Supplementary Information for

Lipophilic β-Cyclodextrin Cyclic-Nitrone Conjugate: Synthesis and Spin Trapping Studies

Yongbin Han,[a] Yangping Liu,[b] Antal Rockenbauer,[c] Jay L. Zweier,[b] Grégory Durand[d] and Frederick A. Villamena[a,]*

Email: frederick.villamena@osumc.edu

Table of contents

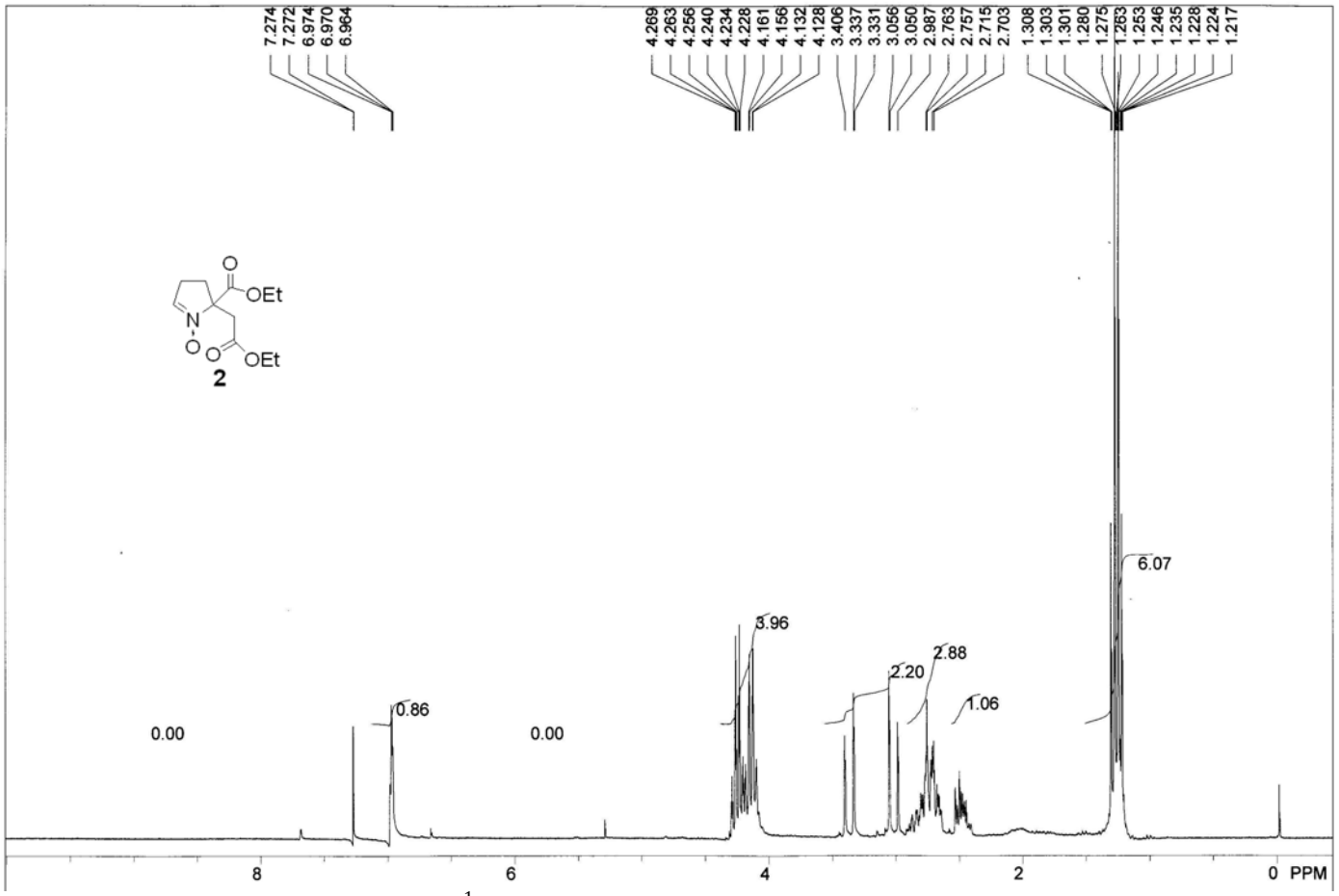


Figure S1. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

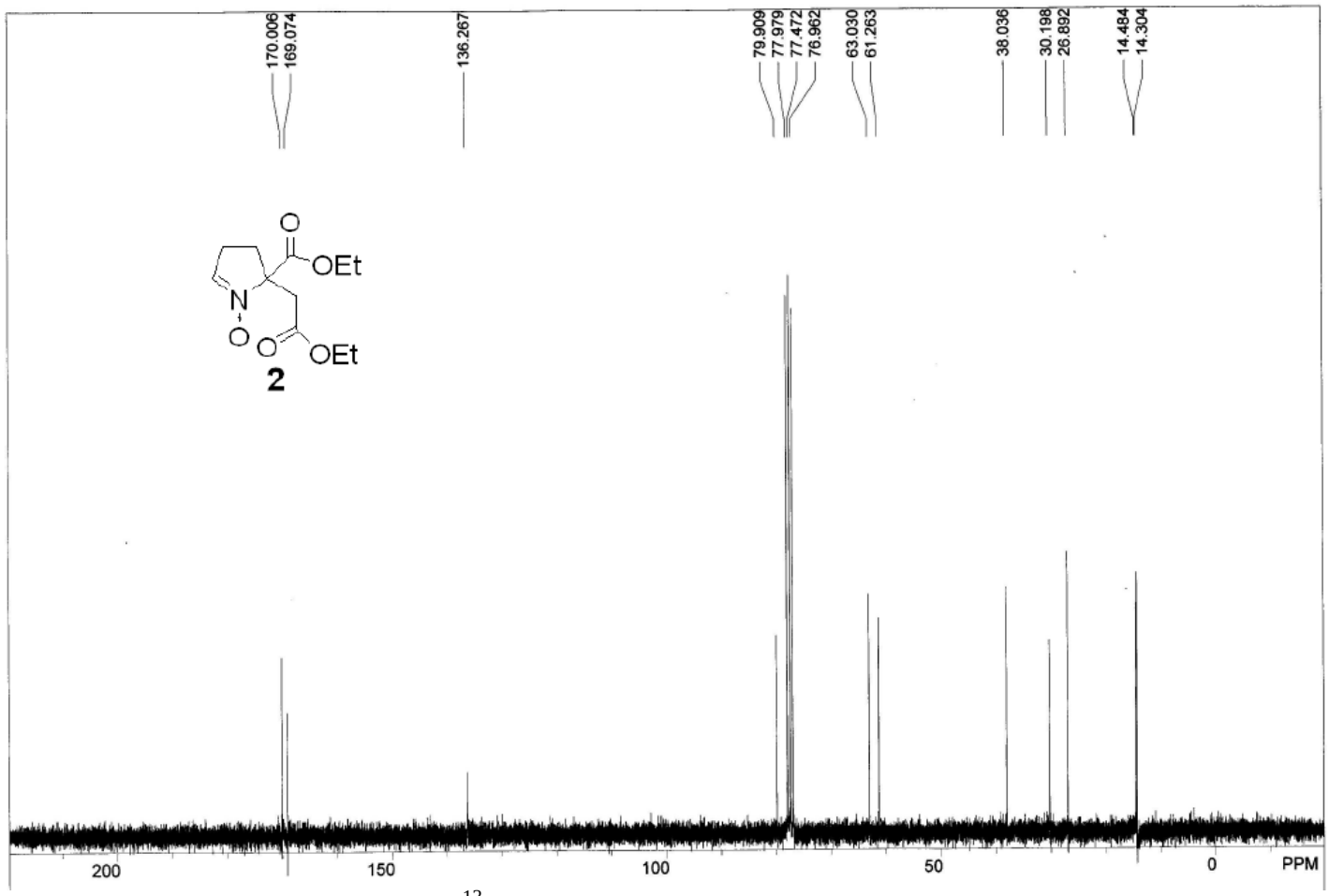


Figure S2. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

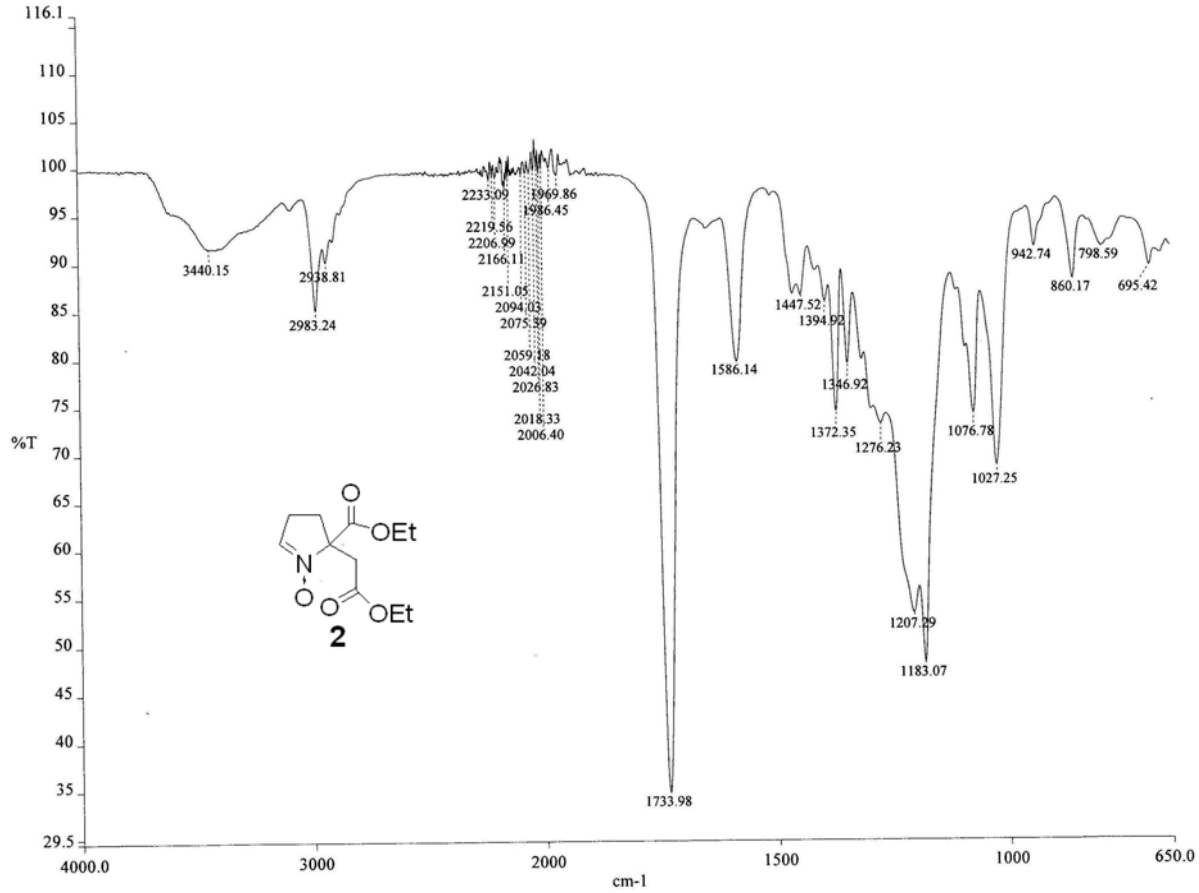


Figure S3. Neat IR spectrum of compound **2**

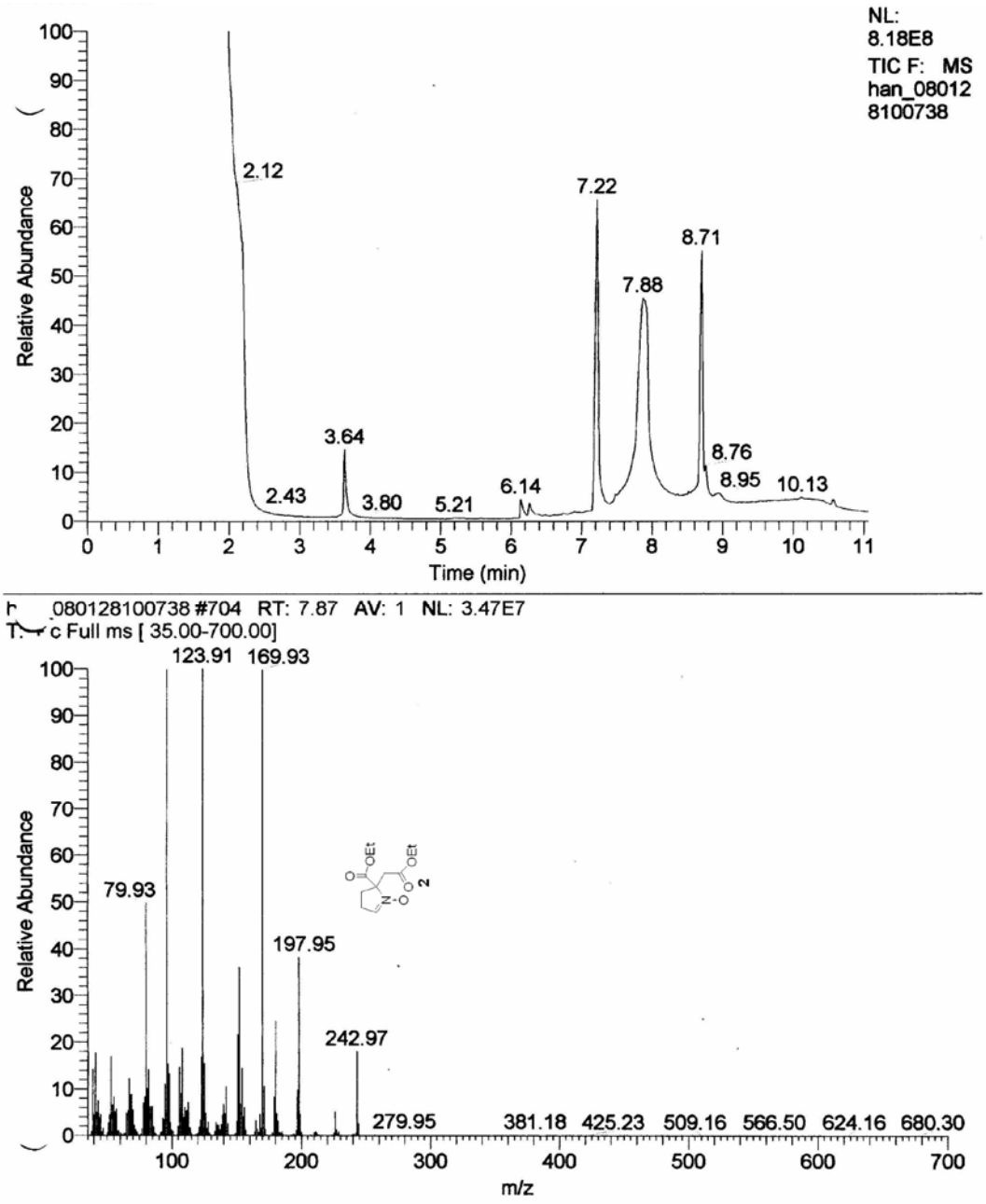


Figure S4. GC-MS spectrum of compound **2**

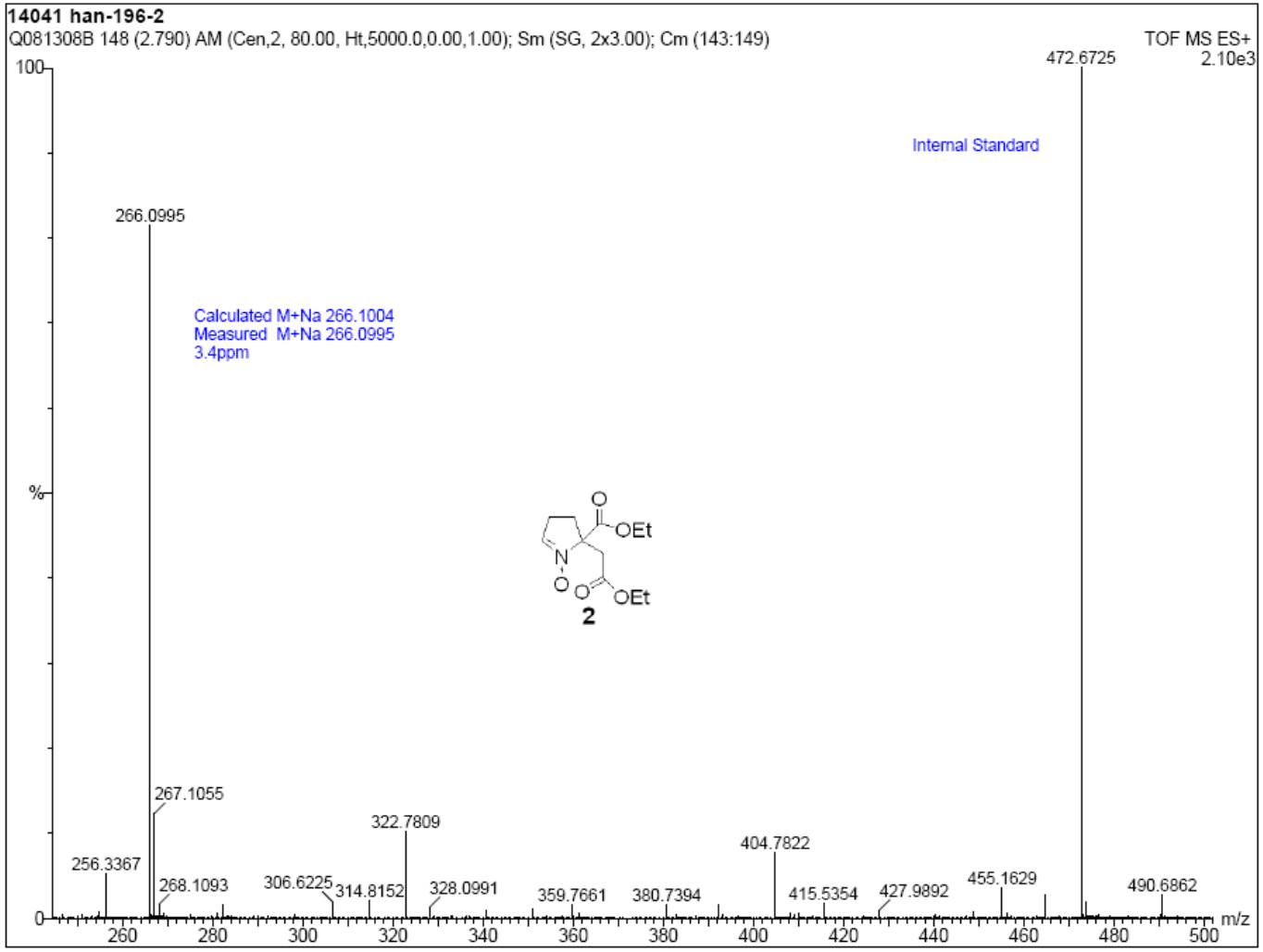


Figure S5. HRMS spectrum of compound **2**

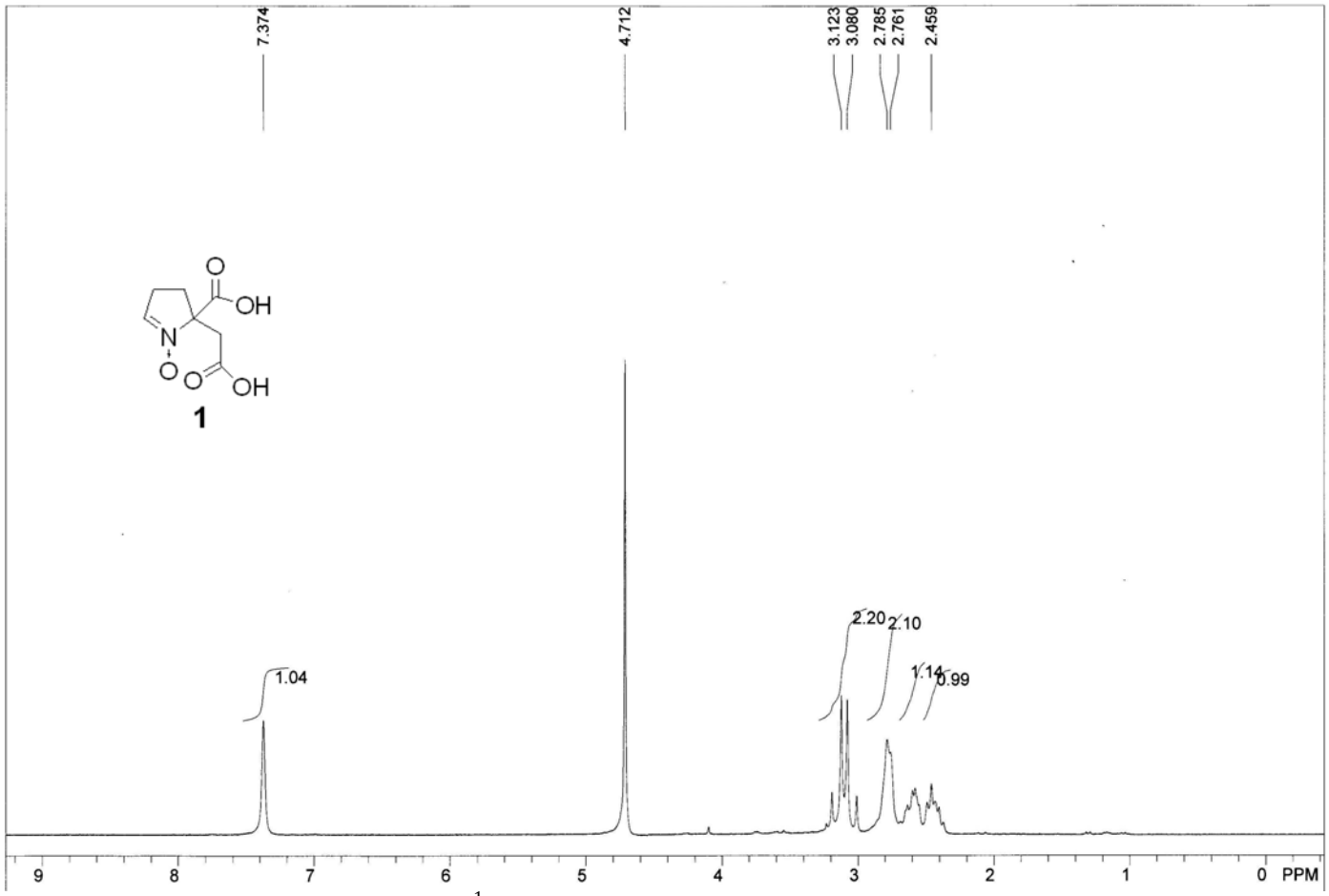


Figure S6. ^{1}H NMR spectrum of compound **1** in D_2O

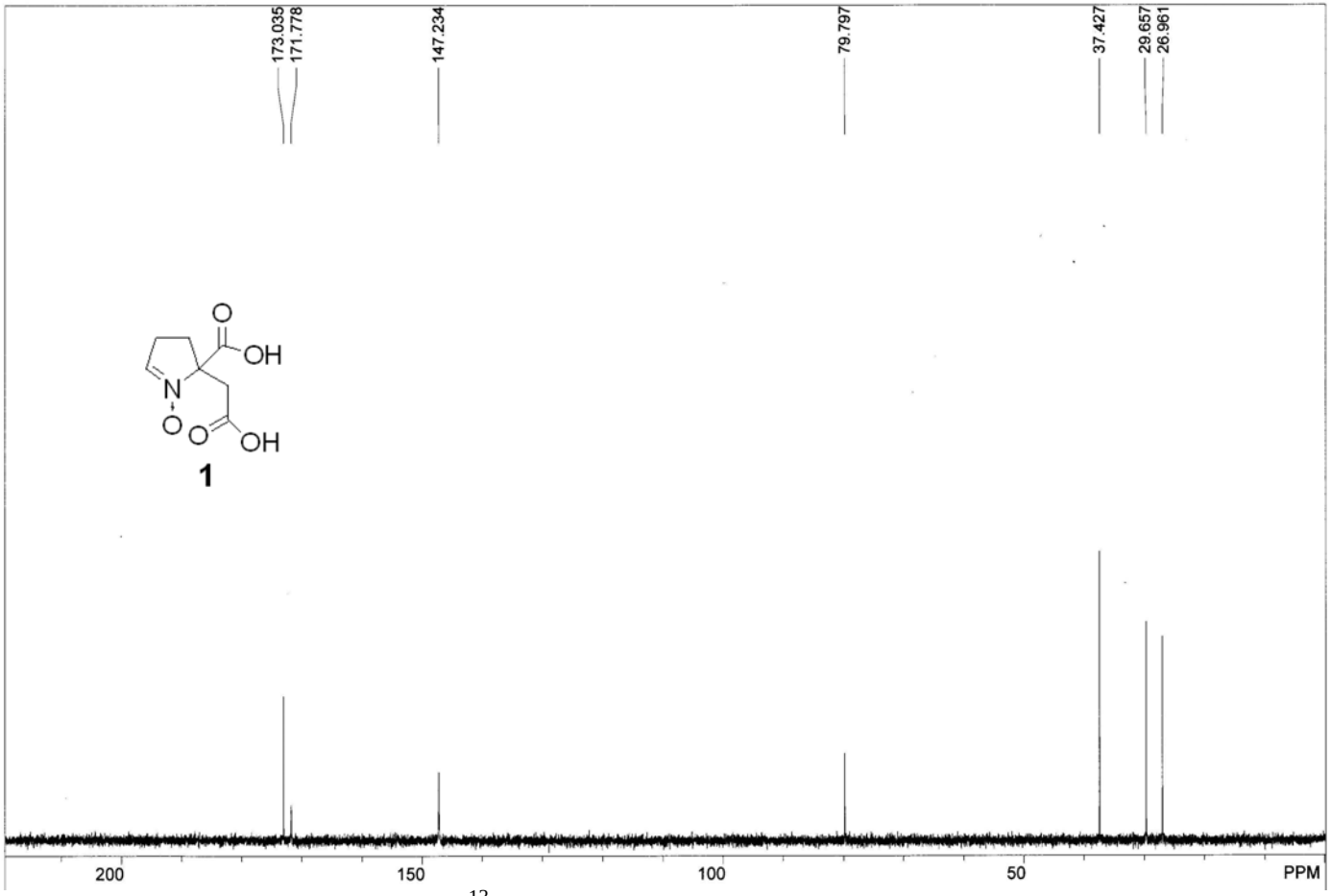


Figure S7. ^{13}C NMR spectrum of compound **1** in D_2O

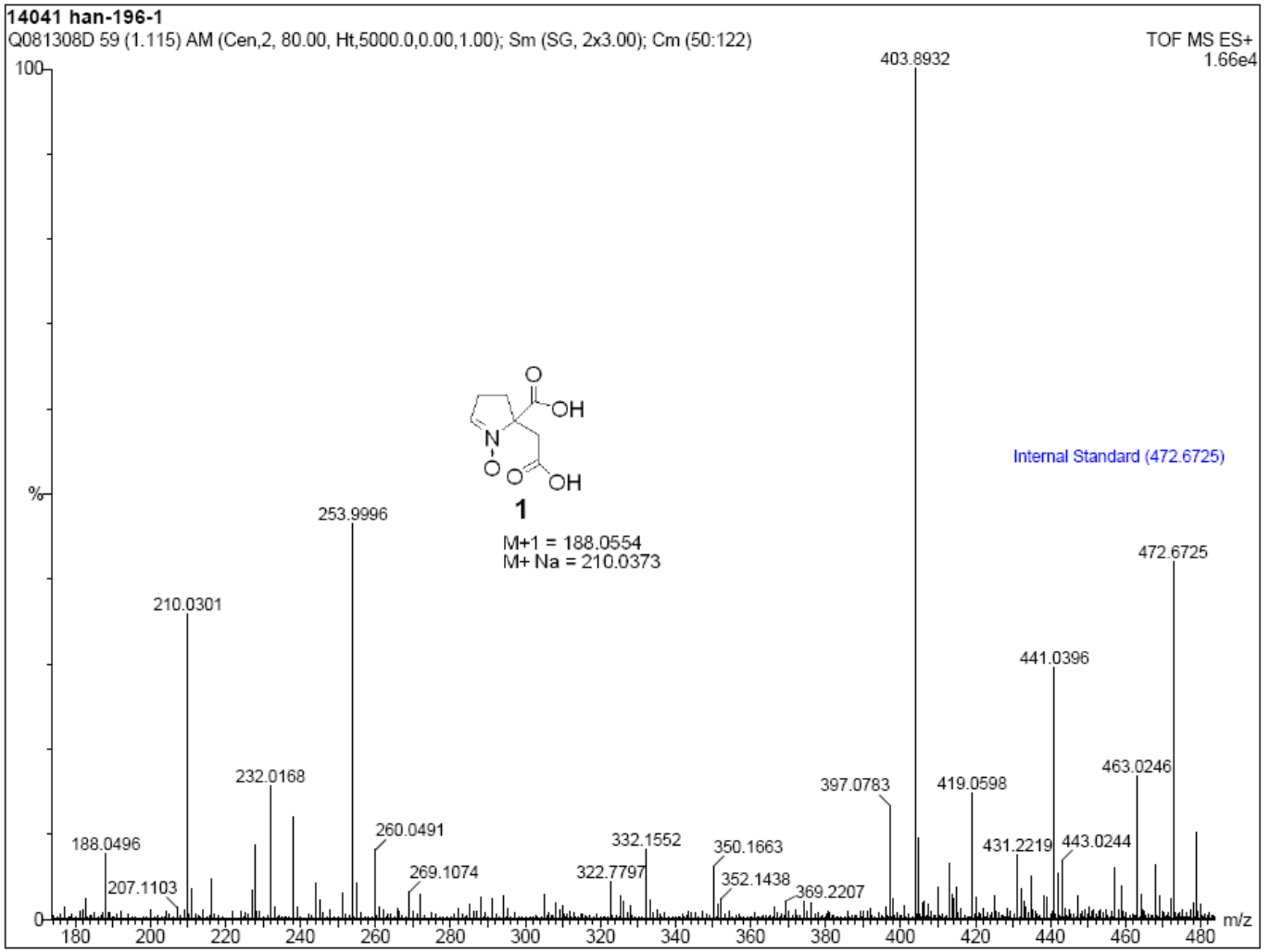
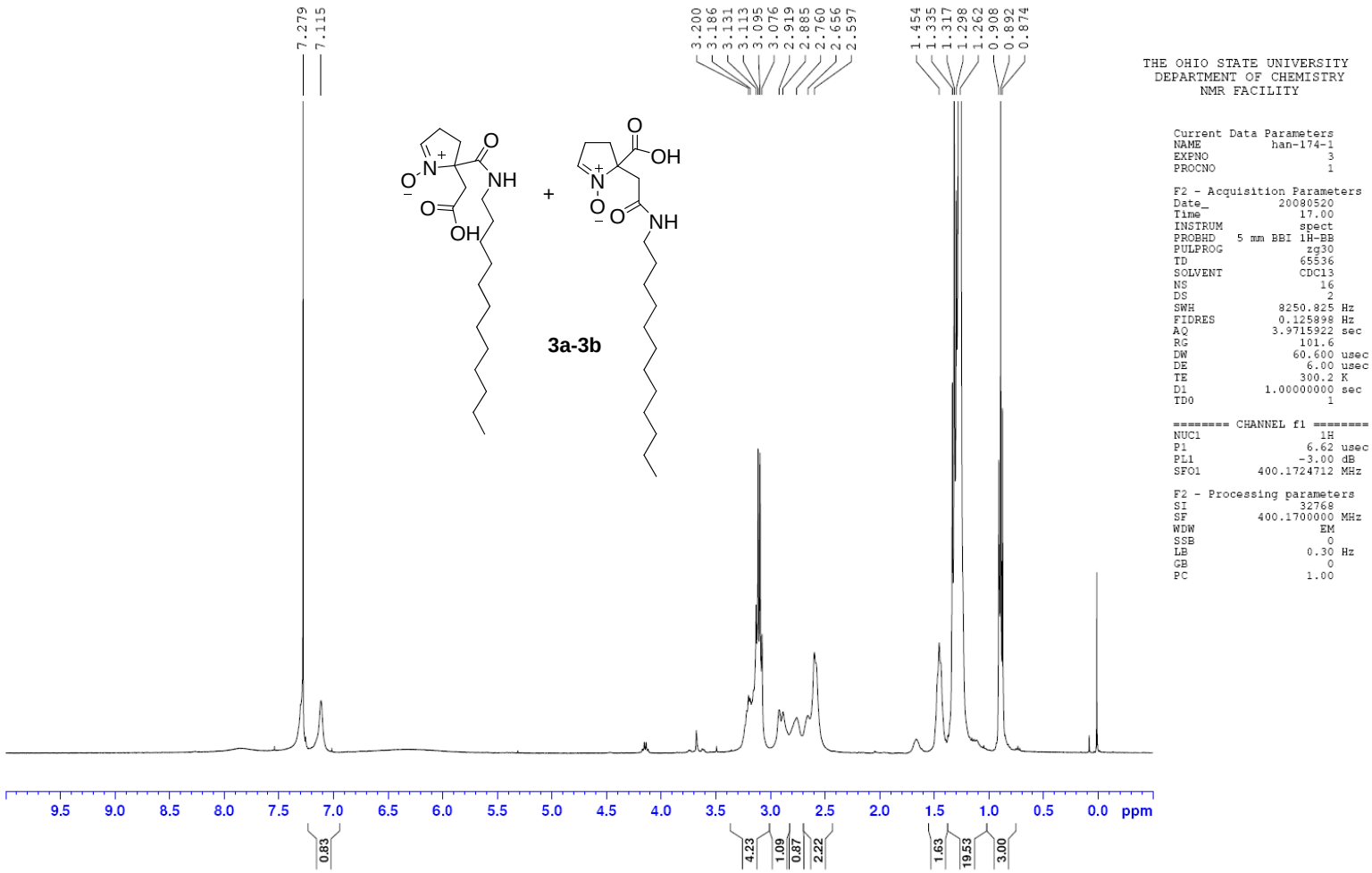


