213	H3	PX	0.04819	0.00000	0.19897	0.05916	-0.02394
214	H3	PY	-0.56000	0.00000	-1.00211	-0.04927	0.08310
215	H3	PZ	0.00000	-0.00307	0.00000	0.00000	0.00000
216	H5	S	-0.19784	-0.71098	-0.35269	-0.01789	0.03059
217	H5	S	-0.10270	-0.44057	-0.19370	-0.05420	0.02038
218	H5	PX	0.15861	0.50274	0.20699	0.00201	-0.00728
219	H5	PY	-0.05918	-0.25740	-0.08314	-0.00525	0.00027
220	H5	PZ	-0.18438	-0.81389	-0.35222	-0.06184	0.02568
221	H7	S	-0.19784	0.71098	-0.35269	-0.01789	0.03059
222	H7	S	-0.10270	0.44057	-0.19370	-0.05420	0.02038
223	H7	PX	0.15861	-0.50274	0.20699	0.00201	-0.00728
224	H7	PY	-0.05918	0.25740	-0.08314	-0.00525	0.00027
225	H7	PZ	0.18438	-0.81389	0.35222	0.06184	-0.02568

MO:	211	212	213	214	215
Eigenvalues:	4.01961	4.19924	4.46531	4.49945	4.55630
(ev):	109.37924	114.26708	121.50731	122.43635	123.98333

		A	A	A	A	A	
1	H1	S	0.05238	0.42060	-0.06761	-0.09032	-0.03515
2	H1	S	0.01356	0.32660	-0.14795	0.02661	-0.03198
3	H1	PX	-0.06556	-0.43544	0.01258	0.02020	0.00685
4	H1	PY	-0.01971	-0.19557	0.05414	-0.01975	-0.01138
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	0.01999	0.04512	0.06293	0.16187	0.03114
7	C1	S	-0.04619	-0.27769	-0.29317	-1.19692	-0.17674
8	C1	PX	-0.05582	-0.30012	-0.00676	0.11692	-0.00723
9	C1	PY	0.06887	-0.08434	0.10595	-0.10577	-0.06703
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.37984	-0.05877	-0.51838	0.08766	0.06404
12	C1	PX	0.08708	-0.50947	0.61954	-0.06755	-0.00018
13	C1	PY	0.18770	0.13066	-0.38015	0.65409	0.33653
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	0.01559	-0.40195	0.26057	0.52667	0.07609
16	C1	DYY	0.02539	0.60482	0.08740	0.72219	0.14779
17	C1	DZZ	0.07429	0.21936	0.22961	0.65584	0.13701
18	C1	DXY	-0.10868	-0.36305	-0.07794	0.04189	0.05479
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000

21	C2	S	-0.03254	-0.07363	0.11051	0.07582	-0.22201
22	C2	S	0.13303	0.35253	-0.74492	-0.52691	1.41148
23	C2	PX	-0.11047	-0.32000	-0.05947	-0.03800	0.10979
24	C2	PY	-0.12884	-0.19698	0.05785	-0.06610	-0.00394
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.31091	0.57541	-0.17422	-0.02858	0.81783
27	C2	PX	0.05714	-0.25511	-0.05617	0.07850	0.07984
28	C2	PY	0.13701	-0.19040	0.05197	0.01583	-0.17378
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	0.18451	0.40217	0.41835	0.28124	-0.92516
31	C2	DYY	-0.25284	-0.70467	0.47280	0.24147	-0.83209
32	C2	DZZ	-0.15799	-0.34741	0.43214	0.30145	-0.83647
33	C2	DXY	0.11911	0.49278	0.07797	-0.02098	-0.13922
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.03354	0.03721	0.22553	0.01669	-0.00069
37	C3	S	-0.09321	-0.12448	-1.52284	-0.16268	0.02789
38	C3	PX	-0.05431	0.08836	0.03605	-0.00775	-0.15385
39	C3	PY	0.06655	-0.16434	0.05906	-0.07350	0.10518
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.65074	-0.59460	-0.22710	0.71858	-0.07820
42	C3	PX	-0.11892	0.47811	-0.62781	0.35906	0.86752
43	C3	PY	-0.33187	0.24652	-0.30534	-0.29222	-0.28731
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	-0.16359	0.16446	0.80085	0.09009	0.04776
46	C3	DYY	0.08562	-0.02752	0.93418	0.02692	-0.16576
47	C3	DZZ	-0.12379	0.13589	0.89966	0.06567	0.02166
48	C3	DXY	0.06089	-0.48724	-0.02334	-0.08949	0.09120
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00436	-0.00375	-0.02745	0.24471	0.02087
52	C4	S	-0.10246	0.03484	0.03021	-1.68713	-0.18352
53	C4	PX	0.00466	0.01836	-0.04067	0.03539	-0.02618
54	C4	PY	0.06286	0.15536	0.03116	0.19308	0.00069
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.21485	-0.01328	0.91840	-1.25031	-0.38393
57	C4	PX	-0.01885	-0.20606	0.37129	-0.82026	-0.41615
58	C4	PY	-0.09793	0.53027	-0.36590	-0.91350	-0.58718
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.09138	-0.56634	-0.07325	0.83555	0.14058
61	C4	DYY	0.12945	0.42866	-0.08616	1.25198	0.13297
62	C4	DZZ	0.01646	-0.04352	-0.09662	0.97941	0.10906
63	C4	DXY	0.09569	0.09651	0.05211	-0.12535	-0.04021
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	0.02315	0.03976	-0.00807	0.22534	-0.06199
67	C5	S	-0.12148	-0.17299	0.05796	-1.38566	0.61563
68	C5	PX	0.07803	0.21768	0.01758	-0.08912	-0.01496
69	C5	PY	-0.15886	-0.30873	0.05657	0.03795	-0.13449
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	-0.41042	-0.37465	-0.05383	-0.99791	-0.34589
72	C5	PX	0.07477	0.20863	-0.05074	-0.40540	-0.34855
73	C5	PY	-0.00342	-0.26822	0.23193	0.17674	0.23719
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

75	C5	DXX	-0.00571	0.11468	-0.05639	0.84479	-0.32066
76	C5	DYY	0.05003	0.00874	-0.11059	0.90651	-0.24310
77	C5	DZZ	0.11939	0.20612	-0.02683	0.86193	-0.24736
78	C5	DXY	0.32048	0.83126	-0.00444	-0.12804	0.00947
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.01696	-0.00645	0.18480	-0.00099	-0.23363
82	C6	S	0.12234	-0.05298	-1.09991	-0.05776	1.31616
83	C6	PX	-0.03291	-0.03362	-0.05681	0.01765	-0.05894
84	C6	PY	-0.09705	0.19202	-0.23172	-0.03329	0.07959
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	-0.39371	0.13958	-2.24508	0.21419	0.28892
87	C6	PX	-0.49657	0.56608	-0.43436	0.04325	0.78034
88	C6	PY	-0.31092	0.25014	0.97916	0.15625	0.75503
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.04410	0.43170	0.58175	-0.02206	-0.79131
91	C6	DYY	0.03900	-0.39870	0.91161	0.02741	-0.96278
92	C6	DZZ	0.02936	0.01322	0.72441	-0.01041	-0.86131
93	C6	DXY	0.10864	-0.20361	0.03490	0.00351	-0.05320
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.07185	-0.05628	0.16091	-0.00690	0.16726
97	C7	S	-0.29192	0.22557	-1.12748	0.14890	-1.03616
98	C7	PX	-0.06768	0.17838	0.09264	0.01377	0.05661
99	C7	PY	0.15070	-0.19337	-0.11562	-0.04993	0.08142
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.61883	0.57561	-0.22347	-0.83128	-0.49679
102	C7	PX	0.65247	-0.08131	-0.11361	0.43866	0.04054
103	C7	PY	0.01226	-0.16872	0.39227	-0.10957	-0.57377
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.24434	0.17728	0.67985	-0.06044	0.76859
106	C7	DYY	0.30826	-0.44821	0.56582	-0.11399	0.61964
107	C7	DZZ	0.32297	-0.23907	0.64082	-0.03516	0.61664
108	C7	DXY	-0.19324	0.11906	0.07442	0.01787	-0.15719
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	0.00788	0.04304	0.02189	-0.30999	-0.14067
112	O1	S	-0.03432	-0.02952	0.01443	-0.29474	-0.14924
113	O1	PX	0.00129	-0.01209	0.01159	-0.10694	-0.04640
114	O1	PY	0.02632	0.09279	-0.00872	0.16350	0.04107
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.00284	-0.56689	-0.21340	3.76790	1.80192
117	O1	PX	0.03887	0.18628	-0.08698	0.53648	0.22410
118	O1	PY	0.07617	0.33040	0.02472	-0.23892	-0.23820
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	0.08159	0.29480	0.07141	-0.94077	-0.45566
121	O1	DYY	-0.04544	-0.11730	0.07566	-1.21863	-0.44666
122	O1	DZZ	0.02575	0.12811	0.07856	-1.04829	-0.48461
123	O1	DXY	0.06685	0.02756	0.02196	-0.06374	-0.03226
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.22385	0.50903	0.00094	-0.20086	0.02974
127	H4	S	0.13849	0.29796	-0.07197	-0.03274	-0.18423
128	H4	PX	0.18874	0.41591	0.00861	-0.10504	0.03014

129	H4	PY	-0.19603	-0.37822	-0.02558	0.13864	-0.00134
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	-0.01223	0.00140	-0.34702	0.02680	-0.06725
132	N1	S	0.10594	0.13094	0.28687	-0.04322	0.09092
133	N1	PX	0.11167	-0.02741	-0.15981	0.01099	-0.06525
134	N1	PY	-0.03901	0.18457	-0.20052	-0.00132	0.12438
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-0.05925	-0.04821	4.42827	-0.25263	1.06290
137	N1	PX	0.26939	-0.29924	0.86802	-0.10374	-0.14208
138	N1	PY	-0.36115	0.31523	0.54607	-0.04736	0.60450
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.23748	-0.20333	-1.04354	0.08676	-0.36600
141	N1	DYY	-0.24407	0.22959	-1.16156	0.07326	-0.01533
142	N1	DZZ	-0.02881	0.00515	-1.10089	0.09095	-0.21733
143	N1	DXY	0.00259	0.06411	0.02702	-0.02515	0.07938
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	-0.18256	-0.50238	-0.08590	-0.02774	0.18270
147	H6	S	-0.05331	-0.30603	0.03516	0.05986	-0.14565
148	H6	PX	-0.22448	-0.53618	-0.05925	-0.01748	0.15721
149	H6	PY	-0.06795	-0.14587	-0.02667	0.01034	0.03025
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.02125	0.00373	0.05600	-0.01328	0.22719
152	C8	S	0.00917	0.00839	-0.47320	0.03205	-1.40937
153	C8	PX	0.02347	-0.05968	-0.12728	0.01893	-0.05201
154	C8	PY	-0.06597	0.05703	0.01759	-0.00490	0.05432
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.46260	-0.03588	-0.80560	0.42349	-0.77918
157	C8	PX	0.59320	-0.38131	1.01949	0.04977	-0.39607
158	C8	PY	0.63985	-0.05400	-0.40167	0.32567	-0.31359
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.34037	0.20348	0.36855	-0.04595	0.93621
161	C8	DYY	0.31135	-0.17232	0.14782	-0.01243	0.81223
162	C8	DZZ	-0.08884	0.01366	0.26245	-0.04932	0.87388
163	C8	DXY	0.54789	-0.12296	-0.11313	0.01978	-0.07895
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	0.21110	-0.21033	-0.10048	-0.00764	-0.17952
167	H8	S	-0.04600	-0.11455	0.13187	-0.11605	0.04454
168	H8	PX	-0.27900	0.24804	0.08306	-0.00346	0.16293
169	H8	PY	0.11133	-0.05603	-0.03499	-0.00304	0.06147
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	0.00273	0.00251	0.06266	-0.00949	0.14411
172	C10	S	-0.02826	0.01936	-0.37344	0.07356	-1.03245
173	C10	PX	-0.66643	0.09712	0.00442	0.00573	0.03998
174	C10	PY	-0.20270	0.09686	0.00485	0.00441	-0.13293
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.22659	-0.00831	-0.41056	0.11917	-0.32244
177	C10	PX	-0.63937	0.12325	-0.21821	-0.08952	0.11720
178	C10	PY	-0.08717	0.05896	-0.15835	0.00267	0.07726
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.35242	0.03256	0.23775	-0.04356	0.66984
181	C10	DYY	0.35324	-0.01470	0.22984	-0.04810	0.55412
182	C10	DZZ	0.02019	0.00544	0.25101	-0.03585	0.54174

183	C10	DXY	1.13664	-0.24974	-0.08317	0.00231	0.00663
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.64166	-0.10022	-0.02476	0.01855	-0.12642
187	H16	S	0.33609	-0.03704	0.10428	0.02219	0.04429
188	H16	PX	-0.74491	0.11376	0.04591	-0.00619	0.09459
189	H16	PY	0.08201	0.01810	0.00859	0.00260	-0.01655
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	-0.68099	0.13862	0.00024	-0.00378	-0.09496
192	H18	S	-0.37589	0.08352	-0.04942	-0.03903	0.15639
193	H18	PX	-0.67291	0.13016	-0.00405	0.00329	-0.05655
194	H18	PY	-0.42637	0.08859	0.02605	0.00426	-0.04170
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.00292	0.01130	0.00487	-0.07958	-0.02992
197	C9	S	-0.00740	-0.08705	-0.03635	0.45887	0.17939
198	C9	PX	0.02418	0.06893	0.00023	-0.03155	-0.01291
199	C9	PY	0.04680	0.07240	0.00125	0.05252	0.00922
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-0.05380	-0.10988	0.06452	-0.56474	-0.24850
202	C9	PX	0.00913	0.04618	-0.01730	0.26417	0.09877
203	C9	PY	0.07192	0.09396	-0.03955	0.06331	0.04008
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.04568	-0.00834	0.00288	-0.16729	-0.05081
206	C9	DYY	0.06795	0.09321	0.02603	-0.31244	-0.13468
207	C9	DZZ	-0.01609	0.02582	0.02905	-0.43285	-0.15698
208	C9	DXY	-0.03038	-0.09392	-0.00212	0.04006	0.02405
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.04774	-0.06284	-0.00650	0.10588	0.05090
212	H3	S	-0.04305	-0.04268	0.00993	0.03247	0.01716
213	H3	PX	-0.00914	0.01227	-0.00402	0.04407	0.01424
214	H3	PY	0.05857	0.07393	0.00370	-0.02470	-0.02433
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.02019	0.01318	-0.01453	0.12670	0.04988
217	H5	S	0.01100	-0.00880	0.00125	0.03032	0.01902
218	H5	PX	-0.00938	-0.01180	0.00432	-0.07579	-0.02415
219	H5	PY	0.00234	0.00417	-0.00085	0.02840	0.00543
220	H5	PZ	0.01291	-0.01067	-0.00189	0.05548	0.02051
221	H7	S	0.02019	0.01318	-0.01453	0.12670	0.04988
222	H7	S	0.01100	-0.00880	0.00125	0.03032	0.01902
223	H7	PX	-0.00938	-0.01180	0.00432	-0.07579	-0.02415
224	H7	PY	0.00234	0.00417	-0.00085	0.02840	0.00543
225	H7	PZ	-0.01291	0.01067	0.00189	-0.05548	-0.02051

MO:	216	217	218	219	220
Eigenvalues:	4.59956	4.67304	4.70236	4.83284	4.88374
(ev):	125.16054	127.15986	127.95773	131.50831	132.89343

		A	A	A	A	A	
1	H1	S	-0.23702	-0.16601	-0.10093	0.07080	-0.21583
2	H1	S	-0.00931	0.29199	0.00026	0.05627	-0.00724
3	H1	PX	0.17444	0.20987	0.07876	-0.04839	0.20319
4	H1	PY	0.09700	0.09270	0.02133	-0.05525	0.06766
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