Figure S8. HRMS spectrum of compound **1**



THE OHIO STATE UNIVERSITY
DEPARTMENT OF CHEMISTRY
NMR FACILITY

Current Data Parameters
NAME han-174-1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080520
Time 17.00
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 101.6
DW 60.600 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 6.62 usec
PL1 -3.00 dB
SFO1 400.1724712 MHz

F2 - Processing parameters
SI 32768
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S9. ^{1}H NMR spectrum of compound **3a** and **3b** mixture in $CDCl_3$

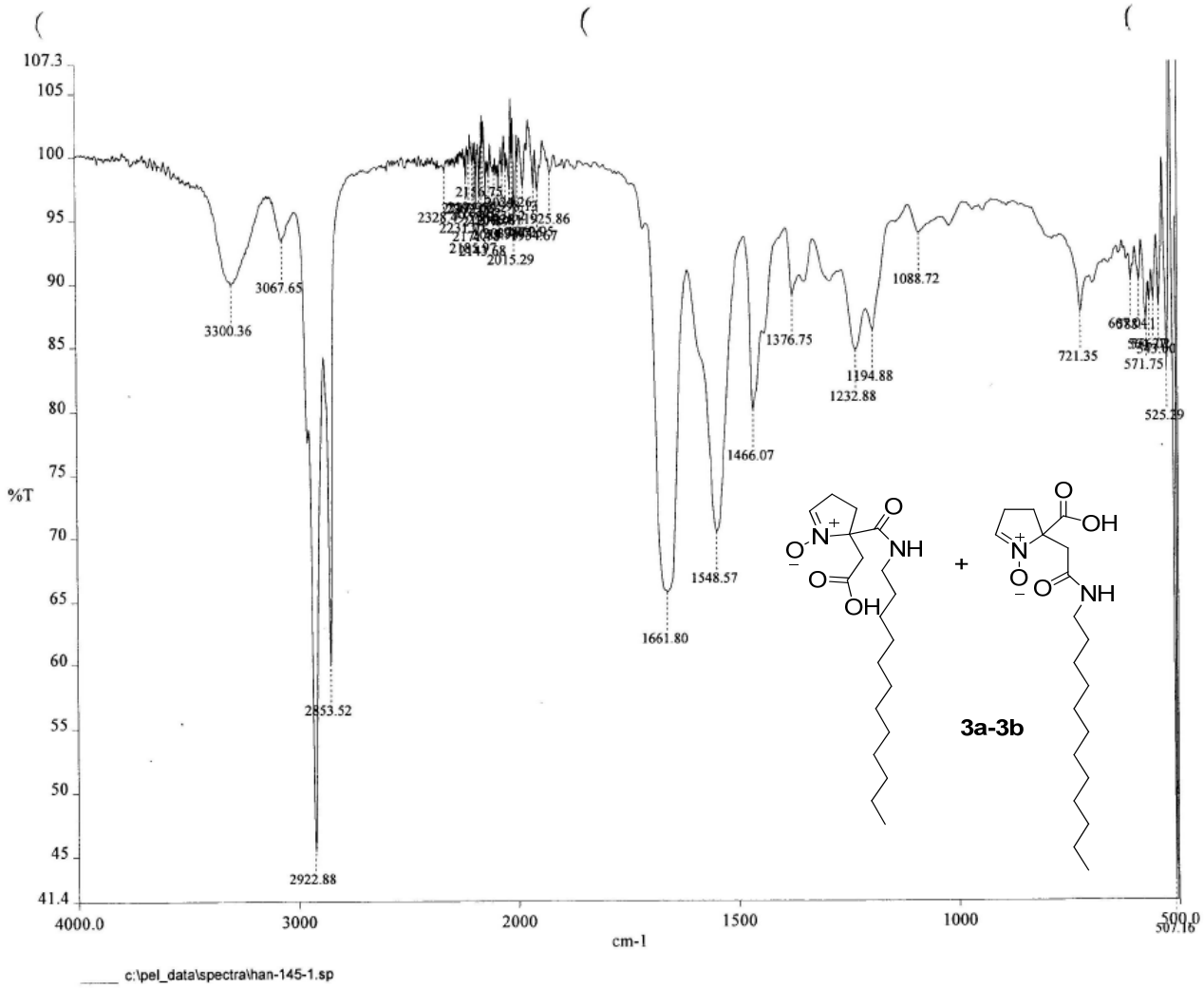


Figure S10. Neat IR spectrum of compound **3a** and **3b** mixture

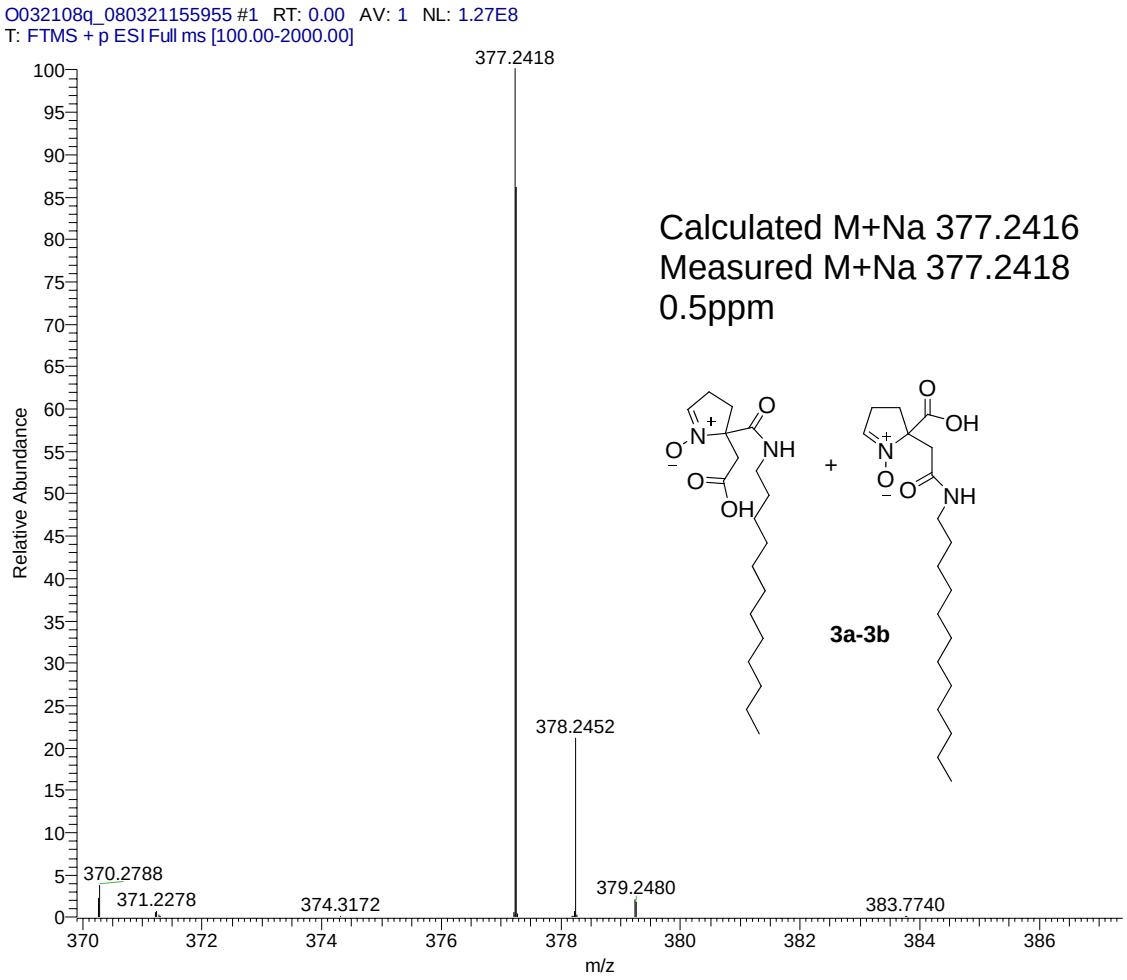


Figure S11. HRMS spectrum of compound **3a** and **3b** mixture

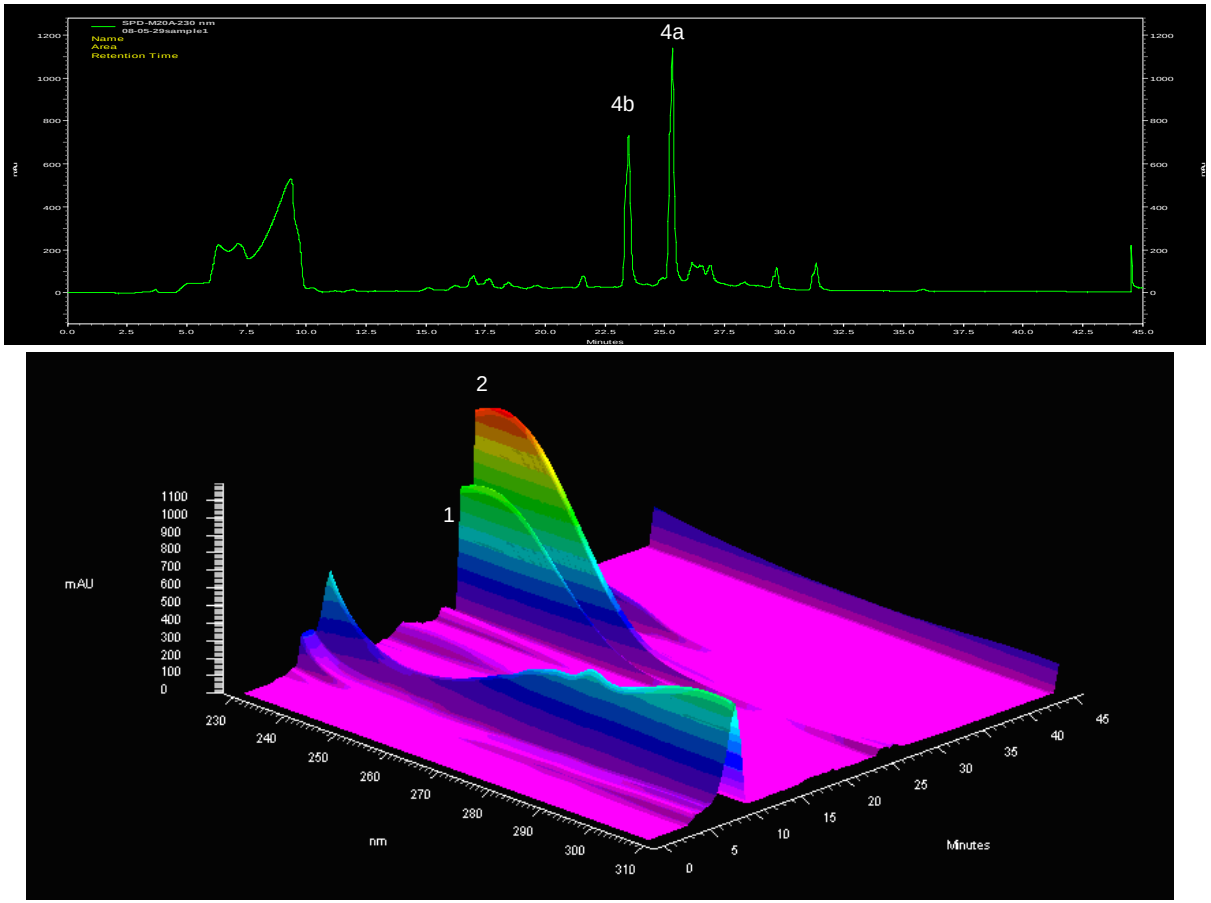


Figure S12. HPLC trace for crude product of **4a** and **4b** (before purification)