6	C1	S	0.22343	0.16795	0.12073	-0.05839	0.22856
7	C1	S	-1.42321	-1.13744	-0.70925	0.25662	-1.27556
8	C1	PX	0.04287	0.08541	0.02106	0.02478	-0.00735
9	C1	PY	0.11549	0.13744	-0.00654	-0.03635	-0.07733
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.31807	-0.43618	-0.53642	0.57502	-1.72029
12	C1	PX	0.28932	-0.39508	0.16287	-0.37658	0.51530
13	C1	PY	-0.22476	-0.59465	0.25951	0.22574	0.17688
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	1.08640	0.95993	0.52779	-0.29664	1.05935
16	C1	DYY	0.76041	0.58369	0.46883	-0.14959	1.03708
17	C1	DZZ	0.84655	0.59650	0.46004	-0.20455	0.82433
18	C1	DXY	-0.02205	0.06129	-0.00314	0.03661	0.08725
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.18761	0.07713	-0.01431	0.05594	0.20479
22	C2	S	1.22312	-0.52336	0.19327	-0.31505	-1.15705
23	C2	PX	0.03966	-0.06708	-0.01033	-0.06408	0.02110
24	C2	PY	0.09869	-0.08269	0.15160	0.13203	0.07154
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	0.32372	-0.48718	-0.35597	0.27026	-1.45564
27	C2	PX	0.16691	-0.07137	-0.13398	0.25138	-0.55155
28	C2	PY	0.25386	0.30870	-0.02369	0.30788	-0.44133
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.84693	0.35837	-0.12992	0.28969	0.99797
31	C2	DYY	-0.67837	0.27481	0.00005	0.26367	0.96904
32	C2	DZZ	-0.72659	0.27167	-0.07066	0.18168	0.72728
33	C2	DXY	-0.03247	0.03215	0.08250	0.19464	0.05129
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	0.20885	0.10994	-0.05899	-0.07183	-0.19306
37	C3	S	-1.33722	-0.70541	0.38799	0.39964	1.21808
38	C3	PX	0.00214	0.00140	0.08414	0.01702	-0.05621
39	C3	PY	-0.07103	-0.09750	-0.14352	0.07309	-0.02630
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	0.03445	-0.68501	0.83563	1.09511	0.45288
42	C3	PX	-0.43950	-0.04198	-0.12515	0.12894	0.02863
43	C3	PY	-0.57256	0.50408	-0.07284	-0.03955	0.48535
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
45	C3	DXX	0.86781	0.45049	-0.27904	-0.34939	-0.74893
46	C3	DYY	0.83977	0.37835	-0.13241	-0.36148	-1.06712
47	C3	DZZ	0.80893	0.40979	-0.23002	-0.26199	-0.70670
48	C3	DXY	-0.03639	0.00383	-0.09388	-0.04419	0.05390
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	0.00572	0.04456	0.02070	0.06792	-0.02227
52	C4	S	-0.14780	-0.13260	-0.20119	-0.34050	0.03381
53	C4	PX	-0.15404	-0.04261	-0.09216	0.03161	-0.13913
54	C4	PY	0.05650	0.05701	0.02844	-0.01560	0.03527
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	0.03088	0.59373	-0.37235	-1.08016	0.45110
57	C4	PX	0.12397	0.66453	-0.06212	-0.43289	0.39796
58	C4	PY	-0.25562	1.65213	-0.34641	-0.00526	-0.21974
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

60	C4	DXX	0.11257	0.08827	0.16020	0.33976	-0.05545
61	C4	DYY	-0.07709	0.00284	0.05980	0.28043	-0.15458
62	C4	DZZ	0.04840	0.11247	0.09640	0.24084	-0.05926
63	C4	DXY	0.10032	0.11719	0.04748	-0.02110	0.10537
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.19065	0.05662	-0.17808	-0.16842	-0.14296
67	C5	S	1.17305	-0.64774	1.09261	0.95383	0.85926
68	C5	PX	-0.03799	-0.06620	0.01437	0.01512	0.08417
69	C5	PY	-0.06423	0.07587	-0.00255	0.04020	0.08751
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.37235	0.53776	0.66316	0.26837	1.27344
72	C5	PX	0.15225	0.71391	0.08389	0.26824	0.07745
73	C5	PY	0.01208	-0.49611	-0.08170	-0.03103	-0.30875
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.76796	0.32649	-0.75137	-0.71027	-0.63589
76	C5	DYY	-0.72151	0.36161	-0.81222	-0.81735	-0.82197
77	C5	DZZ	-0.73849	0.20112	-0.65903	-0.61452	-0.48817
78	C5	DXY	-0.01368	-0.08543	0.02731	0.05786	0.05804
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.00981	0.00425	0.13073	0.17498	-0.11369
82	C6	S	0.07306	-0.10131	-0.71158	-1.01782	0.59394
83	C6	PX	-0.09500	0.01025	0.01927	0.04688	0.07034
84	C6	PY	0.02477	0.04576	-0.04893	0.00192	-0.02914
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	0.00910	2.45219	-0.78808	0.92326	-0.28447
87	C6	PX	-0.60903	0.07322	-0.47914	-0.05260	0.21694
88	C6	PY	-0.44221	-1.42148	0.20905	-1.71882	1.01258
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	-0.10104	-0.02436	0.50674	0.76345	-0.36687
91	C6	DYY	0.05670	-0.04021	0.60112	0.74290	-0.55509
92	C6	DZZ	0.01018	-0.00805	0.48072	0.61777	-0.38834
93	C6	DXY	-0.09288	-0.07837	0.00757	-0.02720	0.13663
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.00870	0.03577	-0.25576	0.10037	-0.01818
97	C7	S	-0.00776	-0.26321	1.63117	-0.46407	0.09228
98	C7	PX	0.03972	0.04914	-0.07919	0.03125	-0.04857
99	C7	PY	-0.15294	0.05404	-0.00790	0.09633	0.14459
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-0.77910	0.51992	0.40229	-0.88280	0.78622
102	C7	PX	0.54319	0.40822	0.00630	0.73908	-0.63494
103	C7	PY	0.33380	-0.28523	-0.00463	-0.35477	-0.00600
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	-0.02747	0.11113	-1.27872	0.43726	0.04081
106	C7	DYY	-0.03741	0.12216	-0.99848	0.31940	-0.02053
107	C7	DZZ	0.03235	0.12498	-0.95394	0.35207	-0.08335
108	C7	DXY	0.13214	-0.07160	0.06478	-0.14025	-0.17312
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.02841	0.30629	-0.06192	-0.00959	-0.00992
112	O1	S	-0.03270	0.42378	-0.08973	-0.08976	0.01571
113	O1	PX	-0.00639	0.08651	-0.01317	0.01191	-0.00203

114	O1	PY	0.00046	-0.09221	0.02333	0.04070	-0.01514
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	0.38070	-4.23414	0.86931	0.22036	0.14587
117	O1	PX	-0.02031	-0.44584	0.07920	0.24429	-0.15917
118	O1	PY	-0.13779	0.66237	-0.16846	-0.01482	-0.09894
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-0.12156	0.96785	-0.19648	0.13243	-0.12787
121	O1	DYY	-0.03260	0.91864	-0.17521	-0.04367	0.00664
122	O1	DZZ	-0.10487	1.06392	-0.21504	-0.06098	-0.02019
123	O1	DXY	-0.00791	0.02024	-0.00147	0.07985	-0.03983
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.11225	-0.05519	0.14563	0.17913	0.16749
127	H4	S	-0.05679	0.35752	-0.07228	0.04499	-0.04546
128	H4	PX	0.06183	-0.07908	0.10623	0.12439	0.13782
129	H4	PY	-0.04155	0.03928	-0.08104	-0.12226	-0.11381
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.08354	0.32783	-0.05731	0.19385	-0.14160
132	N1	S	-0.09199	-0.05407	0.01567	0.16417	0.03845
133	N1	PX	0.05388	0.05722	-0.02078	-0.01759	-0.05427
134	N1	PY	0.00816	0.09429	-0.08550	-0.03305	0.04110
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-1.11517	-5.37241	0.85244	-4.06551	2.54112
137	N1	PX	0.02295	-1.18051	0.27510	-0.89350	0.40758
138	N1	PY	-0.39299	-0.81665	-0.08781	-0.82270	0.63645
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.36194	0.77167	-0.13777	0.32614	-0.46444
141	N1	DYY	0.20741	0.91617	-0.25795	0.34350	-0.30390
142	N1	DZZ	0.26257	1.05857	-0.16806	0.66209	-0.44761
143	N1	DXY	-0.03213	0.00383	-0.05729	0.02178	0.08504
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.19035	-0.05189	0.01301	-0.08547	-0.23025
147	H6	S	0.00514	0.09539	-0.03824	0.10716	-0.08060
148	H6	PX	0.13605	-0.06020	0.00213	-0.11403	-0.20134
149	H6	PY	0.03208	-0.02882	0.00424	-0.04167	-0.06211
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	-0.15084	0.16390	-0.02370	0.15775	0.11415
152	C8	S	0.91522	-1.03423	-0.00453	-0.96729	-0.62044
153	C8	PX	0.04814	0.02600	0.01005	-0.01009	0.00131
154	C8	PY	-0.10497	0.02947	0.21523	-0.09822	-0.08522
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.93127	0.64352	0.06198	0.43864	-1.37084
157	C8	PX	0.25139	-1.56695	0.33203	-0.98218	0.30543
158	C8	PY	0.54209	0.86153	0.03900	0.89092	-0.73896
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	-0.63862	0.57649	-0.07013	0.67931	0.53040
161	C8	DYY	-0.51877	0.72134	-0.10275	0.79495	0.55356
162	C8	DZZ	-0.58103	0.59326	-0.05543	0.55504	0.40936
163	C8	DXY	0.02656	-0.03422	0.12713	-0.08655	-0.02481
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.00180	-0.12087	0.27993	-0.16621	0.00298
167	H8	S	-0.13230	-0.23539	-0.11884	-0.20858	0.17791

168	H8	PX	-0.02840	0.03460	-0.26200	0.10948	0.04597
169	H8	PY	-0.04558	0.03204	0.01786	0.02466	0.02014
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.17145	0.11681	0.28615	-0.10806	-0.14820
172	C10	S	1.15690	-0.88498	-1.78566	0.61256	0.90562
173	C10	PX	-0.02157	0.02057	0.00238	0.01321	0.01245
174	C10	PY	0.09383	-0.16419	-0.02108	-0.11004	-0.04015
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	0.56679	0.36499	-0.92199	0.98859	0.26158
177	C10	PX	-0.12299	0.50031	-0.14692	0.30103	-0.08463
178	C10	PY	0.01449	0.38533	-0.14687	0.30326	-0.03250
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.78854	0.62460	1.32665	-0.49590	-0.76275
181	C10	DYY	-0.70612	0.44062	1.28688	-0.61176	-0.74012
182	C10	DZZ	-0.64096	0.42342	1.04785	-0.37656	-0.50747
183	C10	DXY	-0.01251	0.08550	0.04390	0.03826	-0.00523
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	0.14073	-0.18207	-0.19152	0.04038	0.15849
187	H16	S	-0.05472	-0.09818	0.20777	-0.18720	-0.04903
188	H16	PX	-0.11586	0.08662	0.20409	-0.09337	-0.14652
189	H16	PY	0.02565	-0.03635	-0.06475	0.03210	0.05307
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.11504	-0.08872	-0.25285	0.11579	0.13525
192	H18	S	-0.14119	0.27903	0.08047	0.04618	-0.10210
193	H18	PX	0.08603	-0.06932	-0.19088	0.07837	0.11056
194	H18	PY	0.06744	-0.08711	-0.14997	0.05747	0.10958
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	-0.00942	0.07415	-0.05039	-0.31279	0.13478
197	C9	S	0.02628	-0.47960	0.30243	1.79162	-0.75850
198	C9	PX	-0.01958	0.00203	-0.01503	-0.00527	-0.01631
199	C9	PY	0.00294	-0.01282	0.00145	0.00964	-0.00665
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	0.03700	0.51542	0.04841	1.19174	-0.53494
202	C9	PX	-0.01943	-0.22675	0.01835	0.05833	-0.06863
203	C9	PY	-0.05574	-0.14440	0.02342	-0.10667	0.06237
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	-0.01334	0.17870	-0.17734	-1.28943	0.56455
206	C9	DYY	-0.02663	0.36710	-0.21508	-1.33828	0.58301
207	C9	DZZ	-0.04728	0.36473	-0.24007	-1.36087	0.56716
208	C9	DXY	0.02284	-0.03469	0.02382	0.04139	-0.00065
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	0.01234	-0.12238	0.04237	0.20883	-0.09203
212	H3	S	0.02296	-0.01248	-0.02796	-0.16867	0.06123
213	H3	PX	0.00101	-0.02439	0.00955	0.04760	-0.02109
214	H3	PY	-0.00907	0.07541	-0.03427	-0.21223	0.09395
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	0.00165	-0.11447	0.04554	0.17447	-0.07017
217	H5	S	0.00925	-0.03190	-0.00912	-0.24676	0.13651
218	H5	PX	-0.00526	0.04561	-0.02418	-0.11078	0.04381
219	H5	PY	0.00700	-0.00144	0.01160	0.07179	-0.02718
220	H5	PZ	0.01224	-0.04430	0.03577	0.16701	-0.05924
221	H7	S	0.00165	-0.11447	0.04554	0.17447	-0.07017

222	H7	S	0.00925	-0.03190	-0.00912	-0.24676	0.13651
223	H7	PX	-0.00526	0.04561	-0.02418	-0.11078	0.04381
224	H7	PY	0.00700	-0.00144	0.01160	0.07179	-0.02718
225	H7	PZ	-0.01224	0.04430	-0.03577	-0.16701	0.05924

MO:		221	222	223	224	225
Eigenvalues:		4.89251	4.92769	5.06080	5.28515	0.00000
(ev):		133.13204	134.08936	137.71148	143.81642	0.00000

		A	A	A	A	A	
1	H1	S	0.09346	-0.06041	0.06639	-0.21002	0.00000
2	H1	S	0.04702	-0.10299	-0.11770	0.05064	0.00000
3	H1	PX	-0.10617	0.01232	-0.07722	0.21722	0.00000
4	H1	PY	-0.06427	0.00144	-0.03359	0.06089	0.00000
5	H1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
6	C1	S	-0.08281	0.03569	-0.04754	0.17578	0.00000
7	C1	S	0.47862	-0.12461	0.36196	-1.08680	0.00000
8	C1	PX	-0.00939	-0.15496	0.06027	-0.08382	0.00000
9	C1	PY	-0.04214	0.15465	-0.12731	-0.03084	0.00000
10	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
11	C1	S	-0.33368	-0.88738	-0.35963	-0.77295	0.00000
12	C1	PX	-0.18921	0.38004	0.32227	0.26037	0.00000
13	C1	PY	1.04042	0.80883	0.02492	-0.11260	0.00000
14	C1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
15	C1	DXX	-0.42772	0.25985	-0.39589	1.00996	0.00000
16	C1	DYY	-0.32503	0.17235	-0.23743	1.06417	0.00000
17	C1	DZZ	-0.30377	0.11503	-0.16049	0.57514	0.00000
18	C1	DXY	-0.07650	-0.20896	0.09998	0.02774	0.00000
19	C1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
20	C1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
21	C2	S	-0.02437	0.19802	0.12539	-0.12073	0.00000
22	C2	S	0.42765	-0.96543	-0.80088	0.78448	0.00000
23	C2	PX	-0.04067	0.02161	-0.01137	-0.04662	0.00000
24	C2	PY	0.09087	0.00956	0.09658	-0.04038	0.00000
25	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
26	C2	S	-0.23847	-1.25845	-0.49613	0.54674	0.00000
27	C2	PX	-0.20649	-0.59415	0.10130	0.13753	0.00000
28	C2	PY	0.11268	0.00428	0.11199	0.49312	0.00000
29	C2	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
30	C2	DXX	-0.26847	0.91708	0.72894	-0.70034	0.00000
31	C2	DYY	-0.28255	0.73894	0.68465	-0.75367	0.00000
32	C2	DZZ	-0.09857	0.71030	0.41462	-0.39118	0.00000
33	C2	DXY	0.15299	0.07508	0.08880	0.02072	0.00000
34	C2	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
35	C2	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
36	C3	S	-0.00106	0.11886	-0.05102	-0.23896	0.00000
37	C3	S	-0.06705	-0.68532	0.14849	1.31333	0.00000
38	C3	PX	0.02836	-0.06362	-0.05113	-0.04128	0.00000
39	C3	PY	0.05840	0.03274	0.10010	0.11990	0.00000
40	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
41	C3	S	1.92839	0.77741	0.98672	3.54694	0.00000
42	C3	PX	0.92653	1.15505	-0.61171	-0.45155	0.00000
43	C3	PY	0.01278	-0.58529	0.44803	-1.49973	0.00000
44	C3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000