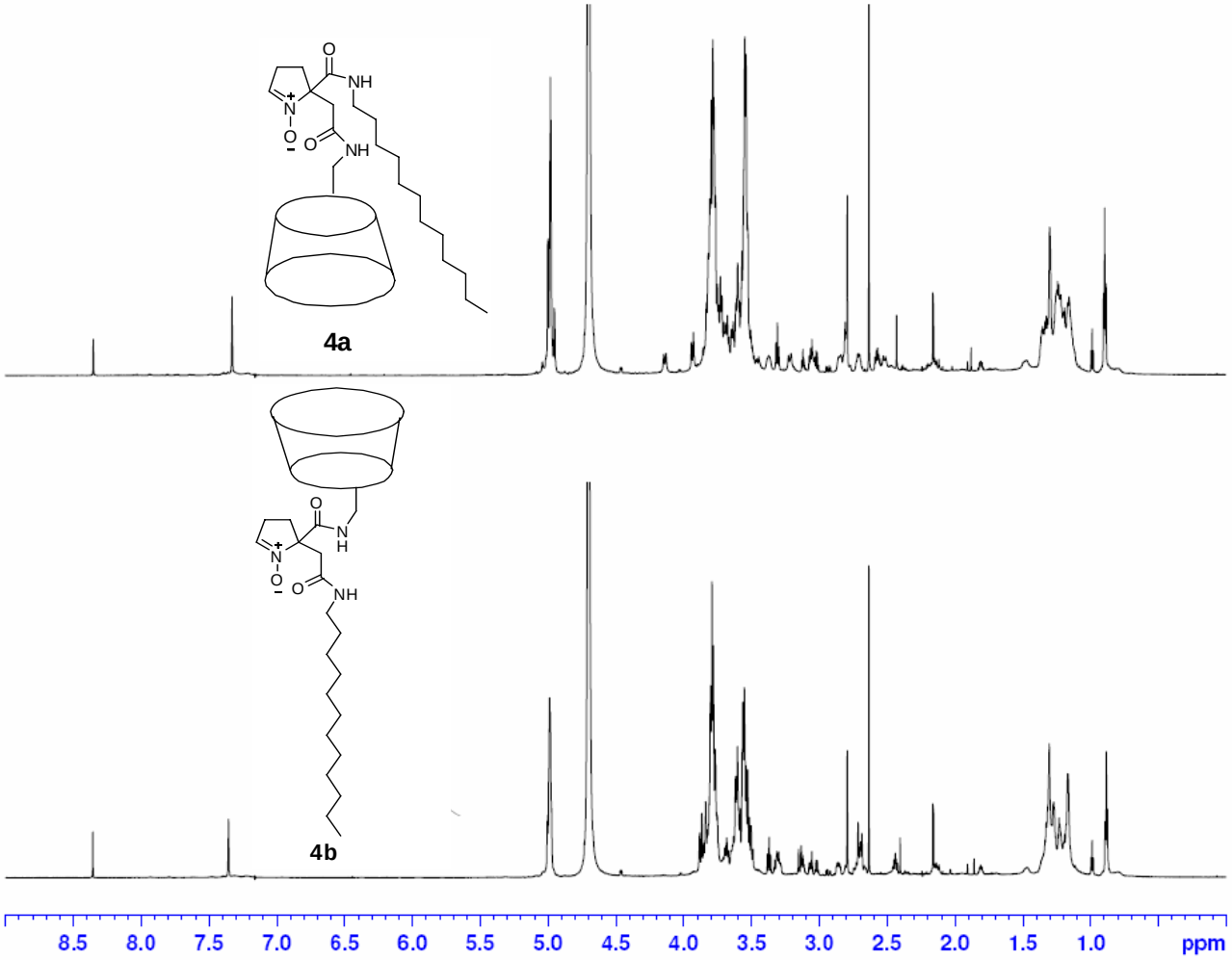


Figure S13. ^{1}H NMR spectra of compound **4a** and **4b** in D_2O

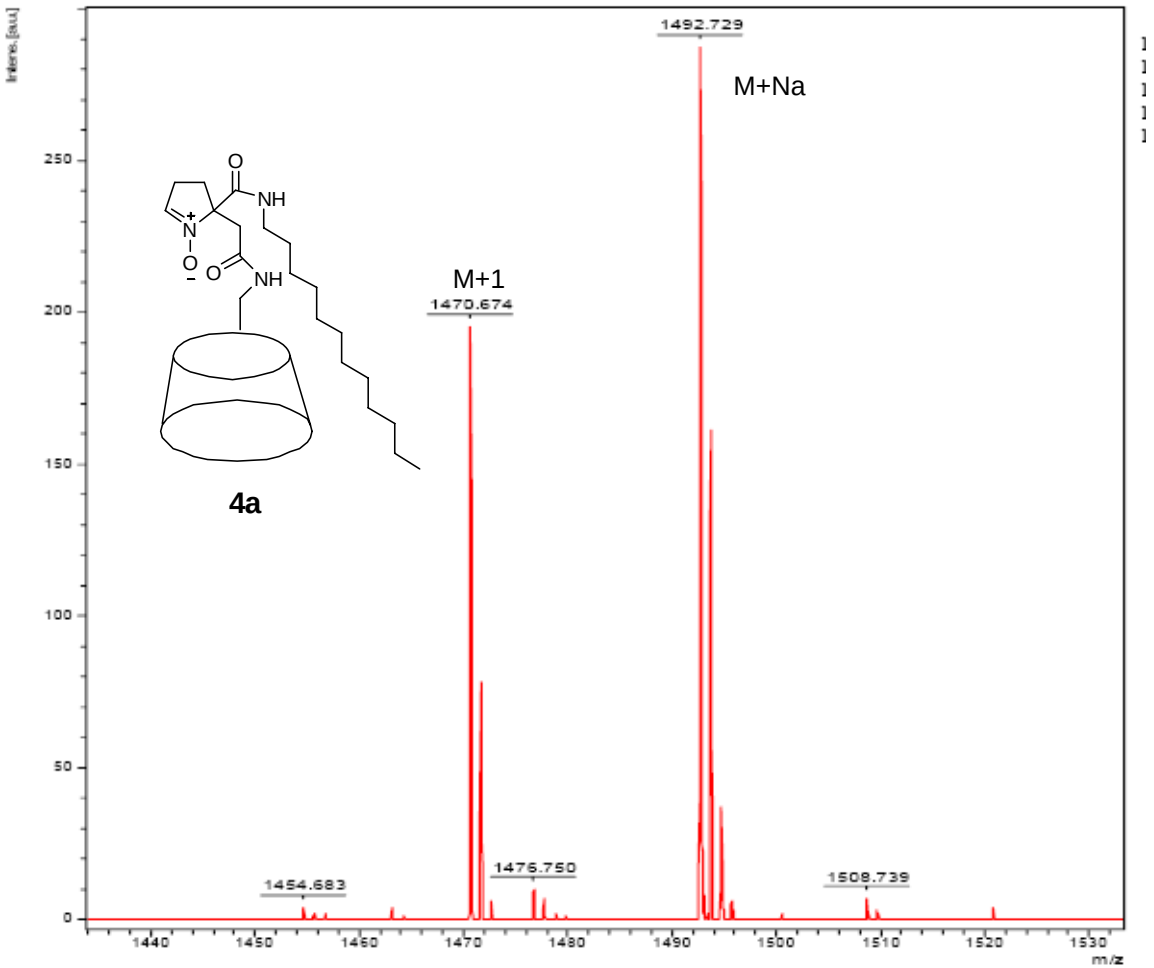


Figure S14. HRMS spectrum of compound **4a**

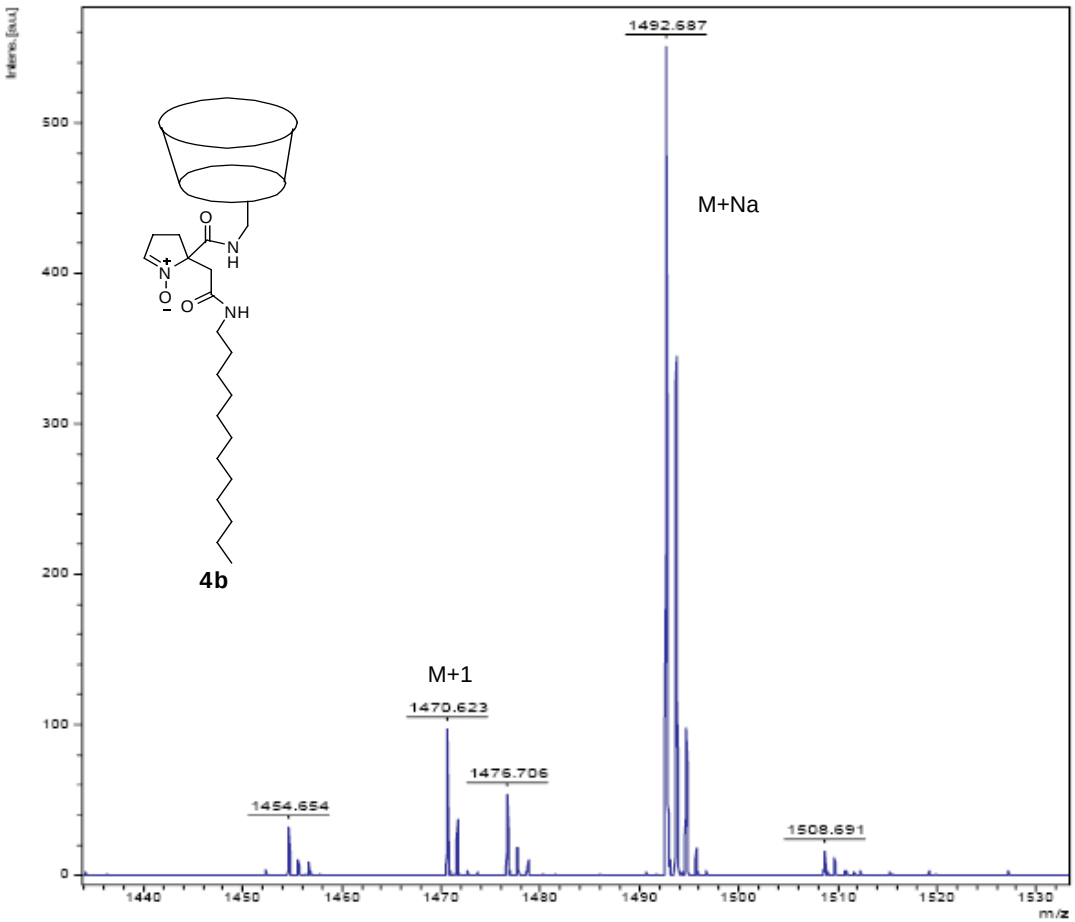


Figure S15. HRMS spectrum of compound **4b**

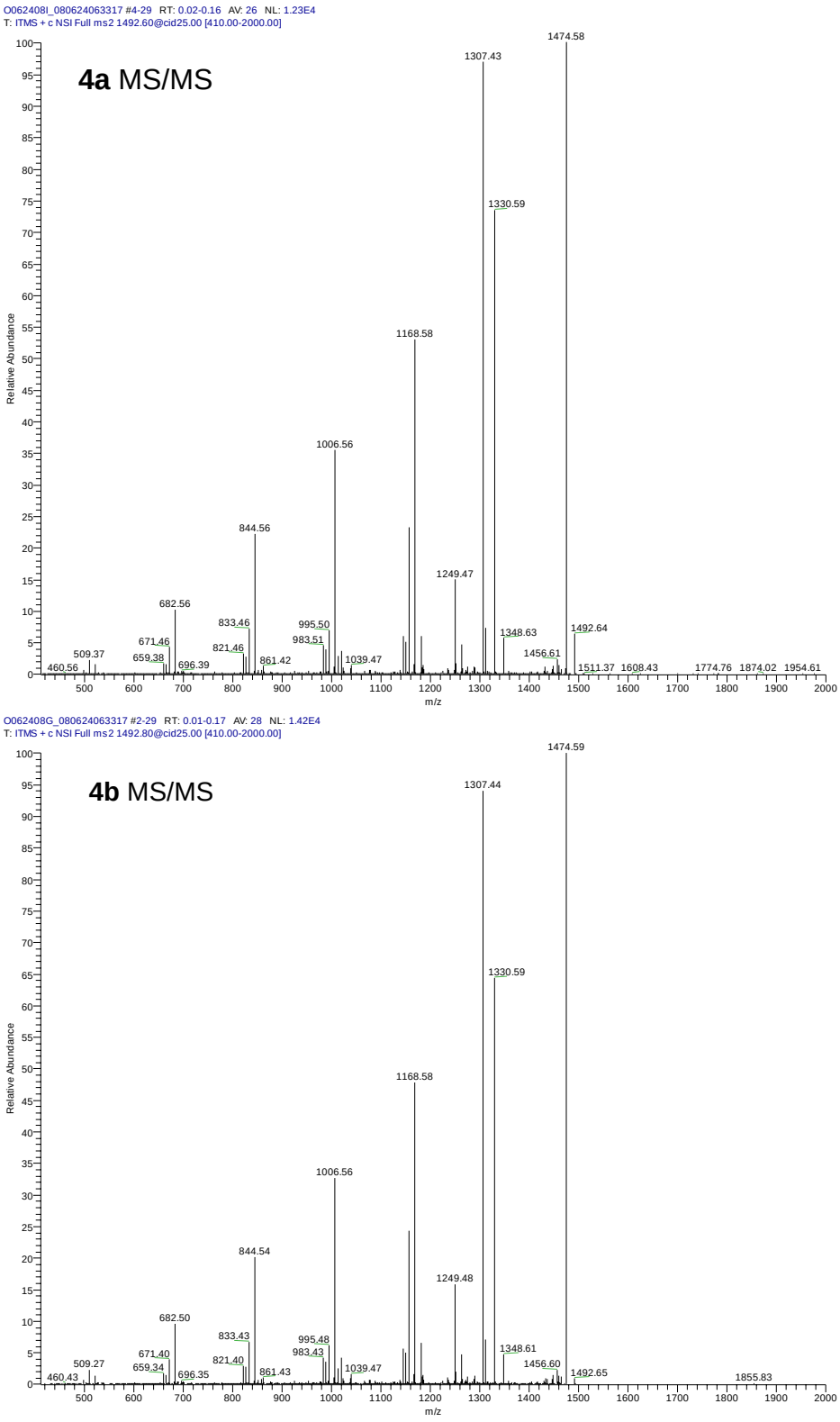


Figure S16. MS - MS analysis of compound **4a** and **4b**

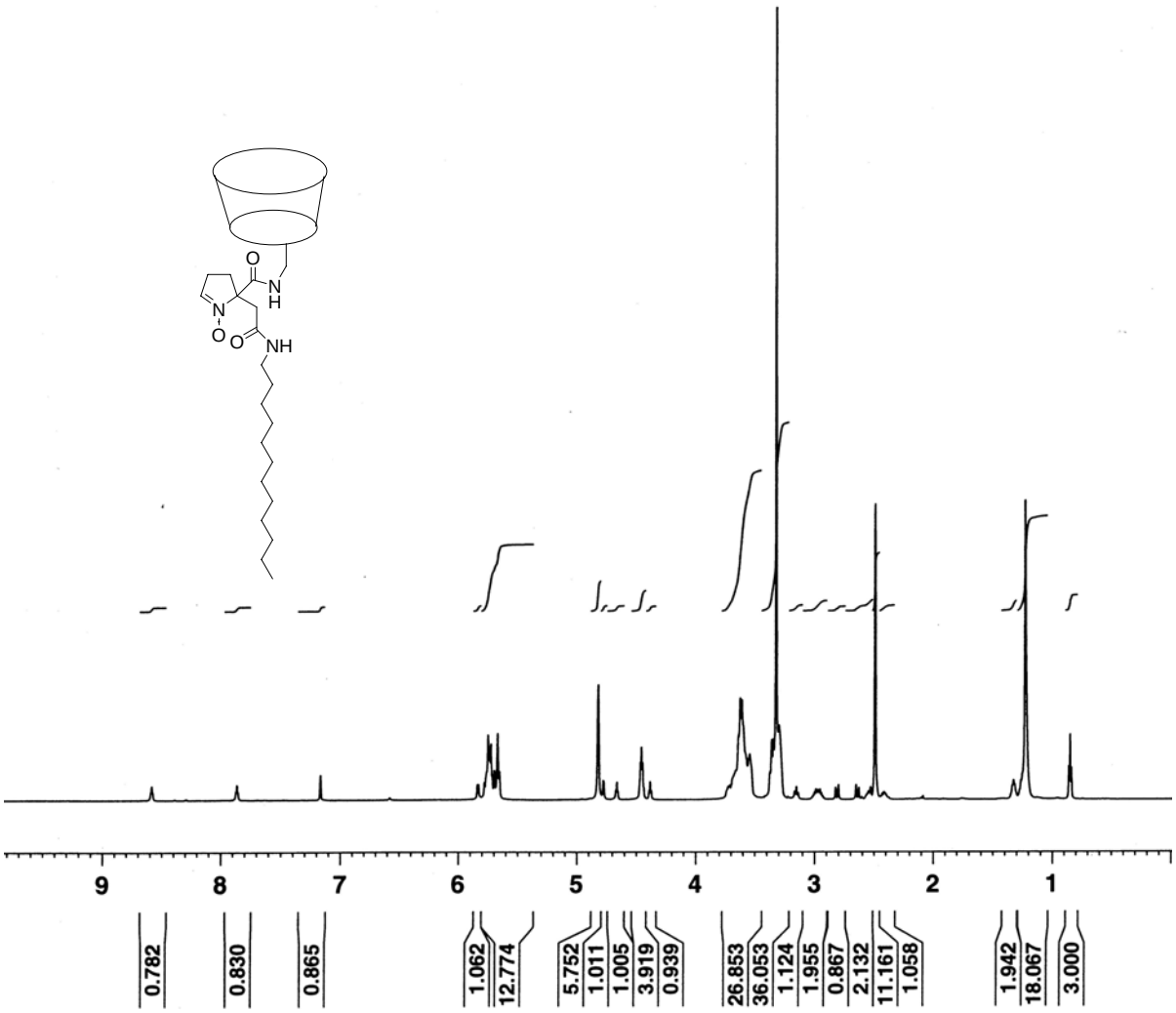


Figure S17. ^{1}H NMR spectrum of compound **4b** in DMSO-d_6

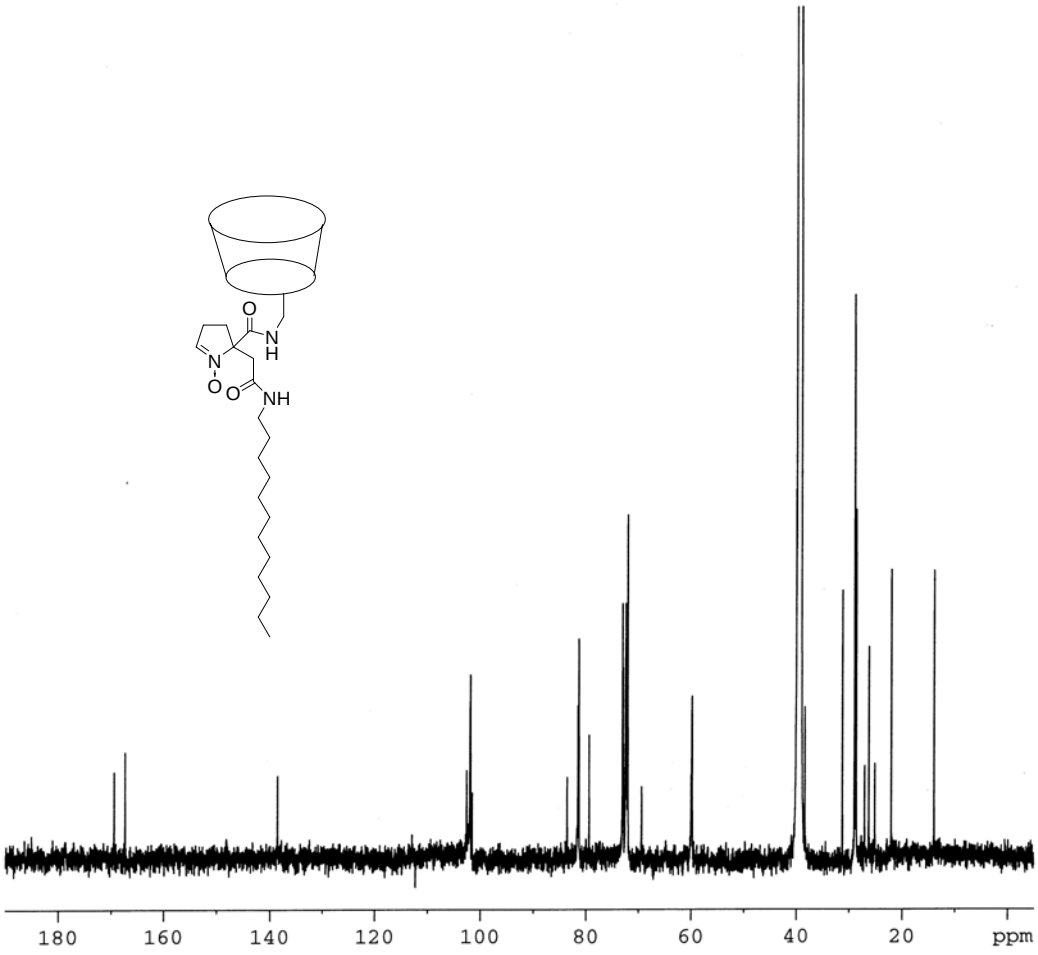


Figure S18. ^{13}C NMR spectrum of compound **4b** in DMSO-d_6

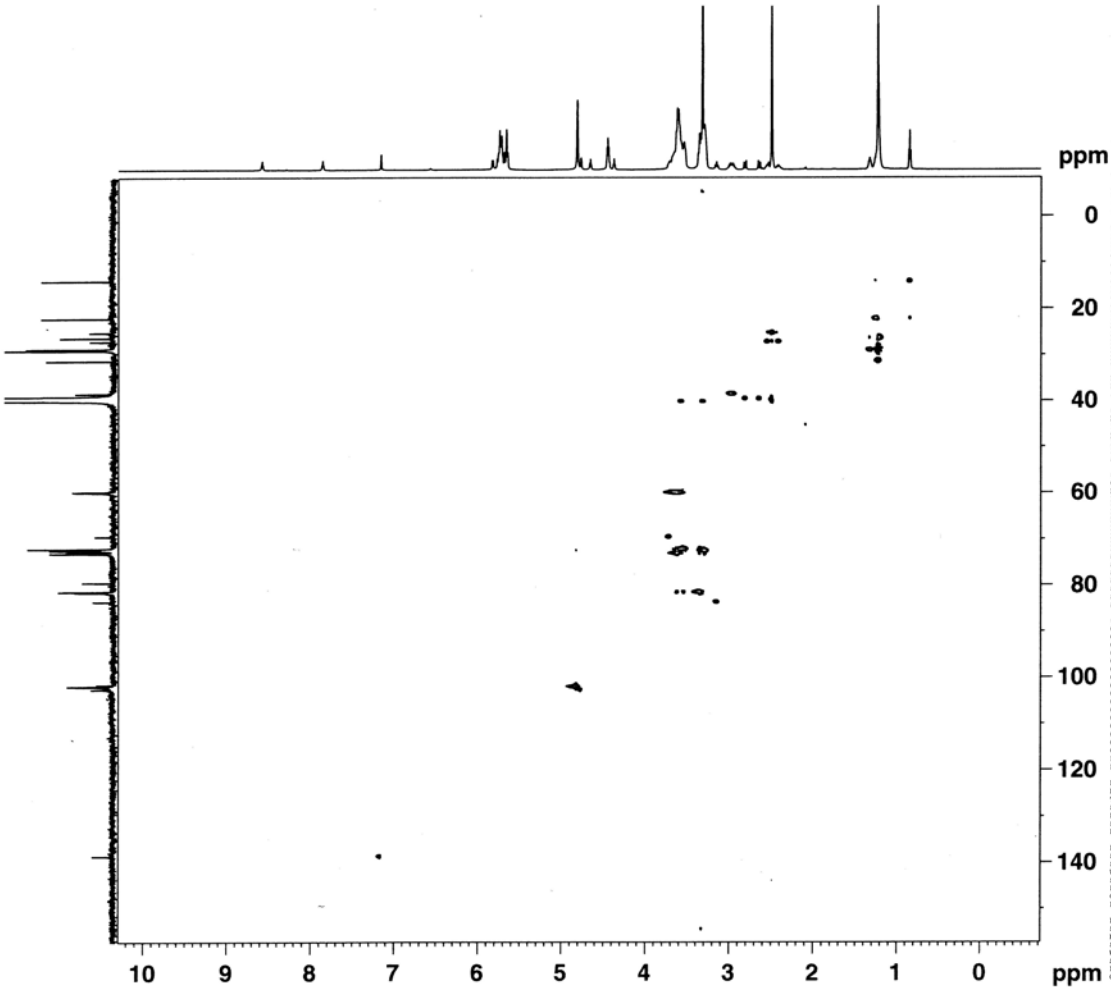


Figure S19. HSQC spectrum of compound **4b** in DMSO-d_6

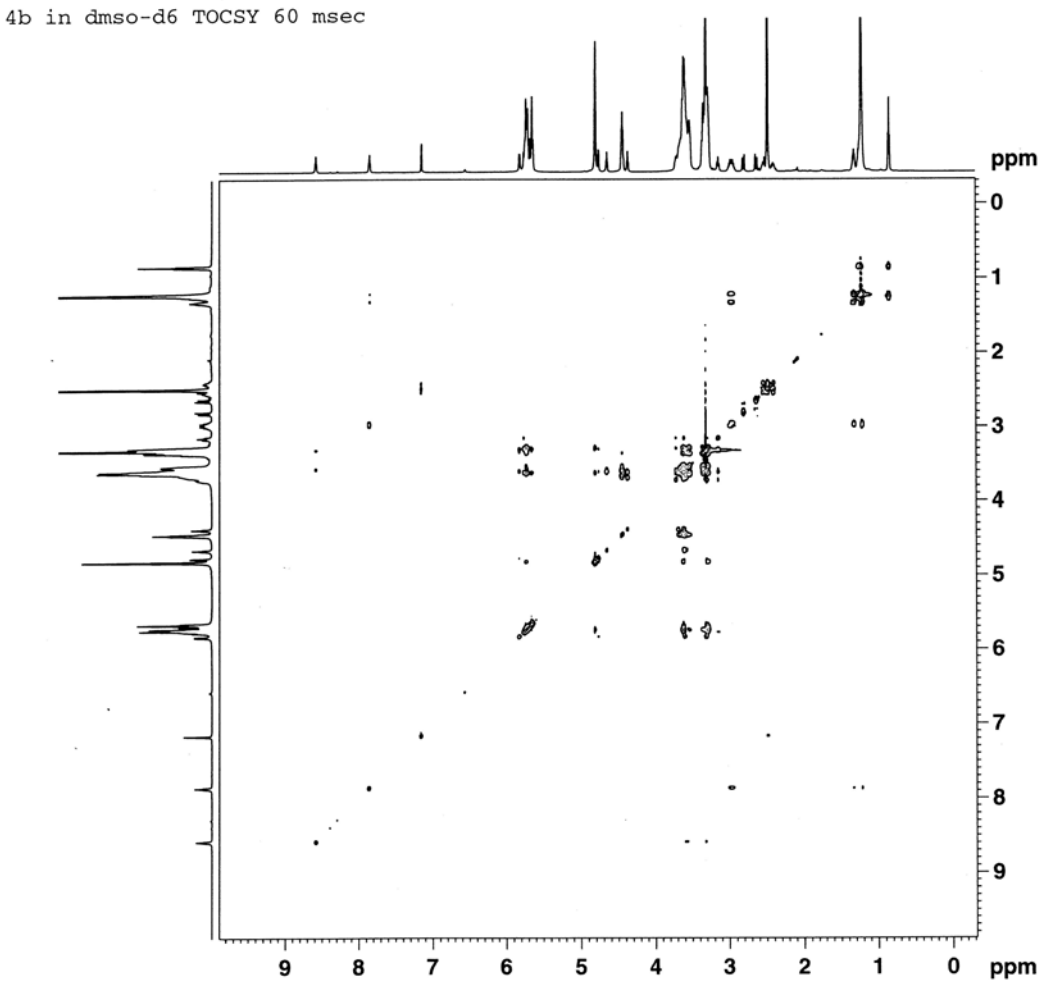


Figure S20. TOCSY spectrum of compound **4b** in DMSO-d_6

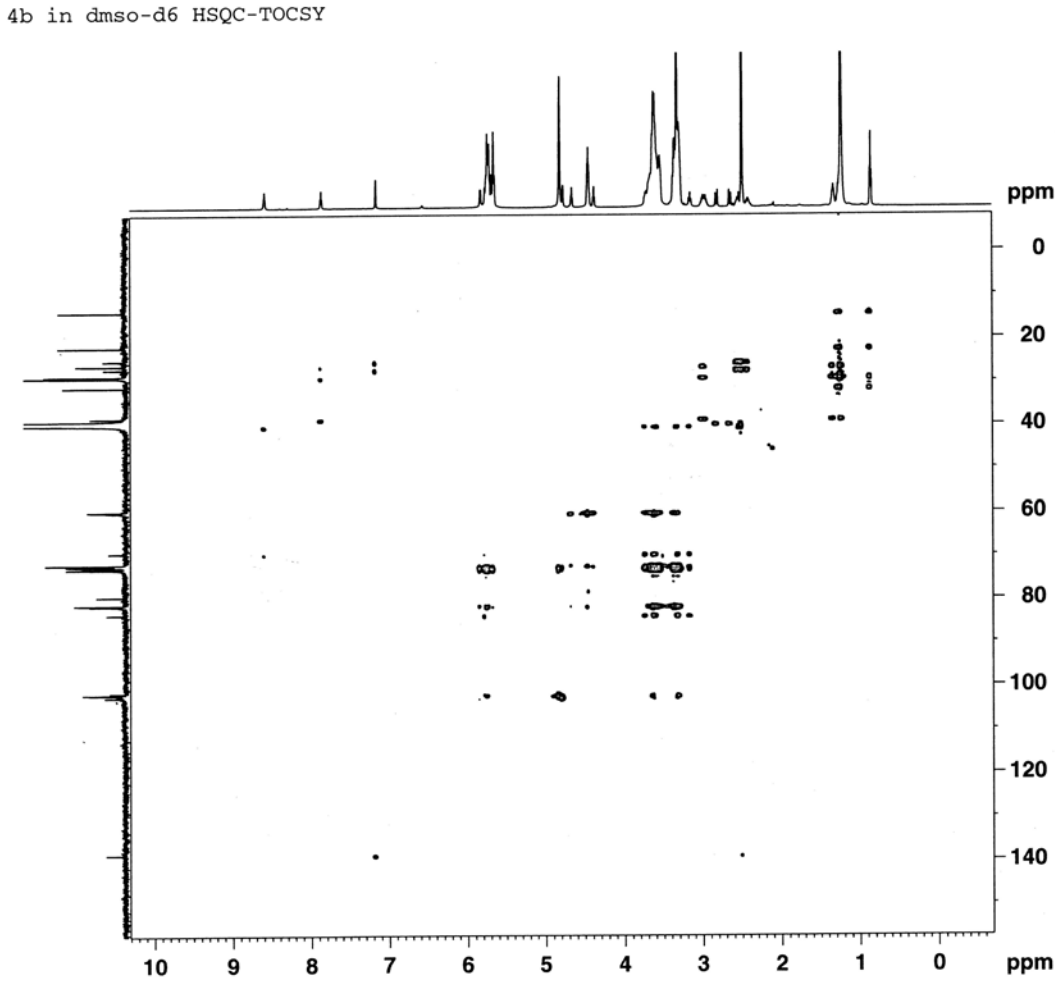


Figure S21. HSQC-COCSY spectrum of compound **4b** in DMSO-d_6

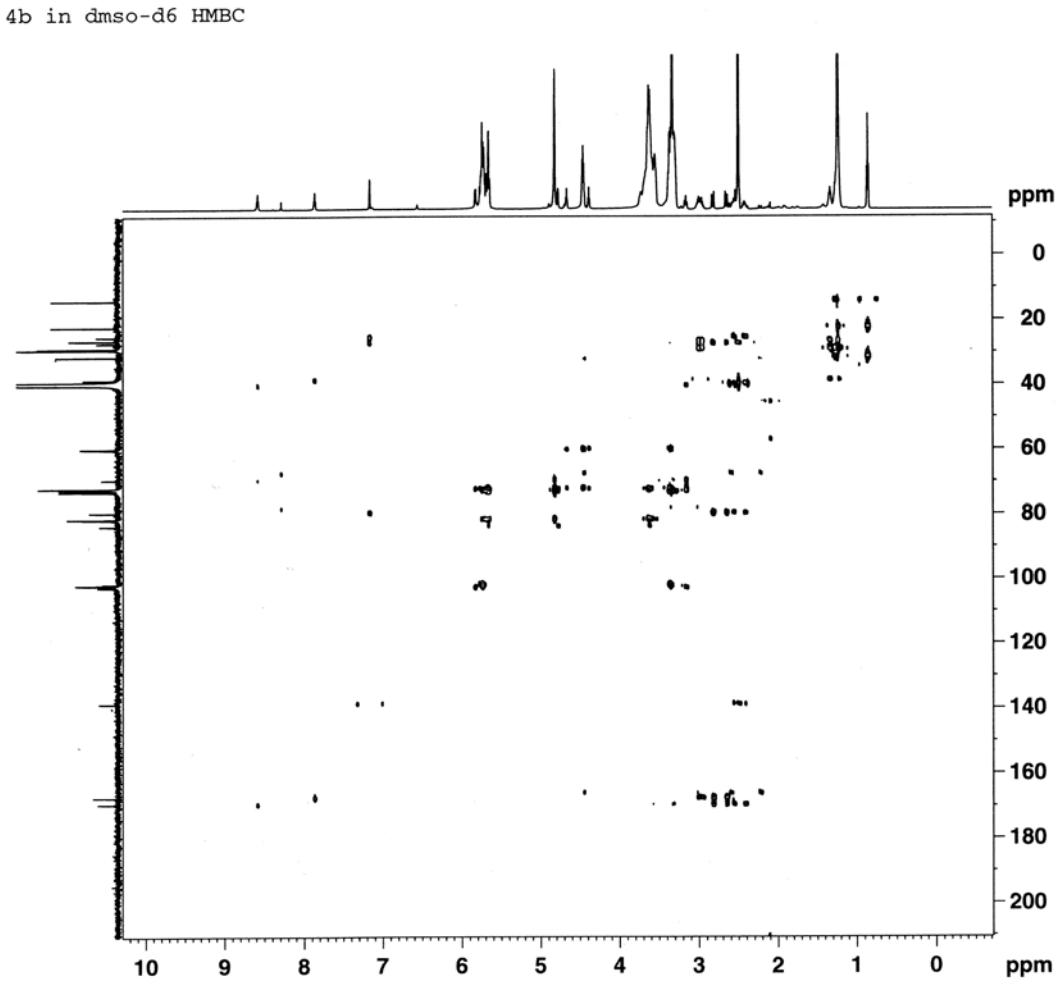


Figure S22. HMBC spectrum of compound **4b** in DMSO-d_6

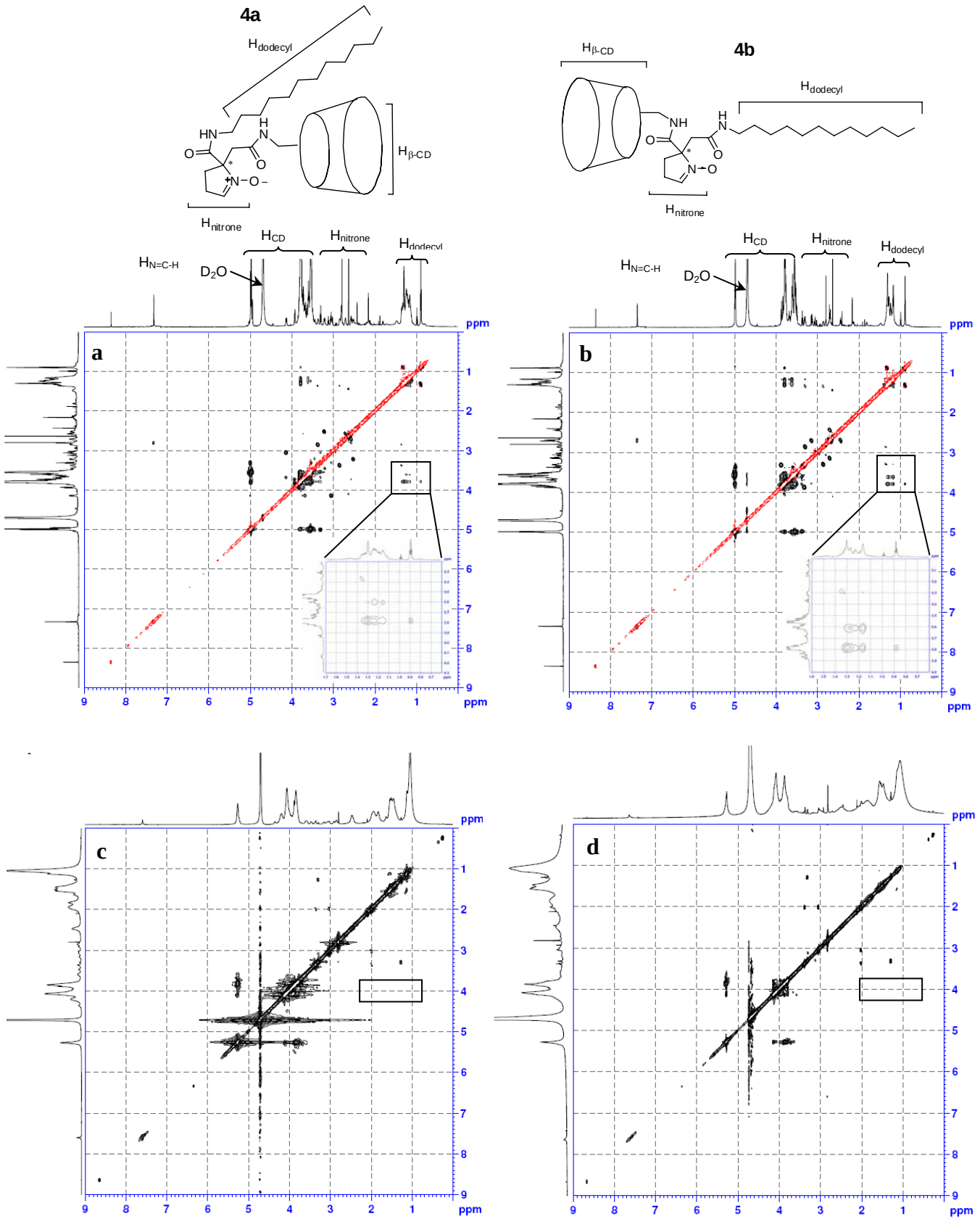


Figure S23. ROESY spectra of compounds a) **4a** and b) **4b** alone, and c) **4a** and d) **4b** in the presence of *l*-borneol in D_2O at 25°C.

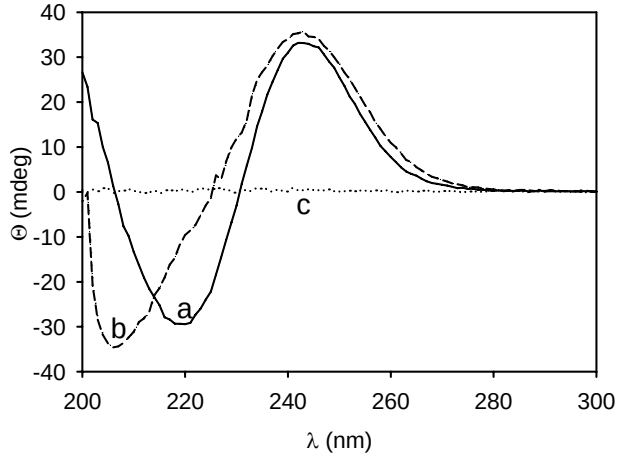


Figure S24. Induced Circular Dichroism spectra of 3.4 mM aqueous solutions of **4a** (a)**,** **4b** (b), and **1** (c).

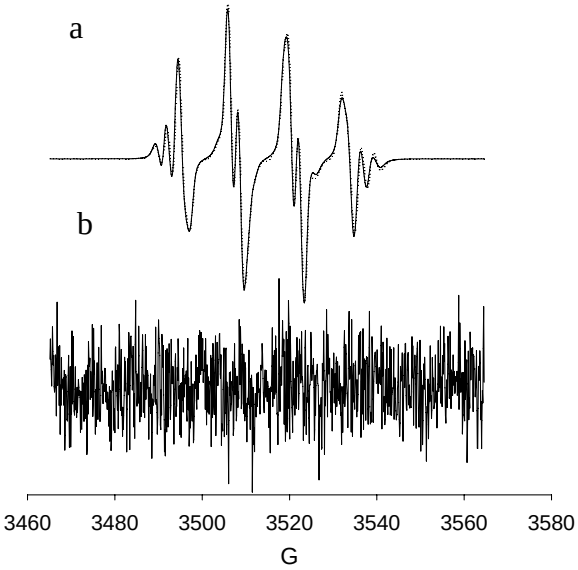


Figure S25. X-band EPR spectra of **1** (20 mM) in the presence of (a) Fe^{2+}/H_2O_2 and (b) xanthine/xanthine oxidase. Simulated spectrum is shown as a trace plot. EPR parameters for (a): **1**-OH': g = 2.0051, a_N = 13.2 G, $a_{\beta\text{-}H}$ = 9.7 G; **1**-OH'': g = 2.0051, a_N = 13.5 G, $a_{\beta\text{-}H}$ = 11.9 G; **1**-alkyl: g = 2.0049, a_N = 14.4 G, $a_{\beta\text{-}H}$ = 20.8 G; unidentified: g = 2.0051, a_N = 14.2 G, $a_{\beta\text{-}H}$ = 16.1 G.

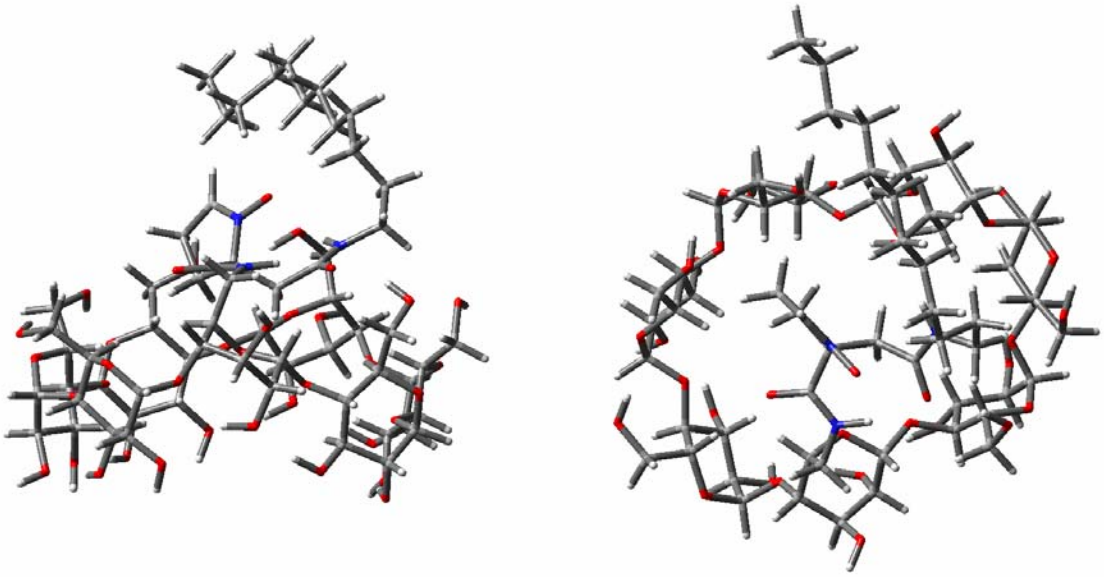
Table S1. Relative bottom-of-the-well energies at the HF/3-21G* level of theory of the various isomers of **4a** and **4b**, and their respective $O_2^{\bullet-}$ adducts.