45	C3	DXX	-0.11252	0.49300	-0.11666	-0.99628	0.00000
46	C3	DYY	0.11879	0.54992	-0.32746	-1.42173	0.00000
47	C3	DZZ	0.00964	0.45045	-0.16608	-0.80478	0.00000
48	C3	DXY	-0.09812	-0.02578	0.06662	0.00518	0.00000
49	C3	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
50	C3	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
51	C4	S	-0.05296	-0.33158	0.15541	-0.16242	0.00000
52	C4	S	0.08884	1.70011	-0.98668	0.96792	0.00000
53	C4	PX	-0.00730	-0.07317	0.02185	-0.07101	0.00000
54	C4	PY	-0.01102	-0.03980	-0.00560	0.03009	0.00000
55	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
56	C4	S	-1.70585	-0.41176	-0.24861	0.79490	0.00000
57	C4	PX	-0.03679	-0.35053	0.32155	0.01884	0.00000
58	C4	PY	-1.32242	-2.80458	0.27834	-0.64663	0.00000
59	C4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
60	C4	DXX	-0.14618	-1.39938	0.82027	-0.89523	0.00000
61	C4	DYY	-0.07287	-1.52755	0.85078	-0.92386	0.00000
62	C4	DZZ	-0.14875	-1.09457	0.52801	-0.51989	0.00000
63	C4	DXY	-0.09316	0.05196	-0.05459	0.08533	0.00000
64	C4	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
65	C4	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
66	C5	S	-0.07279	-0.00762	-0.16721	0.11891	0.00000
67	C5	S	0.24223	-0.04684	1.00836	-0.76651	0.00000
68	C5	PX	-0.00013	0.12863	0.02194	-0.01775	0.00000
69	C5	PY	0.02754	0.11305	0.06007	-0.05061	0.00000
70	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
71	C5	S	0.64915	-0.08422	0.89446	-1.09936	0.00000
72	C5	PX	0.31477	-0.20223	0.23080	-0.03810	0.00000
73	C5	PY	-0.13743	0.21329	-0.08945	0.27026	0.00000
74	C5	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
75	C5	DXX	-0.18161	0.12279	-0.83276	0.68019	0.00000
76	C5	DYY	-0.22224	-0.13890	-0.91561	0.72201	0.00000
77	C5	DZZ	-0.25735	0.00963	-0.57765	0.38957	0.00000
78	C5	DXY	0.07328	0.19239	0.00689	0.03912	0.00000
79	C5	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
80	C5	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
81	C6	S	0.21712	-0.10956	-0.02869	0.17258	0.00000
82	C6	S	-1.30622	0.67355	0.33600	-0.94616	0.00000
83	C6	PX	0.01006	0.02866	0.05497	0.03664	0.00000
84	C6	PY	-0.00620	0.05163	0.05234	-0.03197	0.00000
85	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
86	C6	S	1.61407	2.29136	0.20874	-1.58260	0.00000
87	C6	PX	-0.12085	-0.00564	-0.44926	-1.27490	0.00000
88	C6	PY	-1.38513	-0.04505	-0.87342	-0.11920	0.00000
89	C6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
90	C6	DXX	0.94364	-0.54792	-0.19026	0.85472	0.00000
91	C6	DYY	1.03417	-0.58832	-0.33861	0.85364	0.00000
92	C6	DZZ	0.76754	-0.38966	-0.10778	0.58259	0.00000
93	C6	DXY	-0.09342	0.03984	0.02196	-0.07114	0.00000
94	C6	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
95	C6	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
96	C7	S	0.04941	0.03224	0.22165	0.19696	0.00000
97	C7	S	-0.01281	0.00915	-1.37657	-0.88369	0.00000
98	C7	PX	0.04173	0.03952	-0.00831	-0.06528	0.00000

99	C7	PY	0.02768	-0.08473	-0.00666	0.11046	0.00000
100	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
101	C7	S	-1.74996	-1.71308	-0.94904	-3.34480	0.00000
102	C7	PX	1.04456	0.78614	0.34438	1.50370	0.00000
103	C7	PY	-0.67554	-0.57788	0.26874	-0.07256	0.00000
104	C7	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
105	C7	DXX	0.05693	0.01688	1.31150	1.13803	0.00000
106	C7	DYY	0.02234	-0.00773	0.97939	0.80039	0.00000
107	C7	DZZ	0.16890	0.10434	0.77049	0.62722	0.00000
108	C7	DXY	-0.06143	0.05737	0.03050	-0.14478	0.00000
109	C7	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
110	C7	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
111	O1	S	-0.29479	-0.31360	0.00288	-0.00679	0.00000
112	O1	S	-0.40830	-0.72873	0.12183	-0.13395	0.00000
113	O1	PX	-0.09187	-0.05487	-0.00493	0.00594	0.00000
114	O1	PY	0.07987	0.03579	0.03988	-0.04355	0.00000
115	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
116	O1	S	4.30221	5.26465	-0.30448	0.43167	0.00000
117	O1	PX	0.10611	0.26452	-0.05632	-0.02207	0.00000
118	O1	PY	-0.86678	-1.44792	0.27550	-0.35403	0.00000
119	O1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
120	O1	DXX	-1.16238	-0.99111	-0.05036	0.00698	0.00000
121	O1	DYY	-0.86669	-0.50778	-0.21346	0.22990	0.00000
122	O1	DZZ	-0.96421	-1.17050	0.07947	-0.09158	0.00000
123	O1	DXY	-0.12945	0.08457	-0.06473	0.04718	0.00000
124	O1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
125	O1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
126	H4	S	0.08071	0.07338	0.18114	-0.12123	0.00000
127	H4	S	0.02883	-0.11161	-0.02750	0.05060	0.00000
128	H4	PX	0.04064	0.07618	0.13890	-0.10360	0.00000
129	H4	PY	-0.00147	-0.03597	-0.13509	0.10492	0.00000
130	H4	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
131	N1	S	0.21093	0.14726	0.09760	-0.00031	0.00000
132	N1	S	0.17583	-0.02917	-0.13189	-0.00016	0.00000
133	N1	PX	-0.02006	0.07564	0.10082	-0.01716	0.00000
134	N1	PY	-0.06514	0.11983	0.08081	-0.08267	0.00000
135	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
136	N1	S	-4.42498	-2.30867	-1.49012	-0.11350	0.00000
137	N1	PX	-0.94960	-0.44646	0.03209	0.16656	0.00000
138	N1	PY	-1.01870	-0.39475	-0.41104	-0.35322	0.00000
139	N1	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
140	N1	DXX	0.39911	0.46477	0.50419	0.04735	0.00000
141	N1	DYY	0.32443	0.50624	0.38808	-0.16000	0.00000
142	N1	DZZ	0.72498	0.42907	0.23110	0.02707	0.00000
143	N1	DXY	-0.02206	-0.00108	-0.03864	-0.04840	0.00000
144	N1	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
145	N1	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
146	H6	S	0.03335	-0.20908	-0.15992	0.16014	0.00000
147	H6	S	-0.08007	-0.09102	0.13545	0.00762	0.00000
148	H6	PX	0.01559	-0.19285	-0.17869	0.14517	0.00000
149	H6	PY	0.02045	-0.05205	-0.05673	0.04058	0.00000
150	H6	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
151	C8	S	0.11536	-0.03803	-0.22898	-0.12074	0.00000
152	C8	S	-0.80719	0.18561	1.43806	0.61520	0.00000

153	C8	PX	0.00518	0.03596	-0.02563	-0.02623	0.00000
154	C8	PY	-0.05986	0.02921	0.07084	0.01051	0.00000
155	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
156	C8	S	0.84140	1.04860	1.47076	1.45934	0.00000
157	C8	PX	-1.02884	-0.44385	0.16645	0.53095	0.00000
158	C8	PY	1.49287	0.72345	0.32873	1.14297	0.00000
159	C8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
160	C8	DXX	0.51150	-0.22073	-1.07312	-0.45797	0.00000
161	C8	DYY	0.66431	-0.16036	-1.34656	-0.69701	0.00000
162	C8	DZZ	0.40703	-0.13816	-0.80498	-0.39763	0.00000
163	C8	DXY	-0.04165	0.04173	-0.00788	-0.02217	0.00000
164	C8	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
165	C8	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
166	H8	S	-0.05397	-0.00950	-0.30967	-0.30024	0.00000
167	H8	S	-0.27934	-0.18689	0.02933	-0.25497	0.00000
168	H8	PX	0.00846	-0.00669	0.29606	0.28165	0.00000
169	H8	PY	0.04348	0.02889	-0.04631	-0.01240	0.00000
170	H8	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
171	C10	S	-0.02941	0.06726	0.14305	0.05454	0.00000
172	C10	S	0.13818	-0.40920	-0.82223	-0.26165	0.00000
173	C10	PX	0.01247	0.00586	-0.03342	-0.01735	0.00000
174	C10	PY	-0.09568	0.00428	0.17395	0.12645	0.00000
175	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
176	C10	S	1.05459	0.06772	-0.61864	0.14606	0.00000
177	C10	PX	0.21109	0.02124	-0.00649	-0.27023	0.00000
178	C10	PY	0.33826	0.05003	-0.07421	0.01936	0.00000
179	C10	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
180	C10	DXX	-0.11395	0.35014	0.76414	0.29009	0.00000
181	C10	DYY	-0.25076	0.32313	0.86239	0.34212	0.00000
182	C10	DZZ	-0.09171	0.22821	0.45047	0.16389	0.00000
183	C10	DXY	0.06360	0.03468	-0.09010	-0.08222	0.00000
184	C10	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
185	C10	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
186	H16	S	-0.01345	-0.05988	-0.17128	-0.05348	0.00000
187	H16	S	-0.13817	0.00955	0.09842	0.10513	0.00000
188	H16	PX	-0.02980	0.06282	0.17986	0.08230	0.00000
189	H16	PY	0.00684	-0.02542	-0.05895	-0.02022	0.00000
190	H16	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
191	H18	S	0.02688	-0.08358	-0.12739	-0.05548	0.00000
192	H18	S	0.03786	0.03155	0.08875	-0.06606	0.00000
193	H18	PX	0.01532	-0.05952	-0.10154	-0.03501	0.00000
194	H18	PY	0.00276	-0.05858	-0.10774	-0.02983	0.00000
195	H18	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
196	C9	S	0.29822	-0.10087	0.07642	-0.03611	0.00000
197	C9	S	-1.62497	0.65390	-0.42883	0.19492	0.00000
198	C9	PX	-0.00664	0.03848	-0.03491	0.02533	0.00000
199	C9	PY	-0.00924	0.00335	-0.00482	0.00743	0.00000
200	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
201	C9	S	-1.91832	-0.24309	-0.35666	0.20795	0.00000
202	C9	PX	0.07457	0.09937	0.00461	-0.04599	0.00000
203	C9	PY	0.39597	0.22999	0.01075	-0.01508	0.00000
204	C9	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
205	C9	DXX	1.36754	-0.34854	0.35046	-0.17750	0.00000
206	C9	DYY	1.22742	-0.52374	0.34758	-0.17139	0.00000

207	C9	DZZ	1.22523	-0.45998	0.30688	-0.14085	0.00000
208	C9	DXY	-0.00551	0.02695	0.00728	-0.00537	0.00000
209	C9	DXZ	0.00000	0.00000	0.00000	0.00000	0.00000
210	C9	DYZ	0.00000	0.00000	0.00000	0.00000	0.00000
211	H3	S	-0.14699	0.13096	-0.05146	0.02488	0.00000
212	H3	S	0.13980	-0.05010	0.03971	-0.01266	0.00000
213	H3	PX	-0.03433	0.00266	-0.00059	-0.00429	0.00000
214	H3	PY	0.18446	-0.12806	0.07016	-0.04185	0.00000
215	H3	PZ	0.00000	0.00000	0.00000	0.00000	0.00000
216	H5	S	-0.06975	0.12650	-0.03607	0.01048	0.00000
217	H5	S	0.34042	0.02561	0.07178	-0.01627	0.00000
218	H5	PX	0.08325	-0.03232	0.01390	-0.00241	0.00000
219	H5	PY	-0.08522	-0.00953	-0.00871	0.00298	0.00000
220	H5	PZ	-0.14281	0.06738	-0.03657	0.02290	0.00000
221	H7	S	-0.06975	0.12650	-0.03607	0.01048	0.00000
222	H7	S	0.34042	0.02561	0.07178	-0.01627	0.00000
223	H7	PX	0.08325	-0.03232	0.01390	-0.00241	0.00000
224	H7	PY	-0.08522	-0.00953	-0.00871	0.00298	0.00000
225	H7	PZ	0.14281	-0.06738	0.03657	-0.02290	0.00000

Atomic Charges from Electrostatic Potential

Resolution: 1 points per atomic unit

6944 of 17955 gridpoints used in calculation

Atom	Charge
----	-----
H 1	0.226432
C 2	-0.509826
C 3	-0.264623
C 4	0.121883
C 5	0.493478
C 6	-0.265125
C 7	0.527383
C 8	-0.465662
O 9	-0.396296
H 10	0.176234
N 11	-0.694921
H 12	0.181634
C 13	0.514887
H 14	0.214387
C 15	-0.475365
H 16	0.182448
H 17	0.213304
C 18	0.059467
H 19	0.080931
H 20	0.039674
H 21	0.039674

Total Charge = 0.000000

RMS fit: 1.308314
RRMS fit: 0.179095

Dipole moment from formal charges:

x = 2.6372, y = 1.7305, z = 0.0000 = 3.1543 debye

Q-minus(elesta) = -0.6949

Q-plus(elesta) = 0.2264

Mulliken Population Analysis

AO	atom type		Occupancy
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1	H1	S	0.532517
2	H1	S	0.298367
3	H1	PX	0.009181
4	H1	PY	0.002289
5	H1	PZ	0.003103
6	C1	S	1.996405
7	C1	S	0.655863
8	C1	PX	0.726659
9	C1	PY	0.716440
10	C1	PZ	0.597250
11	C1	S	0.437520
12	C1	PX	0.278377
13	C1	PY	0.218376
14	C1	PZ	0.530178
15	C1	DXX	0.018328
16	C1	DYY	0.019897
17	C1	DZZ	-0.017491
18	C1	DXY	0.014336
19	C1	DXZ	0.005073
20	C1	DYZ	0.005884
21	C2	S	1.996577
22	C2	S	0.674998
23	C2	PX	0.724961
24	C2	PY	0.759276
25	C2	PZ	0.518959
26	C2	S	0.465593
27	C2	PX	0.301499
28	C2	PY	0.165506
29	C2	PZ	0.450104
30	C2	DXX	0.017019
31	C2	DYY	0.020276
32	C2	DZZ	-0.018189
33	C2	DXY	0.016380
34	C2	DXZ	0.002249
35	C2	DYZ	0.008470
36	C3	S	1.996663
37	C3	S	0.673620

38	C3	PX	0.721380
39	C3	PY	0.755201
40	C3	PZ	0.534254
41	C3	S	0.433570
42	C3	PX	0.211720
43	C3	PY	0.230966
44	C3	PZ	0.451643
45	C3	DXX	0.017682
46	C3	DYY	0.031068
47	C3	DZZ	-0.017546
48	C3	DXY	0.014666
49	C3	DXZ	0.004221
50	C3	DYZ	0.011640
51	C4	S	1.996668
52	C4	S	0.679027
53	C4	PX	0.774123
54	C4	PY	0.627839
55	C4	PZ	0.520384
56	C4	S	0.341095
57	C4	PX	0.142984
58	C4	PY	0.030891
59	C4	PZ	0.386812
60	C4	DXX	0.024767
61	C4	DYY	0.031904
62	C4	DZZ	-0.020395
63	C4	DXY	0.022756
64	C4	DXZ	0.008435
65	C4	DYZ	0.019842
66	C5	S	1.996586
67	C5	S	0.674449
68	C5	PX	0.703647
69	C5	PY	0.772905
70	C5	PZ	0.515694
71	C5	S	0.505642
72	C5	PX	0.252806
73	C5	PY	0.246684
74	C5	PZ	0.461436
75	C5	DXX	0.016760
76	C5	DYY	0.021398
77	C5	DZZ	-0.018695
78	C5	DXY	0.015684
79	C5	DXZ	0.003175
80	C5	DYZ	0.007607
81	C6	S	1.996714
82	C6	S	0.692307
83	C6	PX	0.727693
84	C6	PY	0.750531
85	C6	PZ	0.487710
86	C6	S	0.343431
87	C6	PX	0.190641
88	C6	PY	0.130764
89	C6	PZ	0.371023
90	C6	DXX	0.020123
91	C6	DYY	0.030987