	Relative Energies (*E*, kcal/mol)		Relative Energies (*E*, kcal/mol)
4a		**4b**	
5R-**4a** (*ex*)	-15.6	*5R*-**4b** (*ex*)[a]	-27.1
5R-**4a** (*in*)	-25.7	*5R*-**4b** (*in*)[a]	-0.8
5S-**4a** (*ex*)	-8.0	*5S*-**4b** (*ex*)	0.0
5S-**4a** (*in*)	-2.3	*5S*-**4b** (*in*)	-20.3
4a + borneol		**4b + borneol**	
5R-**4a** (*top*)	-53.9	*5R*-**4b** (*top*)[b]	0.0
5R-**4a** (*bottom*)	-33.8	*5R*-**4b** (*bottom*)[b]	-52.3
5S-**4a** (*top*)	-48.6	*5S*-**4b** (*top*)	-34.4
5S-**4a** (*bottom*)	-51.1	*5S*-**4b** (*bottom*)	-55.0
4a-OOH		**4b-OOH**	
2S,5R-**4a**-OOH (*ex*)	-22.6	*2S,5R*-**4b**-OOH (*ex*)	-26.9
2R,5R-**4a**-OOH (*ex*)	-24.6	*2R,5R*-**4b**-OOH (*ex*)	-36.5
2S,5R-**4a**-OOH (*in*)	-17.7	*2S,5R*-**4b**-OOH (*in*)	-12.5
2R,5R-**4a**-OOH (*in*)	-32.6	*2R,5R*-**4b**-OOH (*in*)	-15.2
2S,5S-**4a**-OOH (*ex*)	-37.2	*2S,5S*-**4b**-OOH (*ex*)	0.0
2R,5S-**4a**-OOH (*ex*)	-37.3	*2R,5S*-**4b**-OOH (*ex*)	-20.4
2S,5S-**4a**-OOH (*in*)	-18.6	*2S,5S*-**4b**-OOH (*in*)	-20.5
2R,5S-**4a**-OOH (*in*)	-13.8	*2R,5S*-**4b**-OOH (*in*)	-22.6

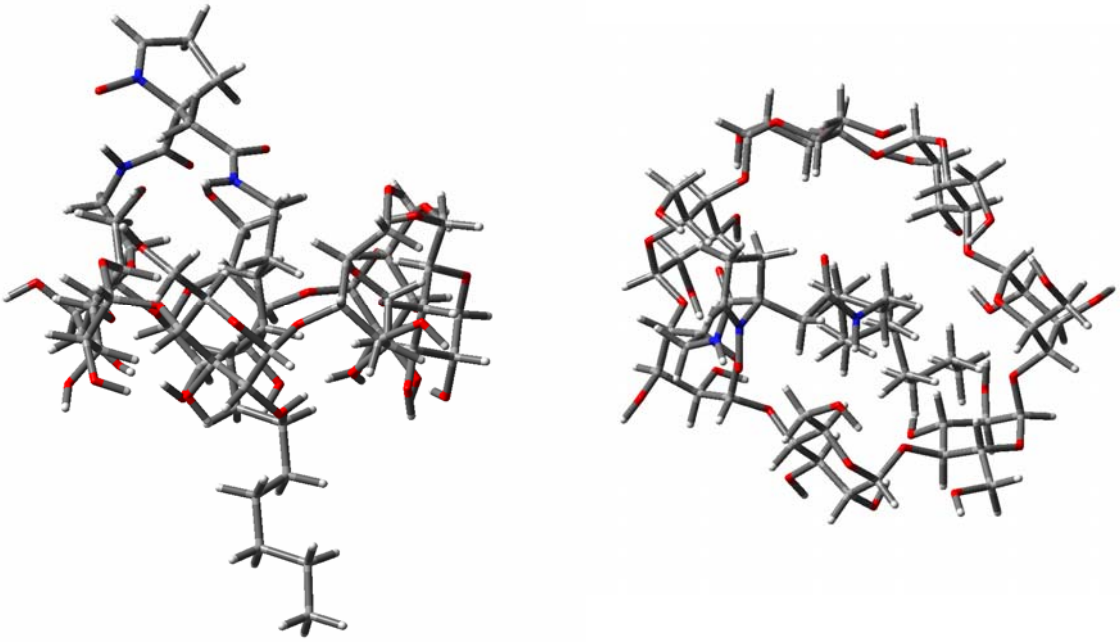
[a] "*ex*" refers to the position of the dodecyl group being outside the β-CD cavity while "*in*" refers to dodecyl group being included (see Figure 11 for example). [b] "*top*" refers to the location of borneol being on the same side of the β-CD annulus as the nitrone group while "*bottom*" is where the borneol being in the opposite side (see Figure 12 for example).

Side View

Top View

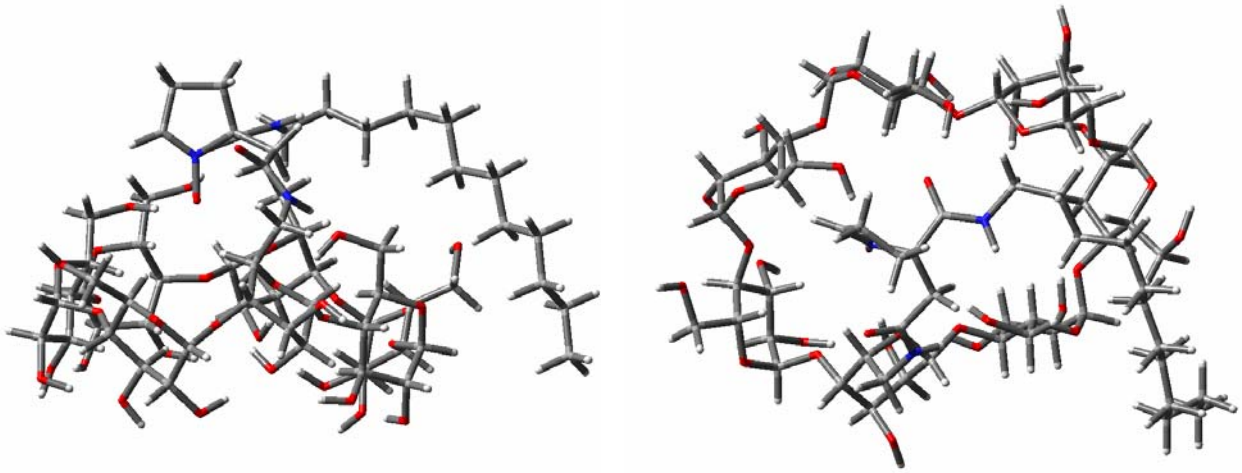


(5*S*)-4b (*excluded*) 27.1 kcal/mol

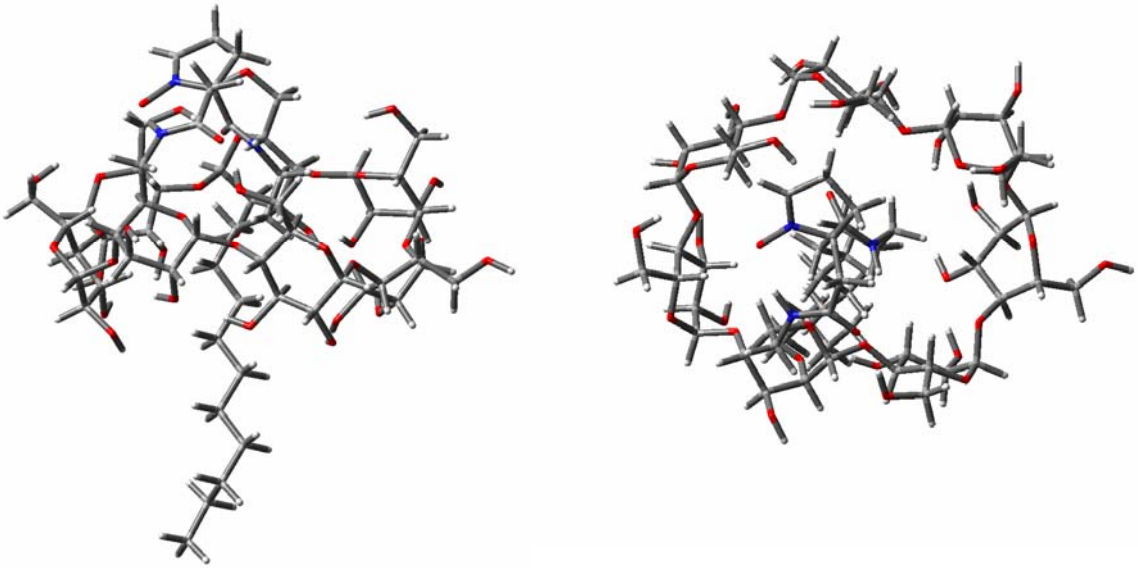


(5*S*)-4b (*included*) 6.8 kcal/mol

Figure S26. Side and top views of the optimized geometries of *(5S)*-**4b** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the *β*-CD cavity and their relative bottom-of-the-well energies.

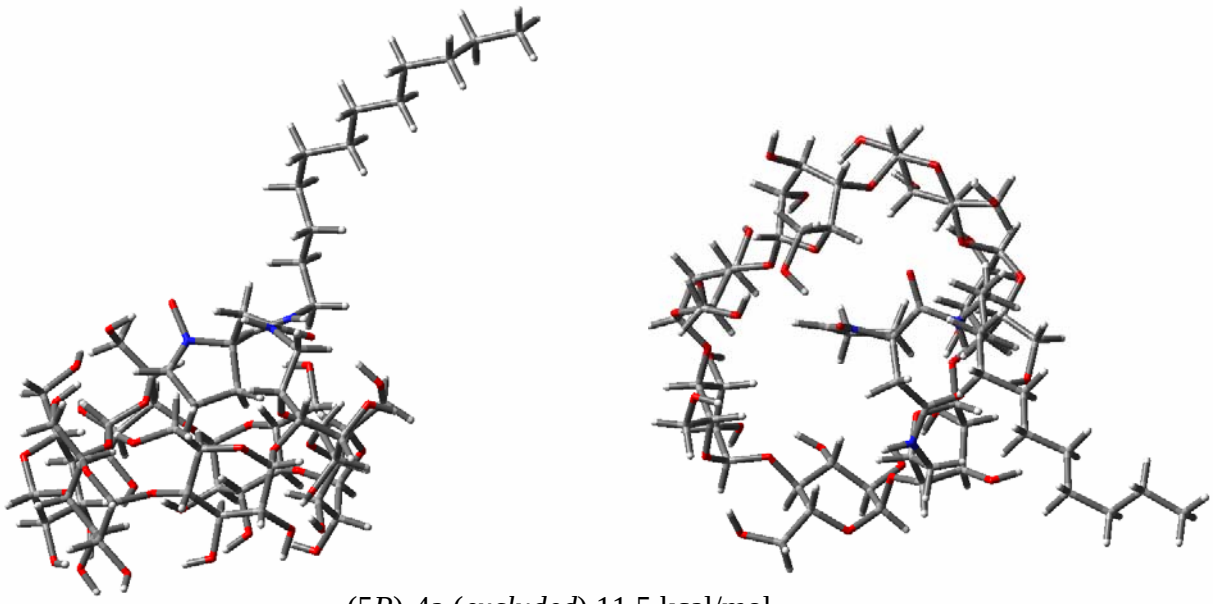


(5*S*)-4a (*excluded*) 19.1 kcal/mol

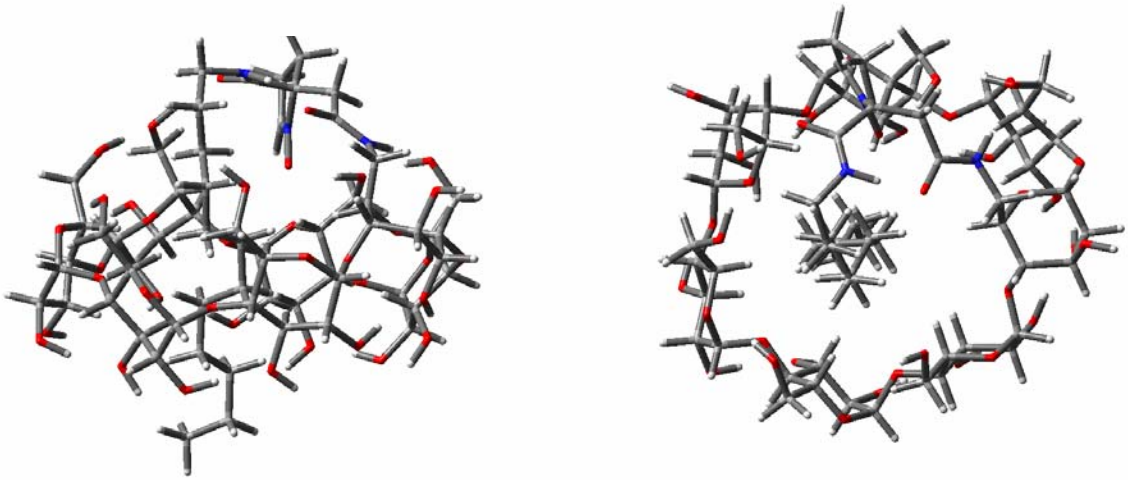


(5*S*)-4a (*included*) 24.8 kcal/mol

Figure S27. Side and top views of the optimized geometries of *(5S)*-**4a** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the *β*-CD cavity and their relative bottom-of-the-well energies.

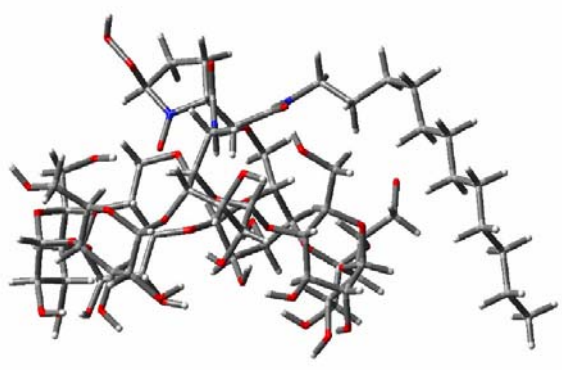


(5*R*)-4a (*excluded*) 11.5 kcal/mol

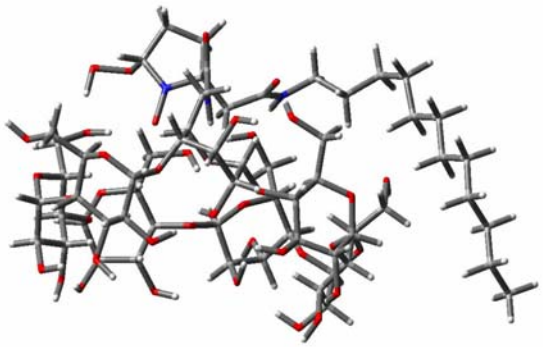


(5*R*)-4a (*included*) 1.4 kcal/mol

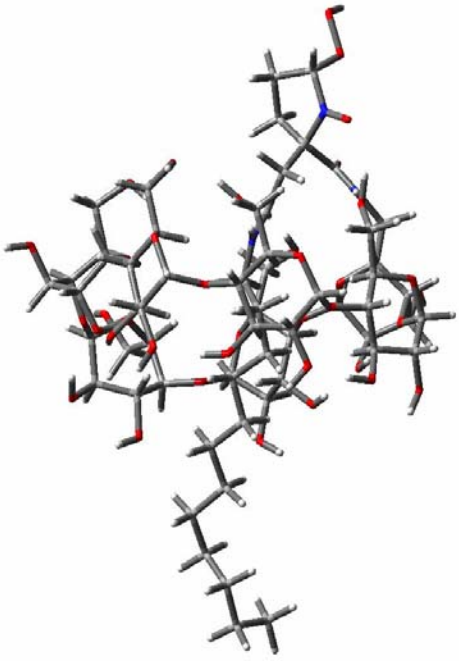
Figure S28. Side and top views of the optimized geometries of *(5R)*-**4a** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the β-CD cavity and their relative bottom-of-the-well energies.



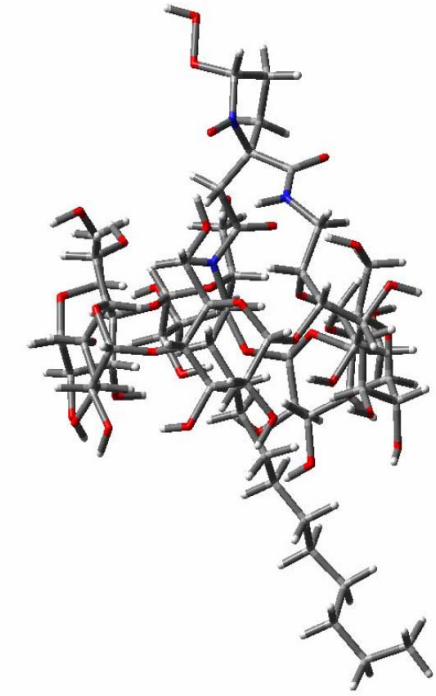
(*2S*,5*R*)-4b-OOH (*excluded*) -26.9 kcal/mol



(*2R*,5*R*)-4b-OOH (*excluded*) -36.5 kcal/mol

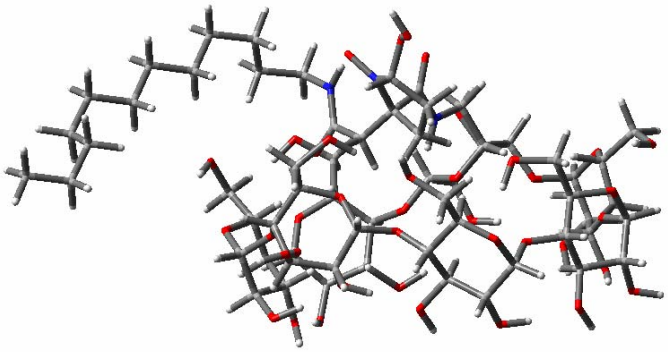


(*2S*,5*R*)-4b-OOH (*included*) -12.5 kcal/mol

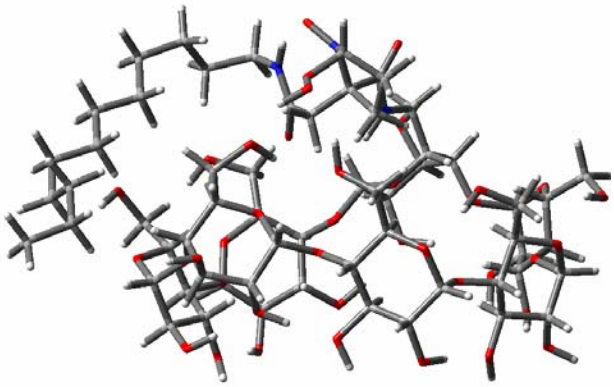


(*2R*,5*R*)-4b-OOH (*included*) -15.2 kcal/mol

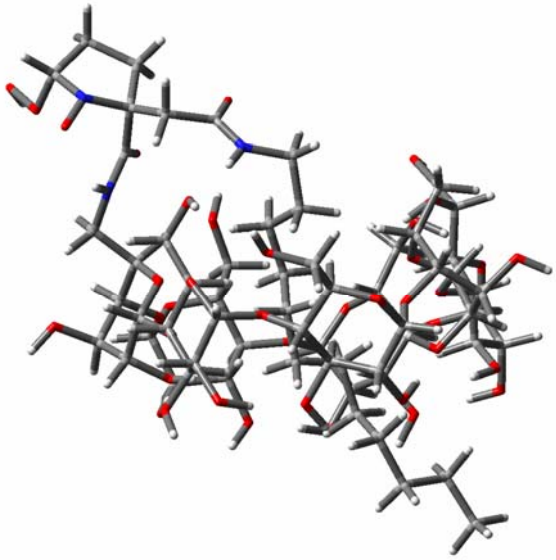
Figure S29. Optimized geometries of the various isomers of (*5R*)-**4b-OOH** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the β-CD cavity and their relative bottom-of-the-well energies.



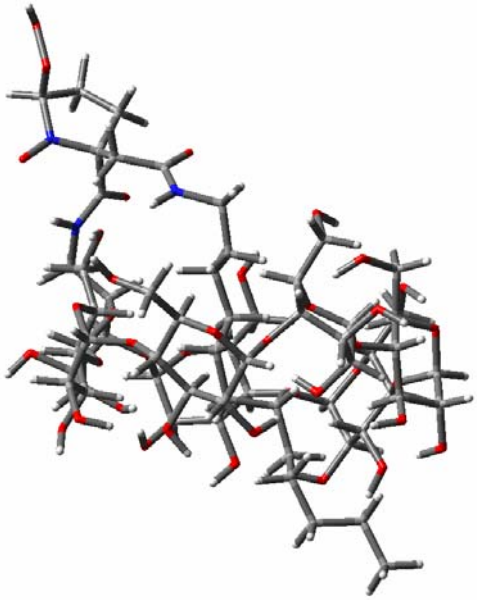
(*2S*,5*S*)-4b-OOH (*excluded*) 0.0 kcal/mol



(*2R*,5*S*)-4b-OOH (*excluded*) -20.4 kcal/mol

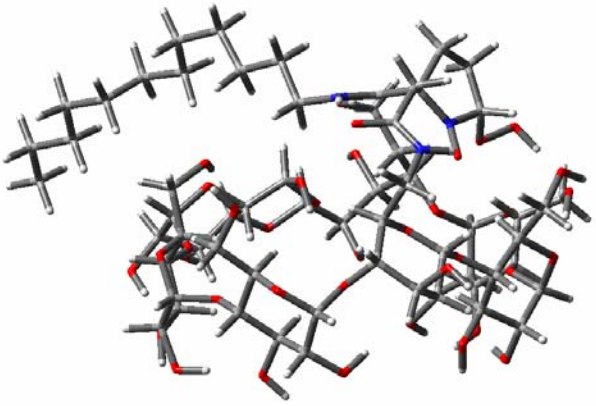


(*2S*,5*S*)-4b-OOH (*included*) -20.5 kcal/mol

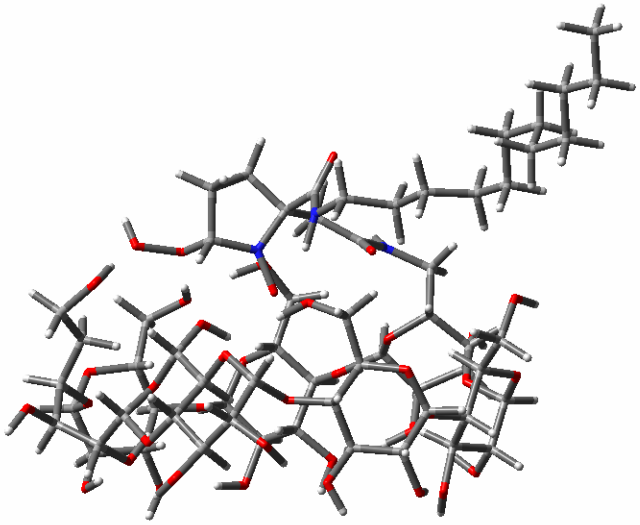


(*2R*,*5S*)-4b-OOH (*included*) -22.6 kcal/mol

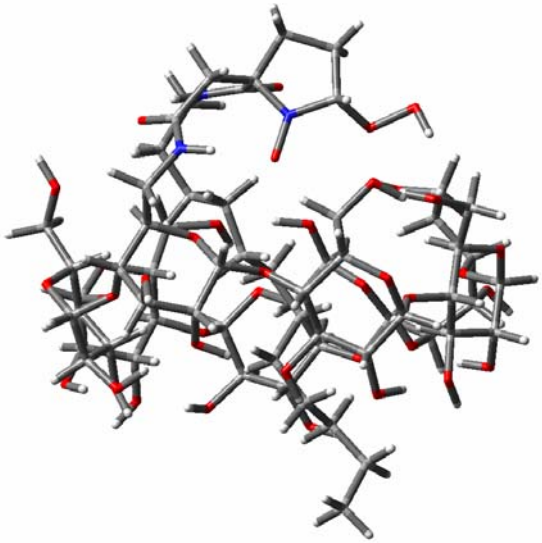
Figure S30. Optimized geometries of the various isomers of (*5S*)-**4b-OOH** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the *β*-CD cavity and their relative bottom-of-the-well energies.



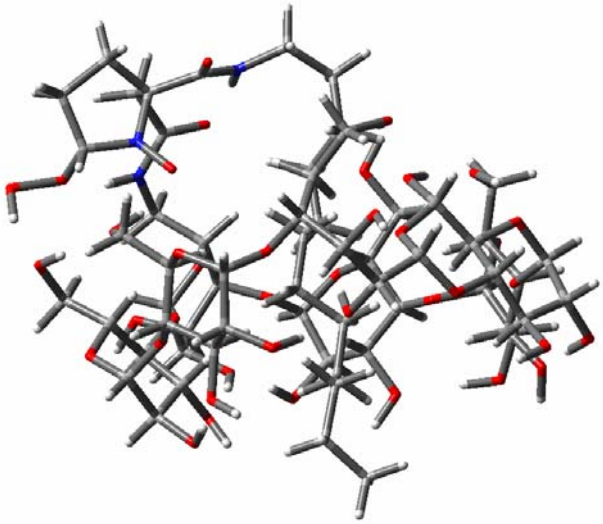
(*2S*,5*R*)-4a-OOH (*excluded*) -4.9 kcal/mol



(*2R*,5*R*)-4a-OOH (*excluded*) -6.8 kcal/mol

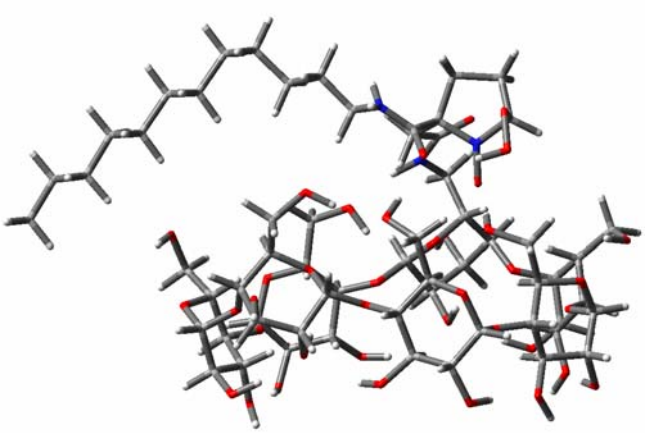


(*2S*,5*R*)-4a-OOH (*included*) 0.0 kcal/mol

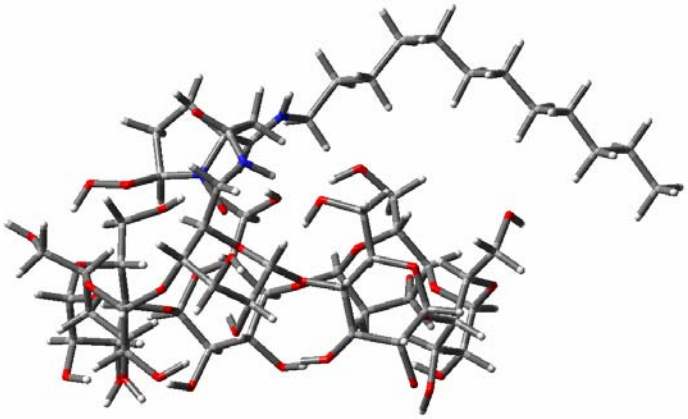


(*2R*,*5R*)-4a-OOH (*included*) -14.9 kcal/mol

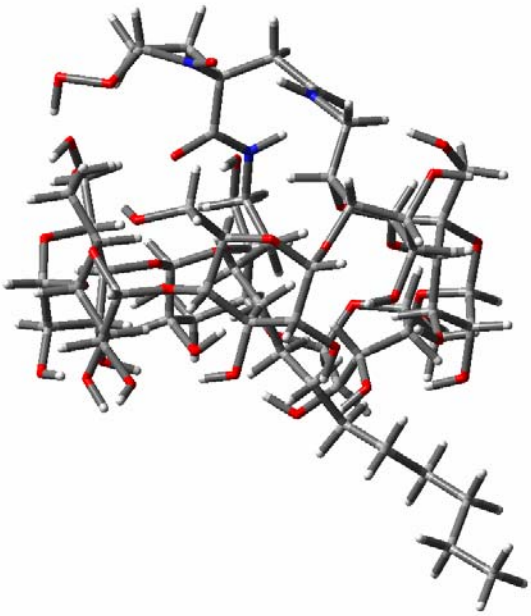
Figure S31. Optimized geometries of the various isomers of (*5R*)-**4a-OOH** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the *β*-CD cavity and their relative bottom-of-the-well energies.



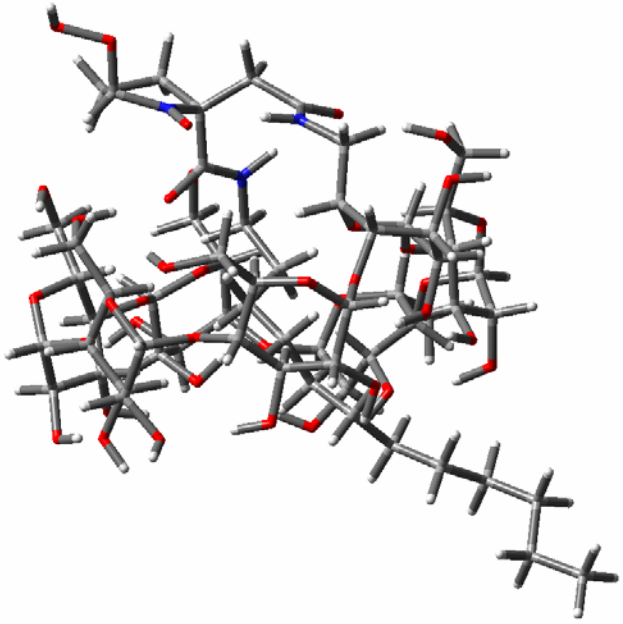
(*2S*,5*S*)-4a-OOH (*excluded*) -23.4 kcal/mol



(*2R*,5*S*)-4a-OOH (*excluded*) -23.6 kcal/mol

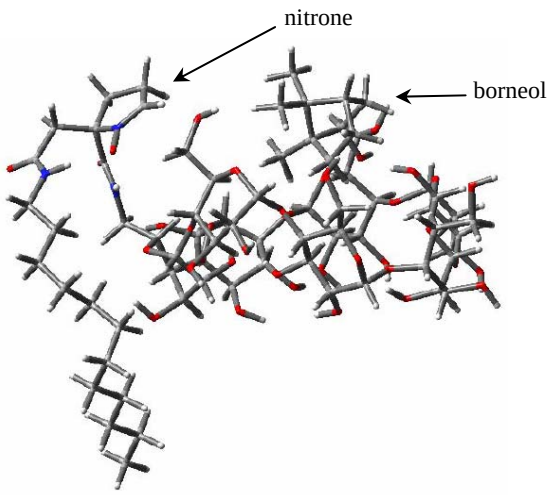


(*2S*,5*S*)-4a-OOH (*included*) -4.8 kcal/mol

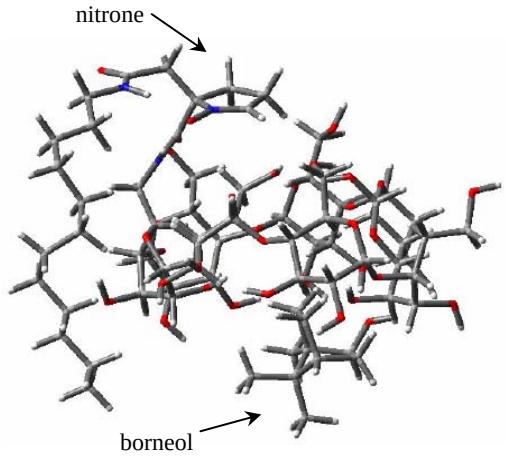


(*2R,5S*)-4a-OOH (*included*) -0.0 kcal/mol

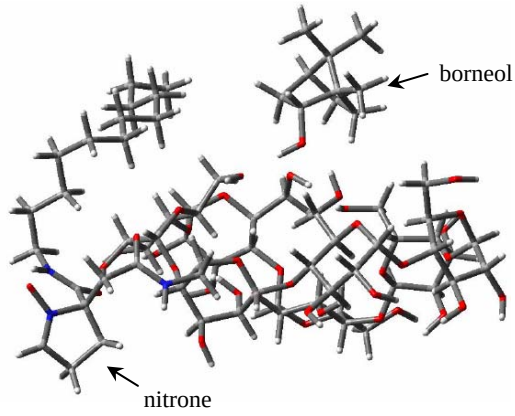
Figure S32. Optimized geometries of the various isomers of (*5S*)-**4a-OOH** at the HF/3-21G* level of theory showing the dodecyl group outside (top) and inside (bottom) of the *β*-CD cavity and their relative bottom-of-the-well energies.