92	C6	DZZ	-0.019967
93	C6	DXY	0.030036
94	C6	DXZ	0.005444
95	C6	DYZ	0.016082
96	C7	S	1.996657
97	C7	S	0.670549
98	C7	PX	0.728845
99	C7	PY	0.733341
100	C7	PZ	0.536088
101	C7	S	0.448949
102	C7	PX	0.320615
103	C7	PY	0.186017
104	C7	PZ	0.480038
105	C7	DXX	0.022761
106	C7	DYY	0.014997
107	C7	DZZ	-0.017778
108	C7	DXY	0.016465
109	C7	DXZ	0.003892
110	C7	DYZ	0.007348
111	01	S	1.995297
112	01	S	0.885512
113	01	PX	0.942983
114	01	PY	0.859023
115	01	PZ	1.115339
116	01	S	0.948862
117	01	PX	0.597882
118	01	PY	0.511108
119	01	PZ	0.738701
120	01	DXX	0.016537
121	01	DYY	0.025687
122	01	DZZ	-0.000113
123	01	DXY	0.006043
124	01	DXZ	0.002863
125	01	DYZ	0.004840
126	H4	S	0.531560
127	H4	S	0.276527
128	H4	PX	0.005579
129	H4	PY	0.006053
130	H4	PZ	0.002260
131	N1	S	1.996242
132	N1	S	0.787125
133	N1	PX	0.865540
134	N1	PY	0.833170
135	N1	PZ	0.661960
136	N1	S	0.962512
137	N1	PX	0.516183
138	N1	PY	0.371284
139	N1	PZ	0.545098
140	N1	DXX	0.008194
141	N1	DYY	0.014474
142	N1	DZZ	-0.011320
143	N1	DXY	0.008872
144	N1	DXZ	0.004584
145	N1	DYZ	0.011447

146	H6	S	0.530699
147	H6	S	0.276199
148	H6	PX	0.009342
149	H6	PY	0.002422
150	H6	PZ	0.002302
151	C8	S	1.996661
152	C8	S	0.680929
153	C8	PX	0.660898
154	C8	PY	0.774976
155	C8	PZ	0.535776
156	C8	S	0.377242
157	C8	PX	0.097228
158	C8	PY	0.120073
159	C8	PZ	0.427158
160	C8	DXX	0.020848
161	C8	DYY	0.029138
162	C8	DZZ	-0.019142
163	C8	DXY	0.025485
164	C8	DXZ	0.010042
165	C8	DYZ	0.010054
166	H8	S	0.531217
167	H8	S	0.294522
168	H8	PX	0.010160
169	H8	PY	0.001670
170	H8	PZ	0.002661
171	C10	S	1.996636
172	C10	S	0.678138
173	C10	PX	0.725035
174	C10	PY	0.768638
175	C10	PZ	0.470293
176	C10	S	0.565066
177	C10	PX	0.360903
178	C10	PY	0.244104
179	C10	PZ	0.451542
180	C10	DXX	0.012351
181	C10	DYY	0.018690
182	C10	DZZ	-0.020290
183	C10	DXY	0.013151
184	C10	DXZ	0.000362
185	C10	DYZ	0.007672
186	H16	S	0.533306
187	H16	S	0.308514
188	H16	PX	0.009115
189	H16	PY	0.002490
190	H16	PZ	0.002273
191	H18	S	0.529207
192	H18	S	0.291436
193	H18	PX	0.006576
194	H18	PY	0.005231
195	H18	PZ	0.002164
196	C9	S	1.996709
197	C9	S	0.648252
198	C9	PX	0.572181
199	C9	PY	0.686169

200	C9	PZ	0.722477
201	C9	S	0.547280
202	C9	PX	0.151609
203	C9	PY	0.318498
204	C9	PZ	0.322838
205	C9	DXX	0.012056
206	C9	DYY	0.010736
207	C9	DZZ	0.004387
208	C9	DXY	0.014913
209	C9	DXZ	0.020755
210	C9	DYZ	0.003392
211	H3	S	0.540886
212	H3	S	0.304305
213	H3	PX	0.001138
214	H3	PY	0.009288
215	H3	PZ	0.002049
216	H5	S	0.540933
217	H5	S	0.327826
218	H5	PX	0.003466
219	H5	PY	0.002066
220	H5	PZ	0.007116
221	H7	S	0.540933
222	H7	S	0.327826
223	H7	PX	0.003466
224	H7	PY	0.002066
225	H7	PZ	0.007116

Atom	Occupancy	Charge
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H1	0.845457	0.154543
C1	6.203094	-0.203094
C2	6.103680	-0.103680
C3	6.070746	-0.070746
C4	5.587132	0.412868
C5	6.175780	-0.175780
C6	5.773520	0.226480
C7	6.148785	-0.148785
O1	8.650564	-0.650564
H4	0.821980	0.178020
N1	7.575365	-0.575365
H6	0.820965	0.179035
C8	5.747366	0.252634
H8	0.840231	0.159769
C10	6.292292	-0.292292
H16	0.855698	0.144302
H18	0.834613	0.165387
C9	6.032253	-0.032253
H3	0.857666	0.142334
H5	0.881406	0.118594
H7	0.881406	0.118594

Total Charge = 0.000000

Natural Atomic Orbital Populations

Nao	Atom	Type	Basis	Occupancy
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1	H1	S	MIN	0.760102
2	H1	S	RYD	0.000860
3	H1	PX	RYD	0.000507
4	H1	PY	RYD	0.000070
5	H1	PZ	RYD	0.000117
6	C1	S	MIN	1.998920
7	C1	S	MIN	0.938227
8	C1	S	RYD	0.000856
9	C1	S	RYD	0.000027
10	C1	PX	MIN	1.201661
11	C1	PX	RYD	0.004427
12	C1	PY	MIN	1.065741
13	C1	PY	RYD	0.005363
14	C1	PZ	MIN	1.134184
15	C1	PZ	RYD	0.002329
16	C1	DXY	RYD	0.001729
17	C1	DXZ	RYD	0.001214
18	C1	DYZ	RYD	0.000560
19	C1	DXX-YY	RYD	0.001401
20	C1	D3ZZ-RR	RYD	0.001197
21	C2	S	MIN	1.998987
22	C2	S	MIN	0.959355
23	C2	S	RYD	0.001088
24	C2	S	RYD	0.000036
25	C2	PX	MIN	1.186574
26	C2	PX	RYD	0.005910
27	C2	PY	MIN	1.075491
28	C2	PY	RYD	0.006953
29	C2	PZ	MIN	0.976752
30	C2	PZ	RYD	0.001688
31	C2	DXY	RYD	0.001824
32	C2	DXZ	RYD	0.000417
33	C2	DYZ	RYD	0.001288
34	C2	DXX-YY	RYD	0.001505
35	C2	D3ZZ-RR	RYD	0.001225
36	C3	S	MIN	1.998989
37	C3	S	MIN	0.878637
38	C3	S	RYD	0.001423
39	C3	S	RYD	0.000050
40	C3	PX	MIN	1.075588
41	C3	PX	RYD	0.008844
42	C3	PY	MIN	1.106043
43	C3	PY	RYD	0.004179
44	C3	PZ	MIN	1.013808
45	C3	PZ	RYD	0.001066
46	C3	DXY	RYD	0.001368
47	C3	DXZ	RYD	0.000397
48	C3	DYZ	RYD	0.001620