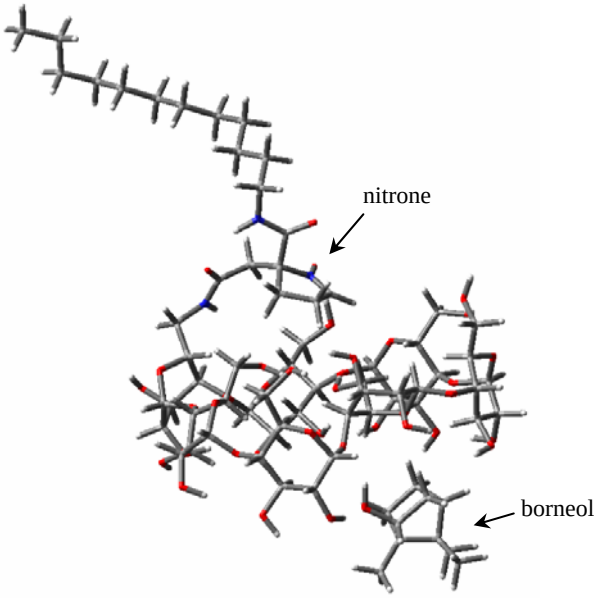
(*5R*)-4b + borneol (*top*) 0.0 kcal/mol



(*5R*)-4b + borneol (*bottom*) -52.3 kcal/mol

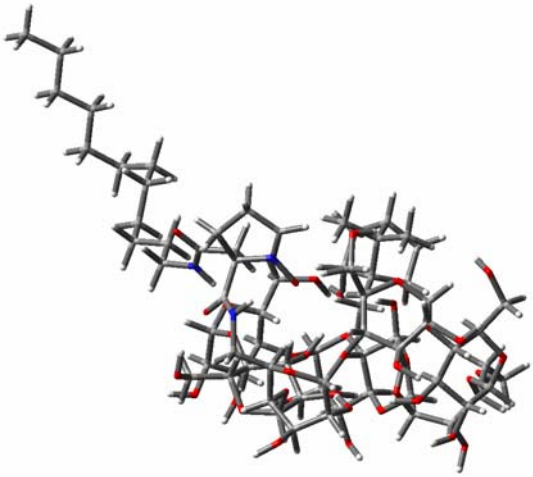


(*5R*)-4a + borneol (*top*) -53.9 kcal/mol

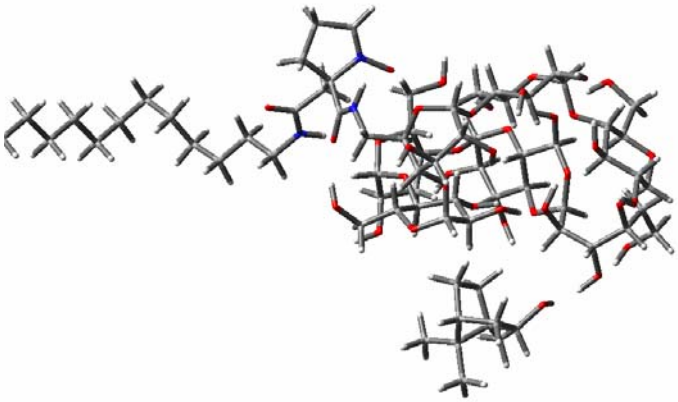


(*5R*)-4a + borneol (*top*) -33.8 kcal/mol

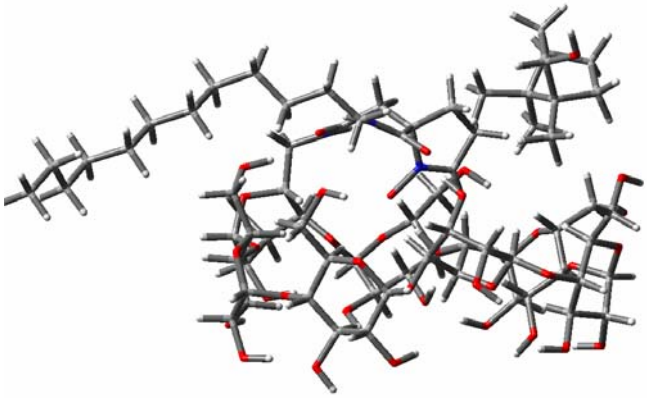
Figure S33. Optimized geometries of the R isomers of **4b/4a**---borneol complex at the HF/3-21G* level of theory showing the location of borneol relative to the nitrone group being on the same (left) and opposite side (right) of the annulus and their relative bottom-of-the-well energies.



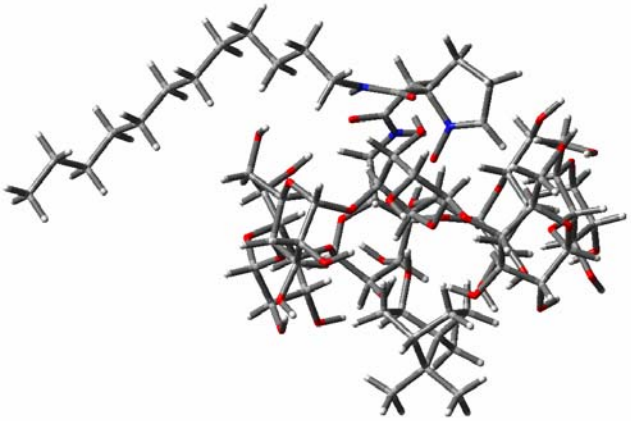
(5*S*)-4b + borneol (*top*) -34.4 kcal/mol



(5*S*)-4b + borneol (*bottom*) -55.0 kcal/mol



(5*S*)-4a + borneol (*top*) -48.6 kcal/mol



(5*S*)-4a + borneol (*bottom*) -51.1 kcal/mol

Figure S34. Optimized geometries of the S isomers of **4b/4a**---borneol complex at the HF/3-21G* level of theory showing the location of borneol relative to the nitrone group being on the same (left) and opposite side (right) of the annulus and their relative bottom-of-the-well energies.

(5*R*)-4b (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.309185	-3.504030	-0.237913
2	6	0	-0.180399	-4.613930	-1.147987
3	6	0	-0.994214	-5.577931	-0.277487
4	6	0	-2.124192	-4.862283	0.457844
5	6	0	-1.684563	-3.578494	1.160302
6	6	0	-1.027339	-3.741874	2.535989
7	6	0	4.730008	-1.336928	-2.102352
8	6	0	4.000273	-2.240165	-3.100237
9	6	0	2.525695	-2.328405	-2.721947
10	6	0	2.375081	-2.611262	-1.239994
11	6	0	3.114402	-1.618682	-0.372592
12	6	0	2.980070	-1.887155	1.119224
13	6	0	4.542417	3.968057	-1.661450
14	6	0	4.380560	3.532495	-3.107111
15	6	0	3.968649	2.071148	-3.151545
16	6	0	4.874915	1.179405	-2.324847
17	6	0	5.014439	1.723727	-0.909902
18	6	0	6.056565	1.048626	-0.041687
19	6	0	-0.040747	4.405732	-0.109200
20	6	0	0.636835	5.161557	-1.246591
21	6	0	1.933664	5.784501	-0.733047
22	6	0	2.819572	4.749933	-0.039991
23	6	0	2.065789	3.874752	0.958737
24	6	0	1.769959	4.542953	2.302156
25	6	0	-5.205548	4.061089	-0.839283
26	6	0	-4.445378	4.669432	-2.018037
27	6	0	-3.012016	4.159065	-1.957626
28	6	0	-2.425067	4.391846	-0.573440
29	6	0	-3.284216	3.843426	0.543660
30	6	0	-2.830328	4.184093	1.954687
31	6	0	-7.336882	-0.907167	-1.087799
32	6	0	-7.378794	-0.005345	-2.302321
33	6	0	-6.238552	0.988581	-2.237976
34	6	0	-6.268639	1.782599	-0.944413
35	6	0	-6.168211	0.797841	0.224467
36	6	0	-6.319778	1.360307	1.640962
37	6	0	-4.189395	-5.235293	-0.854850
38	6	0	-4.610321	-4.827855	-2.253490
39	6	0	-5.009948	-3.366554	-2.227373
40	6	0	-6.090121	-3.085420	-1.203480
41	6	0	-5.695903	-3.617904	0.173285
42	6	0	-6.876668	-3.725996	1.149006
43	8	0	-0.958915	-4.022946	-2.207454
44	8	0	-0.118790	-6.075598	0.756975
45	8	0	-3.049594	-4.437296	-0.569008
46	8	0	-0.832669	-2.822286	0.264854
47	8	0	4.210238	-1.698952	-4.402472
48	8	0	1.914996	-3.414900	-3.433551
49	8	0	0.963647	-2.482719	-0.958842
50	8	0	4.510952	-1.728937	-0.744293
51	8	0	3.408263	4.336184	-3.779376
52	8	0	4.014989	1.558453	-4.493464
53	8	0	4.153641	-0.062692	-2.319197
54	8	0	5.453966	3.109933	-0.993886
55	8	0	6.053112	1.675752	1.255882
56	8	0	0.891348	4.233010	-2.325085
57	8	0	1.601983	6.757358	0.278914
58	8	0	3.251554	3.858156	-1.091064
59	8	0	0.858828	3.391944	0.327496
60	8	0	0.956092	3.670953	3.101055
61	8	0	-5.104423	4.386817	-3.241527
62	8	0	-2.191519	4.882793	-2.891354
63	8	0	-1.151293	3.711332	-0.600962
64	8	0	-4.590587	4.442045	0.379466
65	8	0	-1.613681	3.457999	2.259135
66	8	0	-7.307513	-0.731490	-3.531087
67	8	0	-6.363617	1.912707	-3.333590
68	8	0	-5.127871	2.643149	-0.996141
69	8	0	-7.304704	-0.113599	0.097867
70	8	0	-5.139298	1.966303	2.173015
71	8	0	-3.565040	-5.033543	-3.207871
72	8	0	-5.540351	-2.968150	-3.507640
73	8	0	-6.129081	-1.647101	-1.156473
74	8	0	-5.228633	-4.990856	0.066252
75	8	0	-7.863123	-2.704523	0.968328
76	7	0	-0.725413	-2.415584	3.073659
77	8	0	1.639718	-1.572041	1.570067
78	6	0	-3.486781	0.731925	4.391673
79	7	0	-2.596287	0.581015	3.511462
80	8	0	-2.649563	0.985313	2.165451
81	6	0	-1.575939	-0.155405	5.491308
82	6	0	-1.414835	-0.216387	3.949070
83	6	0	-3.100925	0.076473	5.690174
84	6	0	-0.173746	0.469003	3.380741
85	6	0	3.219708	1.032729	4.960464
86	6	0	4.235764	0.164215	4.199141
87	6	0	5.570495	0.038655	4.963938
88	6	0	6.423342	-1.163103	4.499731
89	6	0	6.695428	-1.169215	2.983997
90	6	0	7.607597	-2.331170	2.546665
91	6	0	7.761853	-2.394406	1.013312
92	6	0	8.627654	-3.584163	0.555389
93	6	0	8.707882	-3.731806	-0.979136
94	6	0	9.470758	-2.586026	-1.672573
95	6	0	9.589491	-2.798017	-3.194412
96	6	0	-1.732947	-1.641238	3.470355
97	8	0	-2.899809	-2.029339	3.496497
98	6	0	10.358170	-1.652333	-3.880700
99	6	0	1.077541	0.163016	4.176340
100	7	0	1.948230	1.172772	4.241684
101	8	0	1.242191	-0.934714	4.710955
102	1	0	0.924859	-3.900650	0.547753
103	1	0	0.647294	-5.123922	-1.614655
104	1	0	-1.405927	-6.375551	-0.881571
105	1	0	-2.604448	-5.532863	1.156066
106	1	0	-2.559181	-2.968668	1.290889
107	1	0	-0.123629	-4.322718	2.487378

108	1	0	-1.729345	-4.241513	3.188697
109	1	0	5.794408	-1.338538	-2.267283
110	1	0	4.422502	-3.231818	-3.088292
111	1	0	2.050010	-1.382874	-2.939317
112	1	0	2.727021	-3.615066	-1.038621
113	1	0	2.755933	-0.625777	-0.583542
114	1	0	3.667438	-1.260667	1.657121
115	1	0	3.215433	-2.921484	1.334113
116	1	0	4.932008	4.970527	-1.581996
117	1	0	5.317242	3.656657	-3.627252
118	1	0	2.974309	1.980236	-2.739949
119	1	0	5.834493	1.071828	-2.814030
120	1	0	4.055515	1.683029	-0.423013
121	1	0	7.027641	1.132179	-0.515983
122	1	0	5.805977	0.016145	0.109866
123	1	0	-0.299433	5.078069	0.687321
124	1	0	-0.025235	5.917431	-1.638327
125	1	0	2.485568	6.223636	-1.553999
126	1	0	3.662321	5.238209	0.430727
127	1	0	2.648987	2.986644	1.138465
128	1	0	1.311516	5.508325	2.171455
129	1	0	2.702779	4.684154	2.829526
130	1	0	-6.229855	4.395177	-0.811533
131	1	0	-4.432485	5.742026	-1.897919
132	1	0	-3.007780	3.098857	-2.160854
133	1	0	-2.291497	5.460106	-0.449390
134	1	0	-3.355787	2.778874	0.440956
135	1	0	-3.630277	3.902251	2.621339
136	1	0	-2.624198	5.238497	2.057269
137	1	0	-8.191104	-1.549963	-1.010631
138	1	0	-8.312665	0.536075	-2.306224
139	1	0	-5.297549	0.460698	-2.293801
140	1	0	-7.187256	2.352217	-0.877736
141	1	0	-5.247996	0.239713	0.140348
142	1	0	-6.638346	0.527049	2.256547
143	1	0	-7.100611	2.105070	1.661373
144	1	0	-3.960021	-6.287342	-0.791765
145	1	0	-5.451130	-5.428064	-2.564258
146	1	0	-4.149287	-2.768150	-1.972897
147	1	0	-7.032970	-3.494464	-1.536490
148	1	0	-4.906235	-2.987873	0.550365
149	1	0	-6.504579	-3.760021	2.165171
150	1	0	-7.371087	-4.658102	0.933187
151	1	0	-1.408694	-3.248385	-1.832252
152	1	0	0.379380	-6.854676	0.478770
153	1	0	3.996938	-0.749397	-4.408146
154	1	0	0.949064	-3.363093	-3.359039
155	1	0	2.551788	4.324384	-3.306902
156	1	0	3.547544	2.162366	-5.089241
157	1	0	6.219258	2.620728	1.130498
158	1	0	1.016018	3.358653	-1.923692
159	1	0	1.290950	7.588379	-0.103014
160	1	0	0.021154	3.663015	2.787935
161	1	0	-5.425196	3.465309	-3.285353
162	1	0	-1.346378	4.421673	-3.003274
163	1	0	-1.812062	2.499030	2.138539
164	1	0	-6.640401	-1.447782	-3.503094
165	1	0	-6.586569	1.419143	-4.137332
166	1	0	-4.302240	1.488043	1.982035
167	1	0	-2.701759	-4.733897	-2.866478
168	1	0	-4.966292	-3.296438	-4.215552
169	1	0	-7.545084	-1.812164	1.171085
170	1	0	0.226327	-2.098685	3.101904
171	1	0	1.009996	-1.536968	0.836397
172	1	0	-4.388569	1.252898	4.151868
173	1	0	-3.328377	0.691917	6.547780
174	1	0	-3.629952	-0.865089	5.762434
175	1	0	-1.200374	-1.046094	5.965323
176	1	0	-1.027666	0.698436	5.867170
177	1	0	3.613698	2.028778	5.117449
178	1	0	3.026475	0.582979	5.926285
179	1	0	4.418991	0.596636	3.222495
180	1	0	3.787061	-0.813341	4.074247
181	1	0	6.141132	0.954225	4.839492
182	1	0	5.368646	-0.075760	6.026057
183	1	0	7.368982	-1.153703	5.034942
184	1	0	5.909973	-2.082064	4.770244
185	1	0	5.752580	-1.265805	2.460646
186	1	0	7.118214	-0.218976	2.679029
187	1	0	8.586432	-2.222937	3.006141
188	1	0	7.187320	-3.269072	2.901269
189	1	0	6.777931	-2.468854	0.558135
190	1	0	8.206561	-1.464997	0.672646
191	1	0	9.631050	-3.479321	0.959166
192	1	0	8.209774	-4.496447	0.972390
193	1	0	9.202952	-4.668909	-1.218449
194	1	0	7.700900	-3.790996	-1.384458
195	1	0	8.969873	-1.641265	-1.487324
196	1	0	10.466569	-2.510772	-1.244010
197	1	0	10.096430	-3.738856	-3.385337
198	1	0	8.595785	-2.876397	-3.625540
199	1	0	10.431177	-1.817145	-4.949880
200	1	0	11.363329	-1.574055	-3.479931
201	1	0	9.855487	-0.704297	-3.719142
202	1	0	-0.009062	0.165098	2.357757
203	1	0	-0.349413	1.529358	3.384069
204	1	0	1.701503	2.065017	3.839066

(5*R*)-4b (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.069707	2.771117	-2.486229
2	6	0	-1.151612	4.243579	-2.109290
3	6	0	-2.499022	4.803645	-2.554486
4	6	0	-3.639239	3.961396	-2.014179
5	6	0	-3.458713	2.478200	-2.289162
6	6	0	-3.804532	1.975431	-3.696149
7	6	0	4.236600	2.275085	-2.631839
8	6	0	3.559587	3.551282	-2.183890
9	6	0	2.220045	3.210086	-1.575770

10	6	0	1.352807	2.545936	-2.627037	66	8	0	-4.072288	1.448966	5.394845
11	6	0	2.035848	1.286344	-3.152764	67	8	0	-2.390002	-0.767182	5.827917
12	6	0	1.375665	0.740774	-4.427674	68	8	0	-2.080017	-2.496258	3.572652
13	6	0	6.079019	-2.310249	-1.138902	69	8	0	-5.402896	-1.037645	3.093045
14	6	0	6.703693	-1.233772	-0.235459	70	8	0	-3.560390	-3.141575	0.838995
15	6	0	5.787138	-0.020761	-0.191161	71	8	0	-3.872533	5.665316	1.668267
16	6	0	5.660407	0.631078	-1.555280	72	8	0	-4.249327	3.750427	3.670623
17	6	0	5.593698	-0.452359	-2.656628	73	8	0	-4.489824	1.071515	2.756477
18	6	0	6.929982	-0.561355	-3.398441	74	8	0	-5.645608	3.028764	-0.110976
19	6	0	2.169079	-4.519650	0.539624	75	8	0	-5.507528	0.175326	-1.082186
20	6	0	3.405138	-4.486162	1.428657	76	7	0	-4.125553	0.560733	-3.513244
21	6	0	4.573258	-5.100562	0.655970	77	8	0	-0.040485	0.895709	-4.436161
22	6	0	4.795351	-4.388236	-0.676652	78	6	0	-5.797996	-2.662574	-4.878364
23	6	0	3.521765	-4.206233	-1.492757	79	7	0	-5.440399	-2.072139	-3.819429
24	6	0	3.060690	-5.438897	-2.264113	80	8	0	-6.317385	-1.683833	-2.807645
25	6	0	-1.667305	-3.697905	4.183083	81	6	0	-3.433152	-2.855805	-4.795974
26	6	0	-0.221383	-3.528220	4.596082	82	6	0	-3.941419	-1.833613	-3.769341
27	6	0	0.649194	-3.248712	3.386751	83	6	0	-4.632840	-3.008705	-5.772884
28	6	0	0.454587	-4.321712	2.325340	84	6	0	-3.485702	-2.017649	-2.331712
29	6	0	-1.019119	-4.477270	2.011183	85	6	0	-3.726461	-0.407082	-4.333402
30	6	0	-1.356866	-5.628145	1.086653	86	8	0	-3.268560	-0.239611	-5.452180
31	6	0	-5.202470	0.257595	3.657514	87	6	0	-0.602647	-0.674177	-0.288160
32	6	0	-4.350607	0.124874	4.905280	88	6	0	-1.058136	0.072084	0.985891
33	6	0	-3.056295	-0.585702	4.576082	89	6	0	-0.235262	1.334850	1.308233
34	6	0	-3.354210	-1.909029	3.892715	90	6	0	1.251347	1.091800	1.634160
35	6	0	-4.171196	-1.665627	2.630041	91	6	0	1.951979	2.414471	2.012839
36	6	0	-4.576557	-2.896491	1.834027	92	6	0	3.469110	2.273245	2.241144
37	6	0	-4.904689	4.237315	0.046289	93	6	0	4.147653	3.647877	2.414517
38	6	0	-4.754517	4.553877	1.525229	94	6	0	5.641480	3.520306	2.769515
39	6	0	-4.236811	3.357901	2.295610	95	6	0	6.380708	4.874153	2.810801
40	6	0	-5.126094	2.155342	2.053484	96	6	0	-2.095524	-1.453710	-2.089550
41	6	0	-5.146991	1.842319	0.570302	97	8	0	-1.401457	-1.031126	-3.017492
42	6	0	-6.041597	0.683939	0.151762	98	7	0	-1.740359	-1.457454	-0.807309
43	8	0	-0.957635	4.426734	-0.699778	99	6	0	5.922985	5.787799	3.965380
44	8	0	-2.632212	4.662571	-3.982815	100	6	0	6.760070	7.078461	4.093655
45	8	0	-3.628061	4.139146	-0.563628	101	6	0	6.564328	8.045965	2.909103
46	8	0	-2.137738	2.065868	-1.858509	102	1	0	-1.097673	2.648519	-3.549479
47	8	0	4.387694	4.234898	-1.246396	103	1	0	-0.353552	4.786759	-2.591419
48	8	0	1.695777	4.459745	-1.109661	104	1	0	-2.605822	5.827478	-2.223204
49	8	0	0.117318	2.180521	-1.973709	105	1	0	-4.577357	4.309173	-2.421533
50	8	0	3.394880	1.619715	-3.580259	106	1	0	-4.133112	1.978964	-1.632302
51	8	0	6.892796	-1.707046	1.106458	107	1	0	-2.996438	2.065726	-4.399672
52	8	0	6.361597	0.927929	0.714540	108	1	0	-4.657741	2.519505	-4.081942
53	8	0	4.470981	1.439754	-1.511138	109	1	0	5.159543	2.491762	-3.147633
54	8	0	5.204547	-1.723134	-2.087610	110	1	0	3.391941	4.156682	-3.067653
55	8	0	6.970478	-1.855067	-4.023571	111	1	0	2.370344	2.521614	-0.761564
56	8	0	3.680112	-3.132093	1.826350	112	1	0	1.173370	3.230229	-3.445817
57	8	0	4.227194	-6.465740	0.346123	113	1	0	2.072956	0.558683	-2.356924
58	8	0	5.291205	-3.096579	-0.262740	114	1	0	1.679486	-0.288512	-4.579749
59	8	0	2.439594	-3.751209	-0.626649	115	1	0	1.763884	1.331435	-5.243027
60	8	0	1.792653	-5.152817	-2.879167	116	1	0	6.809297	-2.920701	-1.645052
61	8	0	-0.141802	-2.420768	5.509173	117	1	0	7.677058	-0.937427	-0.589616
62	8	0	1.981818	-3.209640	3.909043	118	1	0	4.797572	-0.324941	0.119715
63	8	0	1.065604	-3.845501	1.106111	119	1	0	6.519265	1.274207	-1.701934
64	8	0	-1.726665	-4.775169	3.250029	120	1	0	4.807437	-0.215638	-3.348153
65	8	0	-2.803233	-5.736563	1.011806	121	1	0	7.768502	-0.445091	-2.721186

122	1	0	6.977972	0.246457	-4.120463
123	1	0	1.928209	-5.543100	0.299130
124	1	0	3.237868	-5.035465	2.340901
125	1	0	5.482057	-5.027122	1.235480
126	1	0	5.544405	-4.911937	-1.256154
127	1	0	3.669842	-3.386156	-2.171575
128	1	0	3.002035	-6.301238	-1.620663
129	1	0	3.767119	-5.646767	-3.054317
130	1	0	-2.298176	-3.960803	5.016505
131	1	0	0.118938	-4.438815	5.068574
132	1	0	0.356541	-2.302407	2.958682
133	1	0	0.885578	-5.257185	2.661994
134	1	0	-1.401735	-3.560381	1.609011
135	1	0	-0.938610	-6.555062	1.457631
136	1	0	-1.002120	-5.432633	0.089516
137	1	0	-6.178444	0.659564	3.874580
138	1	0	-4.886279	-0.453199	5.645277
139	1	0	-2.482887	0.031359	3.899646
140	1	0	-3.906254	-2.553211	4.566973
141	1	0	-3.649010	-0.993395	1.975350
142	1	0	-5.523137	-2.688012	1.359194
143	1	0	-4.697195	-3.754369	2.485244
144	1	0	-5.486400	4.995825	-0.451503
145	1	0	-5.743188	4.780054	1.907563
146	1	0	-3.237618	3.114162	1.958794
147	1	0	-6.120674	2.335529	2.442944
148	1	0	-4.137334	1.621367	0.265741
149	1	0	-7.047455	1.062011	0.028130
150	1	0	-6.029410	-0.078474	0.915525
151	1	0	-1.790499	4.272632	-0.220193
152	1	0	-2.035517	5.249163	-4.465026
153	1	0	3.819895	4.867373	-0.780733
154	1	0	0.812559	4.381617	-0.693589
155	1	0	6.159687	-2.303861	1.322888
156	1	0	6.622716	0.455327	1.519284
157	1	0	7.666293	-1.893857	-4.692273
158	1	0	3.683416	-2.570689	1.036647
159	1	0	4.543105	-7.086057	1.014877
160	1	0	1.313540	-4.520377	-2.324028
161	1	0	0.791638	-2.183572	5.619259
162	1	0	2.633118	-2.937185	3.230774
163	1	0	-3.122976	-5.914830	1.909098
164	1	0	-3.395775	1.380619	6.085626
165	1	0	-1.543905	-1.247786	5.723122
166	1	0	-3.400297	-4.097836	0.714099
167	1	0	-3.659273	5.756377	2.609075
168	1	0	-4.085984	2.987585	4.259861
169	1	0	-6.026817	-0.500563	-1.580053
170	1	0	-4.611327	0.343166	-2.665778
171	1	0	-0.504939	0.207314	-3.920551
172	1	0	-6.831156	-2.856275	-5.062107
173	1	0	-4.721906	-4.001289	-6.190462
174	1	0	-4.552166	-2.281216	-6.570878
175	1	0	-2.545944	-2.488910	-5.279150
176	1	0	-3.238204	-3.800026	-4.305236
177	1	0	-2.352049	-1.907735	-0.148397
178	1	0	-0.336548	0.044125	-1.044897
179	1	0	0.233927	-1.331708	-0.084175
180	1	0	-2.078136	0.392590	0.811241
181	1	0	-1.066983	-0.607607	1.832799
182	1	0	-0.309066	2.008812	0.465444
183	1	0	-0.693297	1.826310	2.164240
184	1	0	1.750141	0.659511	0.771494
185	1	0	1.342554	0.381851	2.453686
186	1	0	1.490795	2.813638	2.912583
187	1	0	1.782372	3.139491	1.225037
188	1	0	3.646235	1.661063	3.123058
189	1	0	3.931508	1.779438	1.394644
190	1	0	3.622588	4.219580	3.173130
191	1	0	4.063674	4.178415	1.472417
192	1	0	5.742466	3.028520	3.735169
193	1	0	6.101942	2.885617	2.023536
194	1	0	6.239988	5.374926	1.858950
195	1	0	7.446713	4.689722	2.921191
196	1	0	-4.169355	-1.519252	-1.666311
197	1	0	-3.503024	-3.069454	-2.073668
198	1	0	5.995069	5.228738	4.894818
199	1	0	4.880445	6.057574	3.833978
200	1	0	6.482652	7.588911	5.011249
201	1	0	7.810699	6.816435	4.178977
202	1	0	5.515931	8.305052	2.802542
203	1	0	6.899471	7.601999	1.979848
204	1	0	7.124536	8.962237	3.063691

(5*R*)-4a (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.845623	2.614755	2.449038
2	6	0	0.146767	3.597209	3.369864
3	6	0	0.350214	5.002023	2.786140
4	6	0	-0.113461	5.103421	1.340439
5	6	0	0.411692	3.964645	0.469061
6	6	0	1.844160	4.134848	-0.061380
7	6	0	1.345679	-2.014598	4.965722
8	6	0	0.195463	-1.176712	5.501565
9	6	0	-0.161029	-0.134559	4.457133
10	6	0	1.070852	0.662178	4.018053
11	6	0	2.319955	-0.170012	3.727236
12	6	0	3.624045	0.619018	3.872025
13	6	0	0.685042	-6.113577	1.579362
14	6	0	-0.360369	-5.935200	2.667660
15	6	0	-0.397664	-4.462987	3.046994
16	6	0	0.962421	-4.022943	3.534208
17	6	0	2.047665	-4.322171	2.507796
18	6	0	3.438068	-4.211485	3.106195
19	6	0	-1.914074	-4.068982	-1.843732
20	6	0	-2.314787	-5.295300	-1.033973
21	6	0	-1.192454	-6.336666	-1.029838
22	6	0	0.208903	-5.733993	-0.850779
23	6	0	0.444896	-4.486795	-1.699845

24	6	0	0.597433	-4.739874	-3.213489	80	6	0	-0.117068	-1.115782	-1.985928
25	6	0	-6.323428	-1.297647	-2.741419	81	8	0	2.853038	-2.781022	-0.681879
26	6	0	-6.424414	-2.367820	-1.664604	82	6	0	3.001601	-1.568937	-0.585101
27	6	0	-5.034216	-2.589265	-1.102128	83	7	0	4.068736	-1.008950	-0.005031
28	6	0	-4.062775	-2.957888	-2.200172	84	6	0	5.198209	-1.833272	0.455524
29	6	0	-4.069278	-1.908917	-3.305164	85	6	0	6.123260	-2.227436	-0.707923
30	6	0	-3.250217	-2.249860	-4.545601	86	6	0	6.774359	-1.016047	-1.396262
31	6	0	-6.320607	3.958690	-1.462413	87	6	0	7.693522	-1.433935	-2.560705
32	6	0	-7.318641	3.000130	-0.838908	88	6	0	8.303950	-0.241074	-3.326429
33	6	0	-6.743556	1.604263	-0.821524	89	6	0	9.327436	0.564146	-2.501776
34	6	0	-6.388253	1.158426	-2.230862	90	6	0	9.968029	1.703417	-3.318259
35	6	0	-5.387486	2.149546	-2.829762	91	6	0	10.992754	2.512468	-2.499509
36	6	0	-5.080796	1.957953	-4.314542	92	6	0	11.629173	3.650168	-3.322175
37	6	0	-2.353441	6.129965	1.427817	93	6	0	12.608029	4.526402	-2.512417
38	6	0	-3.598022	5.731062	2.188204	94	6	0	13.898669	3.792269	-2.099200
39	6	0	-4.349318	4.671128	1.418057	95	6	0	14.872275	4.725079	-1.352310
40	6	0	-4.689973	5.150478	0.018440	96	6	0	2.500286	0.733797	-1.619507
41	6	0	-3.455751	5.680098	-0.706739	97	6	0	2.637362	1.859249	-0.617695
42	6	0	-3.803381	6.534616	-1.935599	98	8	0	3.231025	1.702951	0.455294
43	8	0	-1.215310	3.219025	3.527199	99	6	0	0.835027	-0.458496	0.098661
44	8	0	1.759706	5.288824	2.697029	100	7	0	1.138734	-1.170381	-2.128671
45	8	0	-1.553212	4.973712	1.325939	101	8	0	1.855058	-1.564780	-3.283946
46	8	0	0.283240	2.702835	1.131240	102	1	0	1.887009	2.836465	2.437773
47	8	0	-0.885378	-2.030479	5.858564	103	1	0	0.641724	3.572860	4.335473
48	8	0	-1.105535	0.779005	5.019243	104	1	0	-0.171315	5.733317	3.392161
49	8	0	0.620352	1.269396	2.778533	105	1	0	0.186818	6.058928	0.931385
50	8	0	2.486709	-1.215735	4.718472	106	1	0	-0.255684	3.904875	-0.377651
51	8	0	-1.649948	-6.382444	2.260838	107	1	0	2.568164	4.114082	0.730565
52	8	0	-1.317565	-4.260055	4.140136	108	1	0	1.940058	5.069547	-0.597153
53	8	0	0.900811	-2.604432	3.745298	109	1	0	1.637149	-2.771236	5.676336
54	8	0	1.949950	-5.718813	2.093920	110	1	0	0.515108	-0.674973	6.401673
55	8	0	4.429948	-4.540846	2.118433	111	1	0	-0.546689	-0.636819	3.583241
56	8	0	-2.632066	-4.918074	0.310235	112	1	0	1.273832	1.404526	4.776529
57	8	0	-1.297681	-6.966045	-2.328486	113	1	0	2.214013	-0.605844	2.749180
58	8	0	0.291879	-5.273979	0.509902	114	1	0	4.448336	-0.007187	3.552913
59	8	0	-0.657078	-3.590947	-1.440953	115	1	0	3.751654	0.833172	4.921217
60	8	0	0.302962	-3.549149	-3.961018	116	1	0	0.778495	-7.144893	1.274931
61	8	0	-7.321647	-2.048795	-0.601933	117	1	0	-0.070635	-6.520728	3.527212
62	8	0	-5.054245	-3.681626	-0.154182	118	1	0	-0.690336	-3.882672	2.186354
63	8	0	-2.776350	-2.980907	-1.570847	119	1	0	1.170013	-4.534975	4.466611
64	8	0	-5.448429	-1.762550	-3.745282	120	1	0	1.946867	-3.691686	1.641183
65	8	0	-1.866596	-1.978228	-4.269969	121	1	0	3.504635	-4.889273	3.949894
66	8	0	-7.568635	3.334092	0.548833	122	1	0	3.622096	-3.203585	3.439045
67	8	0	-7.727163	0.684845	-0.310739	123	1	0	-1.919026	-4.316871	-2.891541
68	8	0	-5.798694	-0.132046	-2.094642	124	1	0	-3.167719	-5.770903	-1.498397
69	8	0	-5.993741	3.476048	-2.764012	125	1	0	-1.390762	-7.035921	-0.229390
70	8	0	-4.198556	0.854056	-4.555905	126	1	0	0.965792	-6.485145	-1.054063
71	8	0	-3.178765	5.200194	3.457049	127	1	0	1.304065	-3.964367	-1.321928
72	8	0	-5.530496	4.417614	2.189039	128	1	0	-0.078944	-5.504331	-3.548468
73	8	0	-5.158767	3.958036	-0.661426	129	1	0	1.612873	-5.074341	-3.397318
74	8	0	-2.738549	6.607941	0.146625	130	1	0	-7.274335	-1.085026	-3.203279
75	8	0	-5.002196	6.115323	-2.602614	131	1	0	-6.771076	-3.279434	-2.127582
76	7	0	2.096134	3.026633	-0.987555	132	1	0	-4.693264	-1.686790	-0.621710
77	8	0	3.614793	1.880068	3.189700	133	1	0	-4.335653	-3.927839	-2.597934
78	6	0	-0.516460	-0.560506	-0.657296	134	1	0	-3.719741	-0.974514	-2.913939
79	6	0	1.916668	-0.581243	-1.020185	135	1	0	-3.592425	-1.593569	-5.329385

136	1	0	-3.420897	-3.277279	-4.845865
137	1	0	-6.707466	4.950383	-1.597764
138	1	0	-8.238548	3.004107	-1.406635
139	1	0	-5.854141	1.594336	-0.211346
140	1	0	-7.285157	1.120229	-2.837432
141	1	0	-4.482058	2.131855	-2.242893
142	1	0	-4.674195	2.890526	-4.685753
143	1	0	-5.990040	1.751076	-4.855780
144	1	0	-1.830896	6.941587	1.907655
145	1	0	-4.231703	6.596129	2.323333
146	1	0	-3.725254	3.793813	1.336762
147	1	0	-5.469179	5.898256	0.062969
148	1	0	-2.829672	4.834019	-0.943774
149	1	0	-2.957379	6.578227	-2.610031
150	1	0	-4.000047	7.528292	-1.571129
151	1	0	-1.855514	3.941553	3.392265
152	1	0	2.215648	5.190885	3.543727
153	1	0	-1.093665	-2.674642	5.156190
154	1	0	-1.298741	1.504879	4.396776
155	1	0	-2.023238	-5.805690	1.549987
156	1	0	-2.116450	-4.785793	3.990801
157	1	0	4.114486	-5.312374	1.625970
158	1	0	-3.449059	-4.374819	0.308720
159	1	0	-0.831622	-7.811705	-2.354964
160	1	0	0.969534	-2.814939	-3.775031
161	1	0	-7.396947	-1.084230	-0.465199
162	1	0	-5.828680	-3.580906	0.420049
163	1	0	-1.222444	-2.720104	-4.329691
164	1	0	-8.260721	4.000803	0.653150
165	1	0	-8.018099	0.973064	0.566483
166	1	0	-3.275186	1.083506	-4.389490
167	1	0	-3.946139	4.803785	3.898966
168	1	0	-6.150001	3.841620	1.707292
169	1	0	-4.920972	5.260700	-3.048412
170	1	0	1.653027	3.078241	-1.879465
171	1	0	3.624012	1.773858	2.223557
172	1	0	-0.985653	0.411075	-0.767264
173	1	0	-0.794181	-1.411141	-2.754553
174	1	0	4.061770	-0.028431	0.193523
175	1	0	5.746797	-1.246169	1.182124
176	1	0	4.824486	-2.723981	0.934913
177	1	0	6.896516	-2.883008	-0.317486
178	1	0	5.541298	-2.795356	-1.424664
179	1	0	7.340418	-0.452512	-0.661027
180	1	0	5.995351	-0.364989	-1.779108
181	1	0	8.494183	-2.062876	-2.180601
182	1	0	7.114901	-2.037262	-3.254212
183	1	0	8.797358	-0.612521	-4.220466
184	1	0	7.505622	0.419528	-3.654280
185	1	0	8.847092	0.986076	-1.625565
186	1	0	10.107513	-0.106629	-2.151546
187	1	0	10.458721	1.285140	-4.192991
188	1	0	9.187897	2.370531	-3.675342
189	1	0	10.499672	2.936308	-1.628619
190	1	0	11.763599	1.839917	-2.139006
191	1	0	12.149876	3.228078	-4.177567
192	1	0	10.834213	4.280131	-3.711841
193	1	0	12.881459	5.392542	-3.108925
194	1	0	12.105880	4.897332	-1.622849
195	1	0	13.656558	2.948164	-1.463979
196	1	0	14.383667	3.399816	-2.988100
197	1	0	15.152507	5.565223	-1.979095
198	1	0	14.410443	5.115040	-0.451227
199	1	0	15.776645	4.198414	-1.067826
200	1	0	3.467274	0.512680	-2.050062
201	1	0	1.854900	1.033755	-2.428627
202	1	0	0.925341	-1.314961	0.751396
203	1	0	0.904894	0.434066	0.685997
204	1	0	-1.210301	-1.242091	-0.189994

(5*R*)-4a (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.849823	1.777497	-0.090013
2	6	0	5.817693	3.278813	0.092627
3	6	0	5.176328	3.879715	-1.147252
4	6	0	3.787281	3.298365	-1.422613
5	6	0	3.754116	1.759469	-1.336674
6	6	0	4.219021	1.120174	-2.649772
7	6	0	4.457389	-1.812534	3.178712
8	6	0	4.595443	-0.425721	3.799852
9	6	0	4.765417	0.622831	2.711816
10	6	0	5.969572	0.214040	1.880194
11	6	0	5.582753	-1.074986	1.160771
12	6	0	6.601029	-1.561374	0.128851
13	6	0	0.161282	-4.747837	2.226636
14	6	0	0.312287	-4.014789	3.555368
15	6	0	1.083117	-2.723101	3.343275
16	6	0	2.408182	-3.063101	2.711156
17	6	0	2.171003	-3.688574	1.350671
18	6	0	3.466440	-4.078551	0.628088
19	6	0	-4.173386	-3.247755	0.487876
20	6	0	-3.774646	-4.010317	1.738504
21	6	0	-2.835276	-5.143560	1.376710
22	6	0	-1.631876	-4.669168	0.568130
23	6	0	-2.007377	-3.747007	-0.597311
24	6	0	-2.426364	-4.544381	-1.835484
25	6	0	-6.151100	1.375674	-0.728188
26	6	0	-6.885525	0.932044	0.521077
27	6	0	-6.072262	-0.168357	1.167093
28	6	0	-5.759384	-1.292048	0.180569
29	6	0	-5.145687	-0.816549	-1.140235
30	6	0	-5.250823	-1.846412	-2.267540
31	6	0	-2.773740	5.396212	0.157729
32	6	0	-3.519903	4.877100	1.376355
33	6	0	-3.869432	3.416865	1.153841
34	6	0	-4.682692	3.268900	-0.111093
35	6	0	-3.896966	3.829214	-1.288563
36	6	0	-4.629628	3.779567	-2.628233
37	6	0	2.533405	5.180788	-0.486138

38	6	0	1.950013	5.507346	0.878306	94	6	0	-1.840102	0.097806	1.727314
39	6	0	0.595600	4.839398	1.015298	95	6	0	-2.137800	0.549015	3.177398
40	6	0	-0.303174	5.275487	-0.121496	96	6	0	-1.273545	-0.145518	4.244860
41	6	0	0.330003	4.826437	-1.433245	97	6	0	-1.545857	0.367241	5.676064
42	6	0	-0.454370	5.210022	-2.666555	98	6	0	-2.937921	-0.029140	6.207324
43	8	0	5.060994	3.656150	1.240862	99	8	0	2.373499	-0.222104	-4.117763
44	8	0	5.970414	3.505639	-2.296601	100	6	0	3.172293	-0.903194	-3.461876
45	8	0	2.848221	3.796998	-0.446703	101	6	0	3.294830	-2.408631	-3.707701
46	8	0	4.527494	1.266108	-0.206335	102	1	0	6.428533	1.532387	-0.962031
47	8	0	3.485885	-0.083586	4.628375	103	1	0	6.843434	3.620015	0.173054
48	8	0	5.036610	1.903783	3.322423	104	1	0	5.126235	4.952501	-1.051957
49	8	0	6.499495	1.241764	1.045800	105	1	0	3.474212	3.606144	-2.410010
50	8	0	5.474052	-2.074059	2.226790	106	1	0	2.741582	1.463606	-1.127548
51	8	0	-0.948588	-3.775454	4.168882	107	1	0	5.241280	1.386024	-2.856929
52	8	0	1.376504	-2.095185	4.606154	108	1	0	3.598756	1.499523	-3.444789
53	8	0	3.170163	-1.859558	2.575057	109	1	0	4.542993	-2.577735	3.933716
54	8	0	1.410122	-4.918331	1.566324	110	1	0	5.490273	-0.413502	4.407066
55	8	0	3.769052	-3.139174	-0.420795	111	1	0	3.880536	0.682801	2.100668
56	8	0	-3.112751	-3.125650	2.649445	112	1	0	6.791469	-0.005434	2.545585
57	8	0	-3.539922	-6.039091	0.490544	113	1	0	4.627678	-0.964024	0.687472
58	8	0	-0.727704	-3.963311	1.443093	114	1	0	7.160199	-2.377886	0.566022
59	8	0	-3.028800	-2.788580	-0.219676	115	1	0	7.280166	-0.765379	-0.125877
60	8	0	-2.560928	-3.683510	-2.973445	116	1	0	-0.226256	-5.742377	2.381240
61	8	0	-7.078824	2.069256	1.357167	117	1	0	0.881289	-4.636832	4.231315
62	8	0	-6.835944	-0.712395	2.254087	118	1	0	0.526053	-2.057175	2.703957
63	8	0	-4.855736	-2.118715	0.976931	119	1	0	2.931541	-3.768457	3.345763
64	8	0	-5.939989	0.310924	-1.625467	120	1	0	1.588040	-3.030786	0.730979
65	8	0	-4.252981	-1.637678	-3.264398	121	1	0	3.338087	-5.073344	0.224893
66	8	0	-2.781036	4.994955	2.591493	122	1	0	4.306920	-4.073836	1.300195
67	8	0	-4.647319	2.935803	2.271897	123	1	0	-4.797013	-3.868168	-0.130872
68	8	0	-4.863380	1.863773	-0.350644	124	1	0	-4.676028	-4.408026	2.188540
69	8	0	-3.570609	5.218961	-1.004790	125	1	0	-2.501442	-5.643437	2.276003
70	8	0	-4.402631	2.535279	-3.309045	126	1	0	-1.140450	-5.548378	0.172535
71	8	0	2.789640	5.085880	1.947643	127	1	0	-1.141694	-3.148514	-0.835871
72	8	0	-0.023253	5.248714	2.252204	128	1	0	-3.360144	-5.048756	-1.666359
73	8	0	-1.574540	4.634293	0.061421	129	1	0	-1.673929	-5.298523	-2.033548
74	8	0	1.618505	5.489908	-1.519357	130	1	0	-6.715550	2.129322	-1.252982
75	8	0	0.066068	4.398861	-3.740904	131	1	0	-7.857722	0.549477	0.253385
76	7	0	4.082485	-0.343999	-2.664478	132	1	0	-5.138430	0.250450	1.507867
77	8	0	5.956024	-1.968936	-1.099195	133	1	0	-6.671936	-1.846480	-0.002448
78	6	0	2.051260	-3.325998	-3.676823	134	1	0	-4.124248	-0.526598	-0.990559
79	6	0	2.424892	-4.774378	-4.123811	135	1	0	-6.231224	-1.725160	-2.704804
80	6	0	1.743530	-5.700572	-3.075789	136	1	0	-5.184913	-2.846870	-1.864828
81	6	0	1.493018	-4.754855	-1.934866	137	1	0	-2.556657	6.449316	0.235368
82	7	0	1.665800	-3.551158	-2.261527	138	1	0	-4.433304	5.443741	1.485889
83	8	0	1.507171	-2.410032	-1.455990	139	1	0	-2.962736	2.845030	1.063352
84	6	0	0.692772	-2.985558	-4.344213	140	1	0	-5.636028	3.763890	0.007568
85	8	0	-0.196431	-3.841134	-4.169503	141	1	0	-2.992815	3.264554	-1.392051
86	7	0	0.569115	-1.883902	-5.027062	142	1	0	-4.209916	4.547309	-3.257626
87	6	0	-0.729798	-1.381284	-5.519788	143	1	0	-5.685652	3.992303	-2.500737
88	6	0	-1.019763	-0.026378	-4.848643	144	1	0	3.401060	5.784547	-0.680954
89	6	0	-1.111599	-0.135331	-3.313812	145	1	0	1.806135	6.578260	0.940824
90	6	0	-1.171247	1.260760	-2.671062	146	1	0	0.720007	3.767959	0.991245
91	6	0	-1.373104	1.220128	-1.141269	147	1	0	-0.418087	6.352667	-0.106558
92	6	0	-0.332210	0.409930	-0.344410	148	1	0	0.463931	3.758505	-1.425835
93	6	0	-0.492802	0.619756	1.181346	149	1	0	-0.305433	6.264152	-2.862319

150	1	0	-1.502596	5.021430	-2.492132
151	1	0	5.213636	3.060924	2.011054
152	1	0	6.743337	4.074562	-2.403047
153	1	0	2.724905	-0.680838	4.499677
154	1	0	4.382815	2.059114	4.022000
155	1	0	-1.635472	-3.478559	3.532999
156	1	0	0.577304	-2.063950	5.150749
157	1	0	2.957034	-2.671934	-0.753850
158	1	0	-3.460044	-2.230387	2.523776
159	1	0	-4.142589	-6.626482	0.964695
160	1	0	-1.739049	-3.685319	-3.511063
161	1	0	-6.266341	2.301688	1.848306
162	1	0	-6.308240	-1.391028	2.694641
163	1	0	-3.586578	-2.353966	-3.202714
164	1	0	-1.810265	4.990508	2.450754
165	1	0	-4.249279	3.270130	3.090013
166	1	0	-4.781321	1.770555	-2.848275
167	1	0	3.515072	4.502213	1.635429
168	1	0	0.629218	5.179143	2.965786
169	1	0	-0.575463	4.318573	-4.457628
170	1	0	4.752359	-0.884136	-2.132415
171	1	0	3.497999	-4.899295	-4.076862
172	1	0	2.085050	-4.980738	-5.125686
173	1	0	2.369071	-6.530648	-2.780696
174	1	0	1.208701	-5.018266	-0.938548
175	1	0	0.796147	-6.062702	-3.447148
176	1	0	5.208413	-2.571659	-0.869729
177	1	0	1.295592	-1.178096	-4.929497
178	1	0	-0.675524	-1.275481	-6.595831
179	1	0	-1.493657	-2.102527	-5.279402
180	1	0	-1.954940	0.360706	-5.238500
181	1	0	-0.229699	0.669239	-5.113778
182	1	0	-2.008899	-0.684642	-3.057294
183	1	0	-0.249052	-0.667119	-2.933422
184	1	0	-2.016263	1.793463	-3.096282
185	1	0	-0.273318	1.817852	-2.919893
186	1	0	-1.352507	2.236483	-0.765481
187	1	0	-2.365087	0.835319	-0.948956
188	1	0	-0.398048	-0.644549	-0.579431
189	1	0	0.663457	0.732615	-0.634602
190	1	0	0.327742	0.130733	1.696720
191	1	0	-0.414876	1.682365	1.395277
192	1	0	-2.638316	0.471952	1.100975
193	1	0	-1.863287	-0.984146	1.648629
194	1	0	-3.187085	0.367771	3.389080
195	1	0	-1.991095	1.623773	3.245429
196	1	0	-1.454039	-1.215391	4.214092
197	1	0	-0.225935	0.010555	4.014730
198	1	0	-0.790706	-0.034105	6.346600
199	1	0	-1.440321	1.447552	5.694957
200	1	0	-3.059225	-1.107363	6.180289
201	1	0	-3.065122	0.299072	7.233261
202	1	0	-3.728059	0.417818	5.616317
203	1	0	3.999055	-2.836696	-3.011050
204	1	0	3.723830	-2.487840	-4.702466

(5*S*)-4b (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.274160	2.744261	-1.798908
2	6	0	-4.740328	3.139910	-1.909777
3	6	0	-5.340172	2.446106	-3.137773
4	6	0	-5.071792	0.942490	-3.126797
5	6	0	-3.617033	0.595167	-2.840001
6	6	0	-2.634288	0.760839	-4.013761
7	6	0	-0.959661	6.174580	1.480894
8	6	0	-2.386465	5.873214	1.908323
9	6	0	-2.857471	4.598540	1.223233
10	6	0	-2.543830	4.599141	-0.274671
11	6	0	-1.133418	5.043955	-0.621855
12	6	0	-0.904038	5.352516	-2.092170
13	6	0	3.523236	3.886421	3.310370
14	6	0	2.440052	4.094660	4.351960
15	6	0	1.091445	4.182753	3.662071
16	6	0	1.088970	5.213249	2.548534
17	6	0	2.192671	4.892490	1.550542
18	6	0	2.430910	5.897531	0.431581
19	6	0	2.914563	-0.836523	2.288742
20	6	0	3.174743	-0.214533	3.654249
21	6	0	4.401188	0.687323	3.562310
22	6	0	4.305412	1.695807	2.421011
23	6	0	3.895253	1.073896	1.095552
24	6	0	4.998202	0.361905	0.320276
25	6	0	-0.654830	-4.739345	3.117037
26	6	0	-0.364537	-3.798197	4.270317
27	6	0	0.153665	-2.500290	3.689791
28	6	0	1.429001	-2.722017	2.906487
29	6	0	1.237472	-3.808798	1.846551
30	6	0	2.526294	-4.431003	1.332161
31	6	0	-5.285117	-4.649024	0.380447
32	6	0	-5.236119	-4.706075	1.899955
33	6	0	-3.960969	-4.053407	2.380401
34	6	0	-2.767899	-4.784745	1.800609
35	6	0	-2.827994	-4.740927	0.273732
36	6	0	-1.819284	-5.646537	-0.432146
37	6	0	-7.013434	-0.267750	-2.188354
38	6	0	-7.591953	-0.513942	-0.812990
39	6	0	-6.643729	-1.386200	-0.023177
40	6	0	-6.375633	-2.695453	-0.739702
41	6	0	-5.924640	-2.470089	-2.179424
42	6	0	-6.068826	-3.726048	-3.049993
43	8	0	-5.452627	2.852400	-0.705150
44	8	0	-4.666254	3.039361	-4.269034
45	8	0	-5.801267	0.423164	-1.982136
46	8	0	-3.180954	1.327134	-1.684847
47	8	0	-2.420051	5.788173	3.334036
48	8	0	-4.272702	4.490594	1.400128
49	8	0	-2.655621	3.194900	-0.624752
50	8	0	-0.844794	6.280500	0.080311
51	8	0	2.445923	3.024119	5.298687
52	8	0	0.078243	4.587046	4.603237

53	8	0	-0.196548	5.065300	1.946938	109	1	0	-0.604442	7.097610	1.910821
54	8	0	3.451502	4.877185	2.303025	110	1	0	-3.034914	6.683417	1.616268
55	8	0	3.634389	5.498222	-0.263708	111	1	0	-2.326344	3.761044	1.650696
56	8	0	2.063456	0.531008	4.144740	112	1	0	-3.284799	5.207077	-0.776694
57	8	0	5.495317	-0.223635	3.301668	113	1	0	-0.458302	4.269845	-0.303182
58	8	0	3.257319	2.603637	2.768230	114	1	0	-1.327498	6.322198	-2.304382
59	8	0	2.797693	0.148098	1.268289	115	1	0	-1.389689	4.605082	-2.701297
60	8	0	4.379031	-0.267220	-0.829614	116	1	0	4.512169	3.938830	3.740477
61	8	0	-1.502556	-3.521220	5.082722	117	1	0	2.624173	5.011360	4.890671
62	8	0	0.455154	-1.586042	4.765811	118	1	0	0.854787	3.220626	3.230650
63	8	0	1.655808	-1.483216	2.217793	119	1	0	1.217397	6.205277	2.964278
64	8	0	0.548905	-4.981098	2.397720	120	1	0	2.024286	3.914641	1.131960
65	8	0	3.355912	-3.380585	0.782492	121	1	0	2.546122	6.888991	0.855082
66	8	0	-6.304052	-3.940556	2.504878	122	1	0	1.637288	5.895528	-0.293744
67	8	0	-3.870108	-4.150289	3.816261	123	1	0	3.706674	-1.524702	2.066686
68	8	0	-1.595237	-4.100839	2.266701	124	1	0	3.432449	-1.011087	4.341588
69	8	0	-4.115984	-5.297563	-0.119603	125	1	0	4.513997	1.213541	4.500349
70	8	0	-0.462032	-5.228065	-0.243802	126	1	0	5.250220	2.217199	2.300851
71	8	0	-7.730480	0.758716	-0.178630	127	1	0	3.487180	1.856646	0.481369
72	8	0	-7.294275	-1.606291	1.236471	128	1	0	5.509172	-0.360853	0.934878
73	8	0	-5.280090	-3.292965	0.006248	129	1	0	5.709146	1.073619	-0.066856
74	8	0	-6.794577	-1.512436	-2.838389	130	1	0	-1.015227	-5.698522	3.452723
75	8	0	-5.831610	-4.942189	-2.324194	131	1	0	0.394150	-4.246337	4.895256
76	7	0	-1.279428	0.593886	-3.499203	132	1	0	-0.587869	-2.077281	3.032823
77	8	0	0.498637	5.398557	-2.384540	133	1	0	2.231809	-2.969764	3.588514
78	6	0	1.438907	-2.816466	-1.868852	134	1	0	0.647726	-3.406708	1.046165
79	6	0	0.386358	-0.588300	-2.144613	135	1	0	2.275164	-5.160619	0.575729
80	6	0	1.971848	-2.028583	-3.030427	136	1	0	3.020980	-4.927306	2.156774
81	6	0	3.392278	3.083766	-2.728627	137	1	0	-6.118722	-5.176657	-0.041892
82	6	0	4.758343	2.569538	-3.208698	138	1	0	-5.266126	-5.734752	2.231982
83	6	0	4.616865	1.589853	-4.389796	139	1	0	-3.947303	-3.023121	2.062995
84	6	0	5.925410	0.857789	-4.755202	140	1	0	-2.772904	-5.811662	2.147946
85	6	0	6.530455	0.045211	-3.587753	141	1	0	-2.734723	-3.721293	-0.062259
86	6	0	7.543050	-1.009817	-4.073550	142	1	0	-2.014725	-5.600731	-1.490615
87	6	0	8.194142	-1.781096	-2.908807	143	1	0	-1.984455	-6.666276	-0.101442
88	6	0	9.182110	-2.858291	-3.398398	144	1	0	-7.688079	0.285399	-2.821112
89	6	0	9.915387	-3.598162	-2.258261	145	1	0	-8.543309	-1.020517	-0.911780
90	6	0	8.989259	-4.505308	-1.423973	146	1	0	-5.707455	-0.863067	0.095820
91	6	0	9.722593	-5.247208	-0.285279	147	1	0	-7.252352	-3.326194	-0.694994
92	6	0	-0.936595	-0.560528	-2.934404	148	1	0	-4.912645	-2.101745	-2.148664
93	8	0	-1.640719	-1.568579	-2.985333	149	1	0	-5.436976	-3.645949	-3.924708
94	6	0	0.426650	-1.824790	-1.209262	150	1	0	-7.096687	-3.765838	-3.368433
95	7	0	1.439726	-0.888182	-3.149752	151	1	0	-5.782982	1.939479	-0.687597
96	8	0	1.664679	0.062208	-4.128924	152	1	0	-5.204930	3.018097	-5.069937
97	6	0	0.688168	0.724481	-1.395425	153	1	0	-1.681642	5.243433	3.658273
98	6	0	1.329021	1.856629	-2.196616	154	1	0	-4.644308	3.794157	0.827581
99	8	0	0.613921	2.682148	-2.796412	155	1	0	2.275940	2.166730	4.849153
100	7	0	2.644490	1.981542	-2.083814	156	1	0	0.133924	4.031683	5.393939
101	6	0	10.708546	-6.318589	-0.792375	157	1	0	4.326010	5.385978	0.402659
102	1	0	-2.761853	3.088419	-2.680480	158	1	0	1.331050	-0.087217	4.351244
103	1	0	-4.817228	4.201225	-2.080117	159	1	0	6.339346	0.121819	3.618854
104	1	0	-6.406297	2.633694	-3.156909	160	1	0	3.675717	-0.851361	-0.508935
105	1	0	-5.412521	0.464341	-4.036377	161	1	0	-2.346986	-3.663666	4.607042
106	1	0	-3.577574	-0.433105	-2.538613	162	1	0	-0.268657	-1.623917	5.410940
107	1	0	-2.717580	1.729497	-4.471515	163	1	0	4.197359	-3.737012	0.467590
108	1	0	-2.849731	-0.000500	-4.752566	164	1	0	-7.143322	-4.420194	2.525864