49	C3	DXX-YY	RVD	0.001625
50	C3	D3ZZ-RR	RVD	0.001064
51	C4	S	MIN	1.998783
52	C4	S	MIN	0.822480
53	C4	S	RVD	0.001487
54	C4	S	RVD	0.000114
55	C4	PX	MIN	1.071846
56	C4	PX	RVD	0.005692
57	C4	PY	MIN	0.753903
58	C4	PY	RVD	0.009798
59	C4	PZ	MIN	0.926714
60	C4	PZ	RVD	0.001710
61	C4	DXY	RVD	0.002106
62	C4	DXZ	RVD	0.001076
63	C4	DYZ	RVD	0.002641
64	C4	DXX-YY	RVD	0.002773
65	C4	D3ZZ-RR	RVD	0.001038
66	C5	S	MIN	1.999024
67	C5	S	MIN	0.966354
68	C5	S	RVD	0.000852
69	C5	S	RVD	0.000031
70	C5	PX	MIN	1.102095
71	C5	PX	RVD	0.005945
72	C5	PY	MIN	1.154844
73	C5	PY	RVD	0.006763
74	C5	PZ	MIN	0.983121
75	C5	PZ	RVD	0.001731
76	C5	DXY	RVD	0.001684
77	C5	DXZ	RVD	0.000281
78	C5	DYZ	RVD	0.001397
79	C5	DXX-YY	RVD	0.001711
80	C5	D3ZZ-RR	RVD	0.001302
81	C6	S	MIN	1.999151
82	C6	S	MIN	0.837925
83	C6	S	RVD	0.003711
84	C6	S	RVD	0.000112
85	C6	PX	MIN	1.033983
86	C6	PX	RVD	0.008355
87	C6	PY	MIN	0.948168
88	C6	PY	RVD	0.009704
89	C6	PZ	MIN	0.875846
90	C6	PZ	RVD	0.001174
91	C6	DXY	RVD	0.002901
92	C6	DXZ	RVD	0.000530
93	C6	DYZ	RVD	0.002381
94	C6	DXX-YY	RVD	0.001822
95	C6	D3ZZ-RR	RVD	0.001023
96	C7	S	MIN	1.998873
97	C7	S	MIN	0.953736
98	C7	S	RVD	0.000711
99	C7	S	RVD	0.000041
100	C7	PX	MIN	1.200778
101	C7	PX	RVD	0.004175
102	C7	PY	MIN	1.040786

103	C7	PY	RVD	0.005468
104	C7	PZ	MIN	1.008539
105	C7	PZ	RVD	0.001671
106	C7	DXY	RVD	0.001779
107	C7	DXZ	RVD	0.000860
108	C7	DYZ	RVD	0.000911
109	C7	DXX-YY	RVD	0.001433
110	C7	D3ZZ-RR	RVD	0.001216
111	O1	S	MIN	1.999715
112	O1	S	MIN	1.570738
113	O1	S	RVD	0.000895
114	O1	S	RVD	0.000026
115	O1	PX	MIN	1.642862
116	O1	PX	RVD	0.002596
117	O1	PY	MIN	1.499321
118	O1	PY	RVD	0.001512
119	O1	PZ	MIN	1.874311
120	O1	PZ	RVD	0.003659
121	O1	DXY	RVD	0.001613
122	O1	DXZ	RVD	0.001127
123	O1	DYZ	RVD	0.001173
124	O1	DXX-YY	RVD	0.003951
125	O1	D3ZZ-RR	RVD	0.002029
126	H4	S	MIN	0.749192
127	H4	S	RVD	0.000751
128	H4	PX	RVD	0.000309
129	H4	PY	RVD	0.000321
130	H4	PZ	RVD	0.000066
131	N1	S	MIN	1.999380
132	N1	S	MIN	1.379731
133	N1	S	RVD	0.000496
134	N1	S	RVD	0.000017
135	N1	PX	MIN	1.511466
136	N1	PX	RVD	0.004266
137	N1	PY	MIN	1.371089
138	N1	PY	RVD	0.003967
139	N1	PZ	MIN	1.227123
140	N1	PZ	RVD	0.001209
141	N1	DXY	RVD	0.002218
142	N1	DXZ	RVD	0.001760
143	N1	DYZ	RVD	0.002970
144	N1	DXX-YY	RVD	0.004686
145	N1	D3ZZ-RR	RVD	0.002870
146	H6	S	MIN	0.748692
147	H6	S	RVD	0.000747
148	H6	PX	RVD	0.000524
149	H6	PY	RVD	0.000079
150	H6	PZ	RVD	0.000072
151	C8	S	MIN	1.999037
152	C8	S	MIN	0.866006
153	C8	S	RVD	0.002899
154	C8	S	RVD	0.000106
155	C8	PX	MIN	0.907783
156	C8	PX	RVD	0.009129

157	C8	PY	MIN	1.089210
158	C8	PY	RYD	0.008116
159	C8	PZ	MIN	1.005298
160	C8	PZ	RYD	0.001574
161	C8	DXY	RYD	0.002297
162	C8	DXZ	RYD	0.001228
163	C8	DYZ	RYD	0.001517
164	C8	DXX-YY	RYD	0.002114
165	C8	D3ZZ-RR	RYD	0.001111
166	H8	S	MIN	0.762543
167	H8	S	RYD	0.000423
168	H8	PX	RYD	0.000592
169	H8	PY	RYD	0.000018
170	H8	PZ	RYD	0.000096
171	C10	S	MIN	1.998991
172	C10	S	MIN	1.045350
173	C10	S	RYD	0.001147
174	C10	S	RYD	0.000015
175	C10	PX	MIN	1.213224
176	C10	PX	RYD	0.004486
177	C10	PY	MIN	1.134888
178	C10	PY	RYD	0.003455
179	C10	PZ	MIN	0.904125
180	C10	PZ	RYD	0.002294
181	C10	DXY	RYD	0.001829
182	C10	DXZ	RYD	0.000071
183	C10	DYZ	RYD	0.001483
184	C10	DXX-YY	RYD	0.002032
185	C10	D3ZZ-RR	RYD	0.001512
186	H16	S	MIN	0.782926
187	H16	S	RYD	0.000407
188	H16	PX	RYD	0.000547
189	H16	PY	RYD	0.000073
190	H16	PZ	RYD	0.000088
191	H18	S	MIN	0.766048
192	H18	S	RYD	0.000814
193	H18	PX	RYD	0.000383
194	H18	PY	RYD	0.000240
195	H18	PZ	RYD	0.000075
196	C9	S	MIN	1.999446
197	C9	S	MIN	1.081286
198	C9	S	RYD	0.001539
199	C9	S	RYD	0.000031
200	C9	PX	MIN	0.814459
201	C9	PX	RYD	0.003582
202	C9	PY	MIN	1.119362
203	C9	PY	RYD	0.003414
204	C9	PZ	MIN	1.206820
205	C9	PZ	RYD	0.000454
206	C9	DXY	RYD	0.002107
207	C9	DXZ	RYD	0.002936
208	C9	DYZ	RYD	0.000667
209	C9	DXX-YY	RYD	0.002293
210	C9	D3ZZ-RR	RYD	0.002076

211	H3	S	MIN	0.783083
212	H3	S	RYD	0.000419
213	H3	PX	RYD	0.000025
214	H3	PY	RYD	0.000607
215	H3	PZ	RYD	0.000030
216	H5	S	MIN	0.806803
217	H5	S	RYD	0.001421
218	H5	PX	RYD	0.000176
219	H5	PY	RYD	0.000059
220	H5	PZ	RYD	0.000484
221	H7	S	MIN	0.806803
222	H7	S	RYD	0.001421
223	H7	PX	RYD	0.000176
224	H7	PY	RYD	0.000059
225	H7	PZ	RYD	0.000484

Total MIN occupancy: 83.713120
 Total RYD occupancy: 0.286880
 Total occupancy: 84.000000

Natural Atomic Populations and Charges

Atom	Occupancy	Charge
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H1	0.761656	0.238344
C1	6.357838	-0.357838
C2	6.219092	-0.219092
C3	6.094699	-0.094699
C4	5.602160	0.397840
C5	6.227136	-0.227136
C6	5.726786	0.273214
C7	6.220977	-0.220977
O1	8.605530	-0.605530
H4	0.750640	0.249360
N1	7.513248	-0.513248
H6	0.750114	0.249886
C8	5.897425	0.102575
H8	0.763672	0.236328
C10	6.314904	-0.314904
H16	0.784041	0.215959
H18	0.767560	0.232440
C9	6.240471	-0.240471
H3	0.784165	0.215835
H5	0.808943	0.191057
H7	0.808943	0.191057

Total Charge = 0.000000

Q-minus(NAO) = -0.6055
 Q-plus(NAO) = 0.2499

Reason for exit: Normal completion

Wall Time: 000:00:00

CPU Time: 000:00:00