165	1	0	-4.682343	-3.804663	4.214980
166	1	0	-0.154721	-5.408424	0.655922
167	1	0	-7.897019	0.623577	0.765908
168	1	0	-6.796115	-2.239285	1.780231
169	1	0	-4.904433	-5.063827	-2.077510
170	1	0	-0.664877	1.389943	-3.460366
171	1	0	0.775512	4.495330	-2.622938
172	1	0	0.942587	-3.721684	-2.192617
173	1	0	2.717519	-2.341650	-3.727125
174	1	0	2.809134	3.432257	-3.567713
175	1	0	3.505477	3.893466	-2.019561
176	1	0	5.258963	2.086353	-2.377429
177	1	0	5.366813	3.419964	-3.500988
178	1	0	3.834361	0.872896	-4.178993
179	1	0	4.281729	2.154834	-5.255782
180	1	0	5.712238	0.182264	-5.579593
181	1	0	6.664582	1.570257	-5.112752
182	1	0	7.038073	0.720240	-2.904907
183	1	0	5.739766	-0.433021	-3.020025
184	1	0	7.038002	-1.713297	-4.730363
185	1	0	8.318982	-0.524482	-4.659893
186	1	0	8.722587	-1.079433	-2.268436
187	1	0	7.411061	-2.236062	-2.311354
188	1	0	8.651613	-3.581632	-4.012017
189	1	0	9.920671	-2.381694	-4.036744
190	1	0	10.708103	-4.198949	-2.690276
191	1	0	10.385440	-2.869085	-1.603337
192	1	0	8.197881	-3.902409	-0.991630
193	1	0	8.518415	-5.233795	-2.079125
194	1	0	10.253508	-4.525004	0.327885
195	1	0	8.986539	-5.727034	0.353258
196	1	0	0.767489	-1.538527	-0.226673
197	1	0	-0.547035	-2.274806	-1.152590
198	1	0	2.225406	-3.077938	-1.177546
199	1	0	-0.252480	1.112384	-1.022227
200	1	0	1.321259	0.499370	-0.551525
201	1	0	10.194114	-7.039736	-1.419107
202	1	0	11.509121	-5.875819	-1.371717
203	1	0	11.155602	-6.852652	0.039167
204	1	0	3.183561	1.219172	-1.716959

(5*S*)-4b (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.426954	-3.592418	1.995946
2	6	0	2.956734	-3.246139	3.381712
3	6	0	4.461150	-3.057609	3.320638
4	6	0	4.865929	-2.043137	2.265831
5	6	0	4.249409	-2.310205	0.897117
6	6	0	5.075686	-3.298583	0.070401
7	6	0	-2.372893	-5.231832	0.332348
8	6	0	-2.177611	-5.377551	1.835116
9	6	0	-1.119393	-4.421215	2.368257
10	6	0	0.165645	-4.517258	1.576812
11	6	0	-0.145535	-4.301619	0.105243
12	6	0	1.008801	-4.497993	-0.853177
13	6	0	-6.300123	-1.708712	-0.576733
14	6	0	-5.768585	-1.751740	0.840892
15	6	0	-4.371024	-2.335563	0.820743
16	6	0	-4.304131	-3.687510	0.132212
17	6	0	-4.949948	-3.618620	-1.252632
18	6	0	-5.294838	-4.964906	-1.864501
19	6	0	-4.055951	2.097379	-2.286180
20	6	0	-5.172754	2.108502	-1.248797
21	6	0	-6.373125	1.302342	-1.737340
22	6	0	-5.971088	-0.031495	-2.360872
23	6	0	-4.846155	0.086496	-3.383327
24	6	0	-5.246984	0.708178	-4.724524
25	6	0	-0.534913	5.884946	-1.116821
26	6	0	-1.741449	5.715834	-0.203435
27	6	0	-2.168045	4.262923	-0.274876
28	6	0	-2.519915	3.905706	-1.698675
29	6	0	-1.308153	4.118539	-2.594121
30	6	0	-1.565640	3.925394	-4.089906
31	6	0	4.393320	4.616467	0.543072
32	6	0	3.535048	5.568650	1.363639
33	6	0	2.084678	5.274798	1.037869
34	6	0	1.824056	5.433202	-0.440757
35	6	0	2.762599	4.547847	-1.259889
36	6	0	2.791867	4.859593	-2.754883
37	6	0	5.292615	0.129899	3.312981
38	6	0	4.387378	1.172835	3.935101
39	6	0	3.717689	1.982494	2.837399
40	6	0	4.747724	2.561313	1.884269
41	6	0	5.503149	1.387696	1.267505
42	6	0	6.554926	1.755758	0.235948
43	8	0	2.334399	-2.061225	3.888032
44	8	0	5.037409	-4.305636	2.873426
45	8	0	4.383779	-0.761046	2.696159
46	8	0	2.854725	-2.688836	0.988053
47	8	0	-3.388244	-5.176654	2.581833
48	8	0	-0.822216	-4.767326	3.732669
49	8	0	1.021812	-3.473882	2.083039
50	8	0	-1.096996	-5.332750	-0.283664
51	8	0	-5.748517	-0.458650	1.445652
52	8	0	-3.925956	-2.540145	2.186283
53	8	0	-2.892419	-3.945499	0.013618
54	8	0	-6.264353	-3.009478	-1.134808
55	8	0	-4.076225	-5.712910	-2.027730
56	8	0	-4.732790	1.612983	0.016102
57	8	0	-7.030462	2.041619	-2.787358
58	8	0	-5.445669	-0.830425	-1.281778
59	8	0	-3.749492	0.810863	-2.783830
60	8	0	-4.099154	0.804265	-5.574837
61	8	0	-1.483115	6.062599	1.154362
62	8	0	-3.334557	4.032163	0.546513
63	8	0	-2.839454	2.509773	-1.692897
64	8	0	-0.884739	5.511420	-2.453371
65	8	0	-2.280856	2.698087	-4.363856
66	8	0	3.752198	5.485833	2.770454

67	8	0	1.218399	6.213662	1.719901	123	1	0	-4.329608	2.756135	-3.091209
68	8	0	0.462730	5.010080	-0.638488	124	1	0	-5.492130	3.138694	-1.132839
69	8	0	4.118807	4.841370	-0.826589	125	1	0	-7.032006	1.121800	-0.898120
70	8	0	1.553561	4.571312	-3.414775	126	1	0	-6.838273	-0.498561	-2.808355
71	8	0	3.376502	0.577354	4.751481	127	1	0	-4.447245	-0.897190	-3.565089
72	8	0	2.968774	3.050505	3.463709	128	1	0	-5.736086	1.656844	-4.581637
73	8	0	4.043080	3.268623	0.849711	129	1	0	-5.946529	0.045579	-5.214151
74	8	0	6.168166	0.707488	2.365583	130	1	0	-0.192188	6.906396	-1.156629
75	8	0	7.137511	0.587969	-0.349636	131	1	0	-2.541605	6.344601	-0.567515
76	8	0	0.506108	-4.321468	-2.199070	132	1	0	-1.356400	3.638683	0.057826
77	6	0	4.446577	-2.421995	-3.565893	133	1	0	-3.356691	4.505406	-2.034478
78	6	0	5.107022	-1.384876	-4.494900	134	1	0	-0.509107	3.477007	-2.264002
79	6	0	6.382010	-2.101390	-5.038108	135	1	0	-0.615658	3.942476	-4.602614
80	6	0	6.104724	-3.550849	-4.731431	136	1	0	-2.186026	4.730704	-4.448061
81	7	0	5.106664	-3.707388	-3.974061	137	1	0	5.445836	4.793924	0.695132
82	8	0	4.606353	-4.916991	-3.479829	138	1	0	3.776860	6.577157	1.064226
83	6	0	2.942647	-2.622138	-3.732037	139	1	0	1.850423	4.267969	1.341648
84	6	0	-0.063170	-0.489393	-2.861740	140	1	0	1.942572	6.475182	-0.714313
85	6	0	-0.571050	-0.324540	-1.421308	141	1	0	2.522561	3.513136	-1.084551
86	6	0	0.548354	0.053472	-0.428179	142	1	0	3.540807	4.231924	-3.207426
87	6	0	-0.015942	0.625324	0.891242	143	1	0	3.093879	5.894185	-2.881183
88	6	0	-0.814059	-0.417748	1.695233	144	1	0	5.910176	-0.367565	4.044103
89	6	0	-1.427618	0.131687	3.001799	145	1	0	4.966447	1.840016	4.555991
90	6	0	-2.576872	1.130302	2.748934	146	1	0	3.046409	1.348960	2.280472
91	6	0	-3.333138	1.545712	4.032085	147	1	0	5.425062	3.219192	2.413526
92	6	0	-4.285225	0.444148	4.543264	148	1	0	4.784561	0.728258	0.808989
93	6	0	-5.061007	0.843235	5.816671	149	1	0	7.357930	2.290663	0.720158
94	6	0	-6.120157	1.936966	5.576091	150	1	0	6.089412	2.394761	-0.505093
95	7	0	4.675932	-3.289181	-1.333825	151	1	0	1.392005	-2.104743	3.663881
96	6	0	4.836373	-2.204229	-2.094675	152	1	0	5.140982	-4.940112	3.593917
97	8	0	5.261052	-1.124024	-1.687333	153	1	0	-3.628361	-4.226040	2.579727
98	8	0	2.649144	-0.246837	-3.603829	154	1	0	-1.659219	-4.943579	4.187238
99	6	0	2.159604	-1.357030	-3.420771	155	1	0	-5.343411	0.224238	0.860900
100	7	0	0.903577	-1.579812	-3.013752	156	1	0	-4.106312	-1.747710	2.711364
101	6	0	-6.920057	2.248229	6.856499	157	1	0	-4.225140	-6.517814	-2.539370
102	1	0	2.721029	-4.601608	1.753370	158	1	0	-4.100364	2.257277	0.388621
103	1	0	2.725074	-4.088869	4.023658	159	1	0	-7.591635	2.745186	-2.436846
104	1	0	4.840341	-2.754851	4.287563	160	1	0	-3.516759	1.528812	-5.291578
105	1	0	5.942063	-2.020314	2.171713	161	1	0	-0.528020	6.046822	1.382309
106	1	0	4.238270	-1.376744	0.371739	162	1	0	-3.215240	4.512925	1.380809
107	1	0	4.979405	-4.298852	0.454426	163	1	0	-1.959305	1.957352	-3.831177
108	1	0	6.115499	-3.002927	0.149305	164	1	0	3.464189	4.613907	3.122208
109	1	0	-2.987178	-6.002680	-0.085609	165	1	0	1.575420	6.390554	2.603376
110	1	0	-1.851014	-6.387960	2.029833	166	1	0	0.851985	5.193798	-3.180629
111	1	0	-1.498860	-3.413410	2.293090	167	1	0	3.069827	-0.267569	4.360605
112	1	0	0.617947	-5.487833	1.738605	168	1	0	2.476429	2.681951	4.213647
113	1	0	-0.584308	-3.330410	-0.040349	169	1	0	6.484129	0.071529	-0.852375
114	1	0	1.413776	-5.495776	-0.736756	170	1	0	5.324191	-0.487053	-3.947122
115	1	0	1.773142	-3.760562	-0.696419	171	1	0	4.436296	-1.143480	-5.302480
116	1	0	-7.328906	-1.385643	-0.612633	172	1	0	7.277012	-1.780788	-4.515774
117	1	0	-6.409806	-2.381874	1.438461	173	1	0	6.664802	-4.395876	-5.066041
118	1	0	-3.708104	-1.658347	0.308143	174	1	0	6.527329	-1.938083	-6.097173
119	1	0	-4.788279	-4.433860	0.743135	175	1	0	-0.290800	-4.865658	-2.293595
120	1	0	-4.313360	-3.043824	-1.903406	176	1	0	-0.909255	-0.675271	-3.515922
121	1	0	-5.784259	-4.785409	-2.812711	177	1	0	0.435162	0.411922	-3.187344
122	1	0	-5.991072	-5.471385	-1.208120	178	1	0	-1.337867	0.442389	-1.429420

179	1	0	-1.050220	-1.247207	-1.112700
180	1	0	1.187466	0.800751	-0.891144
181	1	0	1.170442	-0.808002	-0.210182
182	1	0	0.805689	0.983016	1.506317
183	1	0	-0.643536	1.478345	0.659568
184	1	0	-1.620235	-0.809765	1.086032
185	1	0	-0.155500	-1.249146	1.918003
186	1	0	-1.803466	-0.706387	3.580372
187	1	0	-0.657603	0.612215	3.600103
188	1	0	-2.182522	2.018208	2.267898
189	1	0	-3.286093	0.690136	2.056581
190	1	0	-3.912955	2.437369	3.818671
191	1	0	-2.620511	1.803322	4.811233
192	1	0	-4.987292	0.195774	3.752924
193	1	0	-3.703460	-0.446290	4.766954
194	1	0	-5.562250	-0.035682	6.213110
195	1	0	-4.360563	1.180431	6.576214
196	1	0	-6.797698	1.606217	4.794976
197	1	0	-5.642020	2.844751	5.226522
198	1	0	4.502070	-4.155883	-1.832561
199	1	0	2.757595	-2.857799	-4.776257
200	1	0	2.605562	-3.467579	-3.159787
201	1	0	0.614235	-2.521382	-2.804440
202	1	0	-7.432649	1.360204	7.211294
203	1	0	-7.662545	3.018087	6.676079
204	1	0	-6.259095	2.593983	7.644540

(5*S*)-4a (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.360084	-3.845771	-0.411341
2	6	0	-1.084103	-4.638244	-1.482684
3	6	0	-2.101270	-5.539919	-0.777240
4	6	0	-3.056849	-4.745203	0.117129
5	6	0	-2.347527	-3.737643	1.026875
6	6	0	-1.757081	-4.335392	2.317923
7	6	0	4.346557	-2.350421	-2.286125
8	6	0	3.412291	-3.043563	-3.279905
9	6	0	1.967642	-2.857033	-2.830007
10	6	0	1.832837	-3.216567	-1.361994
11	6	0	2.789309	-2.430895	-0.488111
12	6	0	2.675252	-2.763664	0.992917
13	6	0	5.369739	2.897659	-2.427843
14	6	0	4.820032	2.367645	-3.743002
15	6	0	4.102465	1.052532	-3.490521
16	6	0	4.961652	0.056387	-2.745142
17	6	0	5.557729	0.680135	-1.492208
18	6	0	6.632879	-0.166797	-0.842152
19	6	0	1.240163	4.456035	-0.484186
20	6	0	1.830105	4.793495	-1.851956
21	6	0	3.269167	5.283799	-1.727551
22	6	0	4.109531	4.362823	-0.842408
23	6	0	3.410610	3.977710	0.459050
24	6	0	3.359083	5.089617	1.514384
25	6	0	-3.978388	4.633821	-0.905135
26	6	0	-3.169932	4.995381	-2.148786
27	6	0	-1.837359	4.273896	-2.048323
28	6	0	-1.170615	4.610251	-0.722559
29	6	0	-2.033614	4.317256	0.485198
30	6	0	-1.516724	4.904121	1.792853
31	6	0	-7.147798	0.344070	-0.405396
32	6	0	-7.226304	1.220526	-1.643966
33	6	0	-5.883952	1.888610	-1.883243
34	6	0	-5.422634	2.634047	-0.646485
35	6	0	-5.325111	1.647210	0.510996
36	6	0	-4.940144	2.230978	1.867572
37	6	0	-5.085102	-4.505367	-1.288474
38	6	0	-5.368003	-3.725678	-2.553412
39	6	0	-5.475593	-2.262923	-2.180154
40	6	0	-6.528426	-1.988787	-1.118248
41	6	0	-6.422749	-2.971998	0.059760
42	6	0	-7.724297	-3.163805	0.821260
43	8	0	-1.707859	-3.699443	-2.384252
44	8	0	-1.366607	-6.420300	0.099246
45	8	0	-3.872306	-3.962630	-0.780960
46	8	0	-1.325394	-3.049338	0.257039
47	8	0	3.681568	-2.515605	-4.573138
48	8	0	1.111923	-3.734211	-3.576895
49	8	0	0.485138	-2.862154	-0.977071
50	8	0	4.121510	-2.775059	-0.938777
51	8	0	3.926383	3.300453	-4.352552
52	8	0	3.727788	0.420582	-4.729347
53	8	0	4.030363	-0.970588	-2.369974
54	8	0	6.229345	1.917100	-1.859336
55	8	0	7.187116	0.531901	0.284033
56	8	0	1.778644	3.589650	-2.662498
57	8	0	3.262949	6.566231	-1.069900
58	8	0	4.258553	3.125941	-1.579203
59	8	0	2.086569	3.494917	0.135497
60	8	0	2.545512	4.680156	2.617794
61	8	0	-3.891806	4.680447	-3.331065
62	8	0	-0.963691	4.720690	-3.102019
63	8	0	0.021532	3.793541	-0.669285
64	8	0	-3.296430	5.011548	0.273202
65	8	0	-0.218296	4.378550	2.152122
66	8	0	-7.633731	0.504723	-2.815075
67	8	0	-6.004642	2.851551	-2.950311
68	8	0	-4.156609	3.220171	-0.960687
69	8	0	-6.678019	1.129671	0.675273
70	8	0	-3.530838	2.257748	2.092327
71	8	0	-4.352511	-3.899719	-3.545435
72	8	0	-5.833053	-1.491070	-3.346911
73	8	0	-6.181686	-0.679770	-0.645510
74	8	0	-6.146244	-4.330674	-0.379998
75	8	0	-8.204641	-1.865709	1.202438
76	7	0	-0.897531	-3.339143	2.934085
77	8	0	1.379443	-2.341913	1.498053
78	6	0	-3.281909	0.574694	4.655243
79	7	0	-2.386870	0.100607	3.907042
80	8	0	-2.482355	-0.185795	2.543525

81	6	0	-1.484565	-0.031137	6.070368	137	1	0	-8.089688	-0.076222	-0.120665
82	6	0	-1.077098	-0.064076	4.577301	138	1	0	-7.967225	1.986717	-1.473336
83	6	0	-2.793277	0.806334	6.059647	139	1	0	-5.150664	1.137001	-2.137564
84	8	0	-0.793154	2.173988	3.730310	140	1	0	-6.147250	3.400597	-0.400398
85	6	0	-0.258367	1.179447	4.206448	141	1	0	-4.655271	0.840918	0.263030
86	7	0	1.047042	1.118936	4.477799	142	1	0	-5.460953	1.626948	2.602757
87	6	0	1.937020	2.229321	4.080955	143	1	0	-5.289266	3.248662	1.957167
88	6	0	3.347208	2.049100	4.649294	144	1	0	-5.001654	-5.565142	-1.470601
89	6	0	4.041177	0.750423	4.190297	145	1	0	-6.296918	-4.068079	-2.981598
90	6	0	5.523657	0.701991	4.617348	146	1	0	-4.531030	-1.928033	-1.786785
91	6	0	6.153864	-0.700691	4.484876	147	1	0	-7.510224	-2.005807	-1.569931
92	6	0	6.155578	-1.244969	3.044606	148	1	0	-5.636746	-2.612634	0.701440
93	6	0	6.770132	-2.657243	2.952209	149	1	0	-7.532376	-3.794396	1.679405
94	6	0	6.832294	-3.154015	1.494681	150	1	0	-8.422465	-3.671440	0.168189
95	6	0	7.212111	-4.641644	1.368855	151	1	0	-1.952243	-2.917418	-1.861795
96	6	0	7.108216	-5.155155	-0.084132	152	1	0	-1.054906	-7.214808	-0.352824
97	6	0	8.200284	-4.591778	-1.014777	153	1	0	3.547501	-1.550096	-4.608030
98	6	0	8.080274	-5.153648	-2.445337	154	1	0	0.188083	-3.446621	-3.504988
99	6	0	-0.374310	-1.336012	4.109386	155	1	0	3.117544	3.412478	-3.806996
100	6	0	-1.333053	-2.498112	3.891601	156	1	0	3.326753	1.068935	-5.326438
101	8	0	-2.353068	-2.658060	4.545022	157	1	0	7.448479	1.415831	-0.011098
102	1	0	0.171751	-4.499803	0.257401	158	1	0	1.770396	2.832938	-2.055821
103	1	0	-0.391210	-5.219304	-2.068474	159	1	0	2.983081	7.274935	-1.663901
104	1	0	-2.676476	-6.091933	-1.508572	160	1	0	1.592591	4.672246	2.390821
105	1	0	-3.665643	-5.420944	0.701888	161	1	0	-4.517575	3.944900	-3.194548
106	1	0	-3.034390	-2.950285	1.289243	162	1	0	-0.249870	4.078586	-3.228769
107	1	0	-1.206131	-5.237974	2.110299	163	1	0	-0.338206	3.527038	2.613690
108	1	0	-2.562833	-4.560507	3.000789	164	1	0	-6.977190	-0.175589	-3.069106
109	1	0	5.379324	-2.548581	-2.517352	165	1	0	-6.539862	2.474547	-3.663888
110	1	0	3.628965	-4.099378	-3.313678	166	1	0	-3.121700	1.358230	2.114065
111	1	0	1.690906	-1.819790	-2.955644	167	1	0	-3.456413	-3.866200	-3.159285
112	1	0	2.007244	-4.278182	-1.240847	168	1	0	-5.295544	-1.775243	-4.101006
113	1	0	2.618435	-1.376861	-0.629413	169	1	0	-8.926762	-1.920621	1.839605
114	1	0	3.442819	-2.240607	1.536897	170	1	0	-0.045469	-3.109223	2.455783
115	1	0	2.798493	-3.826251	1.147392	171	1	0	0.793461	-2.053009	0.780331
116	1	0	5.956902	3.790859	-2.570678	172	1	0	-4.253456	0.799011	4.284403
117	1	0	5.638828	2.206058	-4.426433	173	1	0	-2.594644	1.863609	6.195867
118	1	0	3.231612	1.243397	-2.884084	174	1	0	-3.504787	0.476963	6.802449
119	1	0	5.725766	-0.329953	-3.407105	175	1	0	-1.715180	-1.042545	6.368431
120	1	0	4.769408	0.895417	-0.791476	176	1	0	-0.712787	0.389448	6.696933
121	1	0	7.399571	-0.392152	-1.575470	177	1	0	1.454837	0.291378	4.847396
122	1	0	6.205185	-1.079816	-0.468208	178	1	0	1.976282	2.289806	3.004140
123	1	0	1.135718	5.341885	0.115285	179	1	0	1.512617	3.154044	4.436890
124	1	0	1.211526	5.522035	-2.347836	180	1	0	3.914949	2.907628	4.311013
125	1	0	3.721892	5.333347	-2.708619	181	1	0	3.313188	2.078766	5.734242
126	1	0	5.070916	4.819020	-0.647197	182	1	0	3.965204	0.670265	3.111750
127	1	0	3.914578	3.120738	0.874558	183	1	0	3.535296	-0.114347	4.613381
128	1	0	3.028098	6.018449	1.082688	184	1	0	6.088398	1.411480	4.020247
129	1	0	4.359169	5.241020	1.896332	185	1	0	5.599964	1.020881	5.653492
130	1	0	-4.931134	5.139336	-0.898464	186	1	0	7.177454	-0.660916	4.846594
131	1	0	-2.984778	6.059805	-2.144543	187	1	0	5.614532	-1.391180	5.129238
132	1	0	-2.010277	3.209956	-2.099388	188	1	0	5.133365	-1.303179	2.685376
133	1	0	-0.909152	5.662215	-0.745507	189	1	0	6.683845	-0.565840	2.384727
134	1	0	-2.214206	3.266882	0.591156	190	1	0	7.771108	-2.650763	3.374658
135	1	0	-2.243387	4.671122	2.556373	191	1	0	6.173922	-3.345077	3.547086
136	1	0	-1.425060	5.975713	1.694446	192	1	0	5.868192	-3.009578	1.018890

193	1	0	7.548021	-2.541556	0.958350
194	1	0	8.219212	-4.802494	1.743769
195	1	0	6.540821	-5.224036	1.994379
196	1	0	7.180361	-6.239434	-0.087975
197	1	0	6.130276	-4.891416	-0.478468
198	1	0	8.134141	-3.510027	-1.047962
199	1	0	9.176170	-4.841000	-0.609248
200	1	0	8.171325	-6.234668	-2.439339
201	1	0	7.116957	-4.901064	-2.877262
202	1	0	8.854673	-4.752990	-3.090263
203	1	0	0.169726	-1.156748	3.198044
204	1	0	0.337783	-1.640238	4.870795

(5*S*)-4a (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.426056	2.978555	-2.833123
2	6	0	-0.916078	4.321390	-2.319330
3	6	0	-2.341932	4.540544	-2.832859
4	6	0	-3.246788	3.383220	-2.437956
5	6	0	-2.657221	2.018531	-2.788102
6	6	0	-2.816441	1.623654	-4.258936
7	6	0	4.856347	3.024047	-2.264391
8	6	0	4.118793	4.067224	-1.440085
9	6	0	2.677720	3.614679	-1.285407
10	6	0	2.034687	3.346113	-2.643553
11	6	0	2.879086	2.459057	-3.553616
12	6	0	2.522160	2.588780	-5.039387
13	6	0	6.290752	-0.999766	1.055861
14	6	0	5.737202	0.296176	1.677453
15	6	0	4.842638	0.954252	0.637995
16	6	0	5.674961	1.462818	-0.526649
17	6	0	6.677689	0.364411	-0.942615
18	6	0	8.108691	0.750501	-0.568726
19	6	0	2.725061	-4.317179	1.108680
20	6	0	3.438099	-3.920554	2.394355
21	6	0	4.940469	-4.112816	2.219456
22	6	0	5.477121	-3.348465	1.016748
23	6	0	4.664480	-3.572028	-0.250364
24	6	0	4.955883	-4.866618	-1.000631
25	6	0	-2.321679	-4.632025	2.848452
26	6	0	-1.185699	-4.486120	3.854970
27	6	0	0.009147	-3.856941	3.146489
28	6	0	0.397880	-4.703918	1.935932
29	6	0	-0.789482	-4.949900	1.020023
30	6	0	-0.550610	-6.018695	-0.029364
31	6	0	-5.831024	-0.621398	1.903336
32	6	0	-5.359000	-0.979554	3.296693
33	6	0	-3.986576	-1.604219	3.241711
34	6	0	-3.980547	-2.832875	2.338947
35	6	0	-4.410071	-2.378347	0.939434
36	6	0	-4.665340	-3.453181	-0.115401
37	6	0	-4.518949	3.997363	-0.438273
38	6	0	-4.340210	3.991637	1.062175
39	6	0	-4.238005	2.567236	1.551364
40	6	0	-5.412735	1.714314	1.103531
41	6	0	-5.661618	1.839658	-0.395283
42	6	0	-7.041158	1.356024	-0.845855
43	8	0	-0.831281	4.417832	-0.895343
44	8	0	-2.357232	4.517599	-4.272404
45	8	0	-3.351534	3.411811	-0.989876
46	8	0	-1.288337	1.940253	-2.358511
47	8	0	4.804564	4.233232	-0.196259
48	8	0	1.959716	4.643639	-0.596793
49	8	0	0.827961	2.621820	-2.298741
50	8	0	4.262472	2.897166	-3.533595
51	8	0	4.966809	0.050722	2.859052
52	8	0	4.156042	2.058153	1.256014
53	8	0	4.777770	1.744619	-1.615642
54	8	0	6.309930	-0.908390	-0.362562
55	8	0	8.912156	-0.434809	-0.674343
56	8	0	3.106502	-2.552835	2.715683
57	8	0	5.180792	-5.508638	1.942163
58	8	0	5.332309	-1.969055	1.411401
59	8	0	3.234975	-3.508316	0.044450
60	8	0	4.054239	-4.954897	-2.120376
61	8	0	-1.588705	-3.767440	5.006624
62	8	0	1.101182	-3.809328	4.072599
63	8	0	1.356678	-3.966115	1.125979
64	8	0	-1.893130	-5.473273	1.802372
65	8	0	-1.729768	-6.213817	-0.828499
66	8	0	-5.202712	0.207450	4.116017
67	8	0	-3.620865	-2.014100	4.570879
68	8	0	-2.636557	-3.324878	2.352338
69	8	0	-5.737227	-1.777066	1.083867
70	8	0	-3.516728	-4.235504	-0.447944
71	8	0	-3.125270	4.696598	1.339005
72	8	0	-4.177476	2.651679	2.981971
73	8	0	-4.963832	0.371711	1.400558
74	8	0	-5.666260	3.236444	-0.786275
75	8	0	-7.440825	0.126962	-0.224805
76	7	0	-2.561308	0.196513	-4.425563
77	8	0	1.117693	2.612277	-5.303826
78	6	0	-3.471266	-4.112621	-3.423473
79	7	0	-3.112615	-2.906719	-3.542756
80	8	0	-3.968873	-1.811436	-3.289934
81	6	0	-1.230884	-4.199984	-4.176780
82	6	0	-1.658017	-2.736555	-3.814268
83	6	0	-2.361000	-5.096117	-3.608881
84	8	0	-1.437450	-2.887098	-1.441446
85	6	0	-0.985186	-2.393626	-2.478322
86	7	0	0.141050	-1.704014	-2.540960
87	6	0	1.079150	-1.583073	-1.397883
88	6	0	-1.371943	-1.808981	-4.999115
89	6	0	-1.385253	-0.301844	-4.759716
90	8	0	-0.335745	0.330044	-4.934679
91	6	0	0.910866	-0.270054	-0.616534
92	6	0	-0.246649	-0.317217	0.400232
93	6	0	-0.597357	1.076187	0.957805
94	6	0	0.552446	1.764858	1.717849

95	6	0	0.100738	3.095898	2.358311
96	6	0	1.289837	3.988931	2.762546
97	6	0	0.839778	5.271887	3.487503
98	6	0	2.031433	6.180277	3.849374
99	6	0	1.617188	7.516344	4.501024
100	6	0	1.015323	7.357968	5.911041
101	6	0	0.676318	8.721381	6.545536
102	1	0	-0.386638	2.998388	-3.898820
103	1	0	-0.281202	5.101280	-2.717375
104	1	0	-2.734205	5.468959	-2.437311
105	1	0	-4.224164	3.497726	-2.881573
106	1	0	-3.170754	1.283549	-2.191236
107	1	0	-2.161293	2.189901	-4.894146
108	1	0	-3.834769	1.814542	-4.571116
109	1	0	5.885928	3.309967	-2.419022
110	1	0	4.144387	5.008450	-1.967456
111	1	0	2.667155	2.690610	-0.734973
112	1	0	1.815358	4.290330	-3.121803
113	1	0	2.808137	1.447246	-3.190448
114	1	0	3.028998	1.806759	-5.592386
115	1	0	2.916625	3.538169	-5.365665
116	1	0	7.272161	-1.271725	1.412301
117	1	0	6.529309	0.972364	1.958702
118	1	0	4.134928	0.232832	0.261266
119	1	0	6.180062	2.366976	-0.225590
120	1	0	6.601995	0.208408	-2.003091
121	1	0	8.153432	1.152948	0.437240
122	1	0	8.432252	1.531437	-1.248651
123	1	0	2.868582	-5.368653	0.915715
124	1	0	3.074404	-4.517214	3.211560
125	1	0	5.463177	-3.774501	3.102592
126	1	0	6.516139	-3.596121	0.847960
127	1	0	4.839590	-2.736469	-0.903413
128	1	0	4.870024	-5.720694	-0.349473
129	1	0	5.958114	-4.832205	-1.399881
130	1	0	-3.190079	-5.087795	3.296402
131	1	0	-0.903804	-5.478409	4.175039
132	1	0	-0.265890	-2.872393	2.798941
133	1	0	0.825614	-5.636447	2.285455
134	1	0	-1.072199	-4.025002	0.556233
135	1	0	-0.288422	-6.943357	0.469103
136	1	0	0.260017	-5.714292	-0.674346
137	1	0	-6.855013	-0.306504	1.865996
138	1	0	-6.046610	-1.675933	3.756224
139	1	0	-3.281584	-0.884676	2.854456
140	1	0	-4.670920	-3.575958	2.718900
141	1	0	-3.708184	-1.644847	0.574583
142	1	0	-5.037832	-2.936388	-0.991430
143	1	0	-5.425232	-4.126397	0.249808
144	1	0	-4.683854	4.988907	-0.825960
145	1	0	-5.195953	4.467957	1.522208
146	1	0	-3.343253	2.130941	1.141812
147	1	0	-6.295661	1.966574	1.675801
148	1	0	-4.865557	1.309661	-0.890949
149	1	0	-7.063538	1.291355	-1.926088
150	1	0	-7.758911	2.096563	-0.534221
151	1	0	-1.638810	4.103550	-0.454661
152	1	0	-1.823307	5.224329	-4.658347
153	1	0	4.419665	3.656829	0.488705
154	1	0	1.006505	4.439664	-0.529751
155	1	0	4.595529	-0.847948	2.831152
156	1	0	3.877363	1.789318	2.145390
157	1	0	9.852534	-0.219451	-0.625837
158	1	0	2.949158	-2.075905	1.886915
159	1	0	5.184383	-6.043314	2.746499
160	1	0	3.189038	-4.631385	-1.831363
161	1	0	-2.232897	-3.067838	4.792804
162	1	0	1.684632	-3.062790	3.861508
163	1	0	-2.507231	-5.816820	-0.393089
164	1	0	-6.032933	0.492192	4.520309
165	1	0	-3.658251	-1.252049	5.166238
166	1	0	-2.793055	-3.690385	-0.819899
167	1	0	-2.871013	4.540842	2.260451
168	1	0	-4.289259	1.773912	3.386767
169	1	0	-6.865188	-0.619161	-0.446778
170	1	0	-3.267035	-0.475722	-4.110409
171	1	0	0.690079	1.740346	-5.212959
172	1	0	-4.479310	-4.346082	-3.169090
173	1	0	-2.094747	-5.521569	-2.645184
174	1	0	-2.636319	-5.892077	-4.287192
175	1	0	-1.187288	-4.291612	-5.253767
176	1	0	-0.261340	-4.439940	-3.767867
177	1	0	0.358024	-1.156784	-3.349562
178	1	0	0.947231	-2.437502	-0.756666
179	1	0	-0.387121	-2.039149	-5.377964
180	1	0	-2.094249	-2.041032	-5.771813
181	1	0	2.073148	-1.636898	-1.821666
182	1	0	0.755770	0.549974	-1.301947
183	1	0	1.842084	-0.082501	-0.091846
184	1	0	-1.121489	-0.734504	-0.082278
185	1	0	0.015491	-0.991143	1.211754
186	1	0	-0.895372	1.707094	0.129142
187	1	0	-1.447431	0.980314	1.629786
188	1	0	1.369022	1.966900	1.036749
189	1	0	0.931332	1.103184	2.494740
190	1	0	-0.520549	2.884448	3.225880
191	1	0	-0.509607	3.640140	1.646207
192	1	0	1.961397	3.430467	3.411758
193	1	0	1.832079	4.258927	1.863590
194	1	0	0.291125	5.001505	4.384351
195	1	0	0.161242	5.822066	2.840460
196	1	0	2.700066	5.647069	4.520527
197	1	0	2.588290	6.388758	2.941031
198	1	0	0.899602	8.020121	3.858901
199	1	0	2.489771	8.160506	4.570389
200	1	0	1.725038	6.831490	6.542477
201	1	0	0.116693	6.753860	5.862872
202	1	0	1.567402	9.334767	6.629739
203	1	0	-0.044583	9.256072	5.935665
204	1	0	0.255061	8.598031	7.537603

(*2S*,5*R*)-4b-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.292134	-3.425266	0.154355
2	6	0	-0.120041	-4.639752	-0.661773
3	6	0	-0.986701	-5.528705	0.236543
4	6	0	-2.179539	-4.770433	0.813260
5	6	0	-1.814217	-3.391649	1.360481
6	6	0	-1.178725	-3.289846	2.753289
7	6	0	4.721810	-1.511834	-1.946316
8	6	0	3.965833	-2.465330	-2.859007
9	6	0	2.526035	-2.535146	-2.385468
10	6	0	2.428507	-2.798905	-0.885762
11	6	0	3.323199	-1.927403	-0.013483
12	6	0	3.548740	-2.486204	1.390577
13	6	0	4.367692	3.809823	-2.159052
14	6	0	4.119716	3.152689	-3.505340
15	6	0	3.726235	1.701607	-3.287367
16	6	0	4.724128	0.963674	-2.419032
17	6	0	5.000540	1.723959	-1.132489
18	6	0	6.168681	1.191133	-0.330791
19	6	0	-0.152611	4.469282	-0.568270
20	6	0	0.497557	4.967373	-1.844546
21	6	0	1.790673	5.693969	-1.471020
22	6	0	2.702402	4.825605	-0.605086
23	6	0	1.980760	4.158932	0.566045
24	6	0	1.711665	5.055056	1.774944
25	6	0	-5.289941	3.780437	-1.364278
26	6	0	-4.490912	4.303157	-2.559308
27	6	0	-3.046490	3.851607	-2.385255
28	6	0	-2.549399	4.255729	-1.009749
29	6	0	-3.430748	3.769801	0.119100
30	6	0	-3.019203	4.293205	1.491476
31	6	0	-7.381330	-1.177292	-1.102718
32	6	0	-7.411046	-0.432680	-2.428021
33	6	0	-6.268692	0.568013	-2.479568
34	6	0	-6.303452	1.496450	-1.282163
35	6	0	-6.224599	0.646424	-0.018192
36	6	0	-6.291262	1.388406	1.314931
37	6	0	-4.077696	-5.384897	-0.682125
38	6	0	-4.422004	-4.995302	-2.104728
39	6	0	-4.898903	-3.556263	-2.090543
40	6	0	-6.089051	-3.338319	-1.173940
41	6	0	-5.853168	-3.955022	0.213816
42	6	0	-7.137353	-4.279842	0.962545
43	8	0	-0.847586	-4.160813	-1.818320
44	8	0	-0.218672	-5.911308	1.392631
45	8	0	-3.063043	-4.474626	-0.293241
46	8	0	-0.943686	-2.727842	0.402384
47	8	0	4.101557	-1.995388	-4.198960
48	8	0	1.865418	-3.617122	-3.057304
49	8	0	1.037308	-2.506542	-0.604164
50	8	0	4.662215	-1.909164	-0.588911
51	8	0	3.108458	3.844240	-4.240214
52	8	0	3.669451	0.988899	-4.535226
53	8	0	4.057927	-0.260463	-2.095743
54	8	0	5.366577	3.097440	-1.453090
55	8	0	6.356740	2.026665	0.826705
56	8	0	0.739094	3.838282	-2.711105
57	8	0	1.438363	6.828101	-0.652428
58	8	0	3.129157	3.747063	-1.462582
59	8	0	0.746928	3.576629	0.084369
60	8	0	0.948948	4.313268	2.749320
61	8	0	-5.078557	3.866339	-3.773669
62	8	0	-2.200321	4.501354	-3.351117
63	8	0	-1.249963	3.636041	-0.843108
64	8	0	-4.755271	4.276669	-0.141037
65	8	0	-1.659045	3.854633	1.825467
66	8	0	-7.346696	-1.288997	-3.569291
67	8	0	-6.386954	1.375754	-3.665983
68	8	0	-5.170449	2.364203	-1.412498
69	8	0	-7.389628	-0.217085	-0.054657
70	8	0	-4.987529	1.823403	1.744260
71	8	0	-3.313397	-5.123796	-2.997001
72	8	0	-5.312999	-3.168227	-3.417096
73	8	0	-6.157733	-1.906705	-1.048619
74	8	0	-5.224661	-5.261590	0.130753
75	8	0	-7.986151	-3.124257	0.895500
76	7	0	-0.857662	-1.869066	2.868291
77	8	0	2.315582	-2.720118	2.076237
78	6	0	-3.096572	1.381001	4.239802
79	7	0	-2.262946	0.661452	3.300753
80	8	0	-2.701952	0.204975	2.137657
81	6	0	-0.901916	1.101616	5.163190
82	6	0	-0.901697	0.350211	3.812327
83	6	0	-2.054663	2.130984	5.048795
84	6	0	0.131260	0.904403	2.814928
85	6	0	3.504554	1.778667	4.351577
86	6	0	4.614904	0.999069	3.626114
87	6	0	5.940005	1.028778	4.427453
88	6	0	6.784852	-0.250005	4.228765
89	6	0	7.091354	-0.547363	2.750039
90	6	0	7.922758	-1.828453	2.551704
91	6	0	8.072964	-2.186396	1.058354
92	6	0	8.870300	-3.487721	0.844153
93	6	0	8.961971	-3.917958	-0.635452
94	6	0	9.821606	-2.975774	-1.500776
95	6	0	9.948115	-3.469334	-2.955119
96	6	0	-0.862131	-1.179933	4.016056
97	8	0	-0.957828	-1.691748	5.116878
98	6	0	10.811629	-2.525373	-3.814106
99	6	0	1.531466	0.696962	3.356413
100	7	0	2.212144	1.806303	3.637567
101	8	0	1.962821	-0.445485	3.556504
102	8	0	-3.741596	0.350894	5.039983
103	8	0	-4.575028	1.097826	5.990547
104	1	0	0.798367	-3.679562	1.058868
105	1	0	0.731919	-5.186389	-1.032649
106	1	0	-1.338995	-6.389375	-0.317629
107	1	0	-2.677232	-5.369973	1.561879

108	1	0	-2.711246	-2.795444	1.358389
109	1	0	-0.311408	-3.918845	2.859841
110	1	0	-1.898072	-3.557033	3.515279
111	1	0	5.761904	-1.444887	-2.220537
112	1	0	4.405617	-3.448469	-2.817114
113	1	0	2.050191	-1.586451	-2.580787
114	1	0	2.656454	-3.843817	-0.719877
115	1	0	2.914540	-0.931217	0.009675
116	1	0	4.187365	-1.805729	1.933577
117	1	0	4.068864	-3.427893	1.290009
118	1	0	4.711321	4.826484	-2.265947
119	1	0	5.025400	3.193743	-4.089618
120	1	0	2.772597	1.665771	-2.783252
121	1	0	5.629857	0.785808	-2.985068
122	1	0	4.108342	1.724478	-0.530657
123	1	0	7.057503	1.181904	-0.951193
124	1	0	5.955045	0.198089	0.020253
125	1	0	-0.422785	5.296684	0.062207
126	1	0	-0.176540	5.620817	-2.372459
127	1	0	2.326189	5.982647	-2.365771
128	1	0	3.544266	5.407386	-0.254394
129	1	0	2.567449	3.314118	0.886442
130	1	0	1.214460	5.966996	1.490660
131	1	0	2.651906	5.311992	2.239649
132	1	0	-6.320352	4.091950	-1.411565
133	1	0	-4.517442	5.382352	-2.553991
134	1	0	-3.003808	2.777017	-2.474434
135	1	0	-2.464888	5.334923	-0.984057
136	1	0	-3.449487	2.697540	0.134443
137	1	0	-3.715619	3.906743	2.212484
138	1	0	-3.035638	5.372060	1.500634
139	1	0	-8.224707	-1.819096	-0.954792
140	1	0	-8.343494	0.107275	-2.495042
141	1	0	-5.328301	0.035572	-2.478735
142	1	0	-7.224658	2.065556	-1.286179
143	1	0	-5.330442	0.043512	-0.048292
144	1	0	-6.734276	0.709238	2.030469
145	1	0	-6.901407	2.274350	1.246238
146	1	0	-3.752120	-6.409597	-0.602455
147	1	0	-5.207527	-5.638569	-2.469934
148	1	0	-4.097997	-2.923201	-1.747485
149	1	0	-6.978909	-3.737434	-1.640627
150	1	0	-5.233332	-3.268129	0.765297
151	1	0	-6.890784	-4.550803	1.980744
152	1	0	-7.596459	-5.131736	0.479775
153	1	0	-1.291495	-3.344769	-1.530303
154	1	0	0.478488	-6.546730	1.184366
155	1	0	3.799792	-1.073521	-4.280008
156	1	0	0.909330	-3.589209	-2.893213
157	1	0	2.259461	3.851619	-3.754219
158	1	0	3.161346	1.495115	-5.185710
159	1	0	6.450371	2.939862	0.520429
160	1	0	0.904633	3.064896	-2.149441
161	1	0	1.170455	7.593172	-1.177804
162	1	0	-0.001374	4.283447	2.517878
163	1	0	-5.405535	2.946692	-3.723267
164	1	0	-1.396384	3.979937	-3.492522
165	1	0	-1.344852	3.212498	1.172916
166	1	0	-6.591858	-1.912824	-3.527883
167	1	0	-6.636088	0.808776	-4.411261
168	1	0	-4.362625	1.083544	1.789509
169	1	0	-2.471553	-4.848670	-2.583855
170	1	0	-4.661038	-3.482036	-4.061788
171	1	0	-8.624023	-3.088377	1.617082
172	1	0	-0.746062	-1.412238	1.991851
173	1	0	2.074556	-1.968302	2.653701
174	1	0	-1.744910	2.994399	4.475707
175	1	0	-2.443125	2.432547	6.006803
176	1	0	-1.110831	0.385638	5.940642
177	1	0	0.049636	1.574648	5.349759
178	1	0	3.798190	2.810321	4.496916
179	1	0	3.349794	1.331830	5.327073
180	1	0	4.786211	1.411205	2.640907
181	1	0	4.271405	-0.017727	3.524592
182	1	0	6.521100	1.895547	4.130402
183	1	0	5.724689	1.129936	5.488564
184	1	0	7.716739	-0.151451	4.778772
185	1	0	6.246347	-1.092313	4.655047
186	1	0	6.155343	-0.669425	2.220437
187	1	0	7.590329	0.303028	2.301322
188	1	0	8.905938	-1.703316	2.997540
189	1	0	7.437421	-2.653630	3.066699
190	1	0	7.085653	-2.293421	0.616865
191	1	0	8.568896	-1.363897	0.552460
192	1	0	9.872902	-3.369489	1.246540
193	1	0	8.390951	-4.281908	1.409963
194	1	0	9.388025	-4.916257	-0.686855
195	1	0	7.960085	-3.976445	-1.052504
196	1	0	9.391343	-1.979746	-1.504093
197	1	0	10.813462	-2.896713	-1.063498
198	1	0	10.385580	-4.463031	-2.958323
199	1	0	8.958008	-3.553159	-3.392966
200	1	0	10.890062	-2.887176	-4.833374
201	1	0	11.813127	-2.446347	-3.404223
202	1	0	10.378271	-1.530930	-3.841217
203	1	0	0.045298	0.403148	1.860883
204	1	0	-0.075015	1.948491	2.660814
205	1	0	1.795082	2.701796	3.432185
206	1	0	-3.846496	1.958375	3.738617
207	1	0	-4.559710	0.481449	6.740761

(*2S*,5*R*)-4b-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.890743	2.367311	-2.833242
2	6	0	-0.788908	3.886094	-2.791421
3	6	0	-2.113706	4.496585	-3.237771
4	6	0	-3.265497	3.931963	-2.426913
5	6	0	-3.267349	2.412583	-2.383804
6	6	0	-3.812001	1.690967	-3.621109

7	6	0	4.311640	1.244312	-3.231275	63	8	0	0.845922	-3.529324	1.919294
8	6	0	3.807905	2.655897	-3.033019	64	8	0	-1.807807	-3.653810	4.409026
9	6	0	2.500914	2.610579	-2.277594	65	8	0	-3.210918	-4.860770	2.494485
10	6	0	1.478467	1.846258	-3.096110	66	8	0	-3.101562	3.158796	5.359712
11	6	0	1.983947	0.434574	-3.385336	67	8	0	-1.667407	0.860474	6.146881
12	6	0	1.165009	-0.276759	-4.472437	68	8	0	-1.834520	-1.328492	4.311391
13	6	0	5.771539	-3.135059	-0.938448	69	8	0	-4.985226	0.459199	3.803242
14	6	0	6.572788	-1.986772	-0.302443	70	8	0	-3.704710	-2.273478	1.877578
15	6	0	5.794579	-0.688565	-0.455056	71	8	0	-2.844308	6.408027	0.753309
16	6	0	5.641386	-0.300633	-1.913858	72	8	0	-3.197078	5.041830	3.176687
17	6	0	5.377739	-1.560906	-2.771187	73	8	0	-3.865381	2.292700	2.923231
18	6	0	6.636275	-1.970101	-3.543429	74	8	0	-5.136531	3.740448	-0.186976
19	6	0	1.797359	-4.439559	1.408946	75	8	0	-5.545175	0.779694	-0.507369
20	6	0	3.110817	-4.420708	2.179556	76	7	0	-4.220367	0.367838	-3.158775
21	6	0	4.110237	-5.320853	1.451261	77	8	0	-0.220721	0.048236	-4.428733
22	6	0	4.283236	-4.896500	-0.005949	78	6	0	-6.102225	-3.485675	-3.545115
23	6	0	2.965978	-4.685048	-0.741825	79	7	0	-5.655132	-2.260672	-2.935058
24	6	0	2.276037	-5.957884	-1.223310	80	8	0	-6.483401	-1.474556	-2.255481
25	6	0	-1.517871	-2.446174	5.110010	81	6	0	-3.711492	-3.291405	-3.749732
26	6	0	-0.028256	-2.409603	5.371288	82	6	0	-4.185871	-2.040301	-2.986919
27	6	0	0.742529	-2.478730	4.067834	83	6	0	-4.835814	-4.334446	-3.544446
28	6	0	0.309078	-3.687104	3.250587	84	6	0	-3.677170	-1.953401	-1.547230
29	6	0	-1.197338	-3.690553	3.085893	85	6	0	-3.895260	-0.765030	-3.800124
30	6	0	-1.761553	-4.935182	2.432790	86	8	0	-3.431815	-0.801561	-4.925244
31	6	0	-4.561580	1.800699	4.044848	87	6	0	-0.565726	-0.512235	0.062568
32	6	0	-3.593378	1.814753	5.212311	88	6	0	-0.823509	0.535727	1.167385
33	6	0	-2.442826	0.869416	4.946180	89	6	0	0.150135	1.730518	1.137246
34	6	0	-2.979173	-0.509544	4.605818	90	6	0	1.626479	1.384342	1.412059
35	6	0	-3.898280	-0.423832	3.395142	91	6	0	2.498826	2.657991	1.416478
36	6	0	-4.526756	-1.729930	2.931316	92	6	0	4.004498	2.379103	1.589560
37	6	0	-4.237728	4.832082	-0.382741	93	6	0	4.849903	3.645613	1.342026
38	6	0	-3.865018	5.434303	0.961892	94	6	0	6.344144	3.416271	1.639550
39	6	0	-3.397609	4.369263	1.931090	95	6	0	7.234541	4.622329	1.273548
40	6	0	-4.445017	3.282144	2.054046	96	6	0	-2.233233	-1.487975	-1.460435
41	6	0	-4.694155	2.668374	0.689392	97	8	0	-1.530538	-1.375289	-2.467357
42	6	0	-5.778492	1.607446	0.660341	98	7	0	-1.823606	-1.230114	-0.220086
43	8	0	-0.429176	4.345080	-1.480381	99	6	0	6.990110	5.857506	2.163454
44	8	0	-2.415028	4.077623	-4.582353	100	6	0	7.976534	7.013288	1.891114
45	8	0	-3.068904	4.410272	-1.059790	101	6	0	7.784394	7.657300	0.503352
46	8	0	-1.955916	1.942617	-1.983873	102	8	0	-6.501087	-3.146414	-4.899729
47	8	0	4.778400	3.426136	-2.327151	103	8	0	-6.991715	-4.416257	-5.454215
48	8	0	2.152589	3.984219	-2.065104	104	1	0	-1.035674	2.021675	-3.836213
49	8	0	0.279624	1.768751	-2.291411	105	1	0	0.002628	4.213698	-3.447763
50	8	0	3.327988	0.511211	-3.959983	106	1	0	-2.081275	5.572498	-3.132565
51	8	0	6.809752	-2.210491	1.095594	107	1	0	-4.204025	4.299921	-2.814933
52	8	0	6.526904	0.341717	0.217712	108	1	0	-3.917004	2.140029	-1.582359
53	8	0	4.553822	0.639698	-1.972466	109	1	0	-3.088616	1.572915	-4.406724
54	8	0	4.897986	-2.642240	-1.939961	110	1	0	-4.657654	2.239919	-4.017766
55	8	0	6.492436	-3.355848	-3.897123	111	1	0	5.204278	1.237170	-3.838014
56	8	0	3.586847	-3.067602	2.286988	112	1	0	3.622752	3.073668	-4.016218
57	8	0	3.566556	-6.656566	1.439700	113	1	0	2.654290	2.096848	-1.343632
58	8	0	4.971012	-3.633390	0.118108	114	1	0	1.289552	2.362063	-4.028148
59	8	0	2.045283	-3.931900	0.103415	115	1	0	2.015460	-0.115181	-2.457603
60	8	0	0.989645	-5.612668	-1.765572	116	1	0	1.340651	-1.344726	-4.417620
61	8	0	0.277947	-1.175863	6.043226	117	1	0	1.545688	0.080716	-5.416741
62	8	0	2.115314	-2.535236	4.470203	118	1	0	6.391639	-3.916060	-1.347861

119	1	0	7.543109	-1.881723	-0.758634
120	1	0	4.802488	-0.809855	-0.043353
121	1	0	6.552222	0.193236	-2.228968
122	1	0	4.571808	-1.370934	-3.454367
123	1	0	7.530215	-1.825598	-2.947348
124	1	0	6.716668	-1.329057	-4.414514
125	1	0	1.410040	-5.445636	1.382447
126	1	0	2.971249	-4.768667	3.190032
127	1	0	5.074965	-5.272423	1.935001
128	1	0	4.900081	-5.613991	-0.531209
129	1	0	3.146254	-4.029377	-1.574091
130	1	0	2.186499	-6.677102	-0.426022
131	1	0	2.860699	-6.397001	-2.018434
132	1	0	-2.089780	-2.460406	6.023519
133	1	0	0.244055	-3.257196	5.984134
134	1	0	0.527993	-1.593335	3.489367
135	1	0	0.653495	-4.597489	3.726779
136	1	0	-1.503764	-2.819849	2.540497
137	1	0	-1.419105	-5.826338	2.942805
138	1	0	-1.490665	-4.975034	1.391962
139	1	0	-5.448345	2.377887	4.249457
140	1	0	-4.107241	1.493334	6.107501
141	1	0	-1.877295	1.238223	4.103002
142	1	0	-3.522677	-0.910873	5.453165
143	1	0	-3.374692	0.012545	2.565584
144	1	0	-5.516766	-1.508771	2.561291
145	1	0	-4.614109	-2.429953	3.753796
146	1	0	-4.777392	5.542054	-0.987669
147	1	0	-4.761097	5.879712	1.378027
148	1	0	-2.482871	3.921766	1.565602
149	1	0	-5.354832	3.684721	2.482908
150	1	0	-3.769386	2.240008	0.340347
151	1	0	-6.735171	2.107611	0.598285
152	1	0	-5.730849	1.009317	1.556142
153	1	0	-1.218541	4.412989	-0.915073
154	1	0	-1.808131	4.458670	-5.229759
155	1	0	4.317232	4.206246	-1.983221
156	1	0	1.305000	4.103513	-1.588372
157	1	0	6.036202	-2.662912	1.466543
158	1	0	6.798125	0.000609	1.083344
159	1	0	7.126639	-3.605258	-4.581509
160	1	0	3.564000	-2.661357	1.407513
161	1	0	3.894994	-7.194480	2.170728
162	1	0	0.667712	-4.814537	-1.321707
163	1	0	1.240256	-1.058497	6.038691
164	1	0	2.723928	-2.483531	3.704949
165	1	0	-3.456885	-4.839273	3.431412
166	1	0	-2.366160	3.146155	5.991032
167	1	0	-0.917139	0.234566	6.089774
168	1	0	-3.650227	-3.248388	1.932366
169	1	0	-2.503638	6.675646	1.619979
170	1	0	-3.054161	4.406626	3.905926
171	1	0	-6.299491	0.222269	-0.742651
172	1	0	-4.706406	0.341241	-2.287976
173	1	0	-0.710438	-0.470070	-3.761099
174	1	0	-4.741066	-4.822983	-2.582619
175	1	0	-4.870855	-5.075964	-4.324632
176	1	0	-3.625035	-3.030703	-4.791737
177	1	0	-2.748583	-3.615718	-3.389583
178	1	0	-2.444217	-1.436345	0.542809
179	1	0	-0.277507	-0.010156	-0.845173
180	1	0	0.200963	-1.218413	0.358089
181	1	0	-1.818445	0.930334	1.000172
182	1	0	-0.817325	0.059710	2.143430
183	1	0	0.069545	2.205339	0.168428
184	1	0	-0.173612	2.450864	1.885851
185	1	0	1.992766	0.706974	0.646047
186	1	0	1.717434	0.874946	2.369310
187	1	0	2.163102	3.314943	2.214840
188	1	0	2.345005	3.191429	0.485606
189	1	0	4.188626	2.002231	2.593516
190	1	0	4.330108	1.622514	0.885672
191	1	0	4.462682	4.464661	1.939878
192	1	0	4.747368	3.909373	0.295583
193	1	0	6.472261	3.184074	2.695053
194	1	0	6.661604	2.553992	1.067581
195	1	0	7.067068	4.872383	0.231446
196	1	0	8.278009	4.331551	1.369813
197	1	0	-4.284471	-1.271884	-0.970407
198	1	0	-3.764585	-2.928977	-1.081512
199	1	0	7.082206	5.554974	3.203456
200	1	0	5.977371	6.220612	2.024065
201	1	0	7.844001	7.776816	2.652031
202	1	0	8.993986	6.644275	1.982704
203	1	0	6.767094	8.018418	0.392384
204	1	0	7.979546	6.946348	-0.289975
205	1	0	8.457377	8.498309	0.372560
206	1	0	-6.947713	-3.896955	-3.025324
207	1	0	-6.906109	-4.222056	-6.401414

(*2R*,5*R*)-4b-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.226465	-3.428874	0.280527
2	6	0	-0.144875	-4.678809	-0.501435
3	6	0	-1.041766	-5.538680	0.393529
4	6	0	-2.262701	-4.767203	0.884817
5	6	0	-1.930778	-3.363290	1.390925
6	6	0	-1.370492	-3.207291	2.807043
7	6	0	4.747130	-1.655553	-1.729315
8	6	0	4.024297	-2.661189	-2.611799
9	6	0	2.563451	-2.687301	-2.203313
10	6	0	2.397040	-2.850976	-0.695797
11	6	0	3.254541	-1.927755	0.158587
12	6	0	3.404433	-2.392952	1.606251
13	6	0	4.529604	3.639859	-2.405232
14	6	0	4.288145	2.866547	-3.690470
15	6	0	3.848478	1.452014	-3.352942
16	6	0	4.803313	0.771885	-2.395123

17	6	0	5.043446	1.635714	-1.169617	73	8	0	-6.104007	-1.967987	-1.120778
18	6	0	6.142072	1.137315	-0.257375	74	8	0	-5.258435	-5.336869	0.072346
19	6	0	0.043830	4.475492	-0.805363	75	8	0	-8.039123	-3.189301	0.722907
20	6	0	0.662897	4.937729	-2.109958	76	7	0	-1.089455	-1.776744	2.912499
21	6	0	1.971386	5.661411	-1.782779	77	8	0	2.132401	-2.553927	2.242330
22	6	0	2.896580	4.804197	-0.919903	78	6	0	-3.390838	1.232224	4.513634
23	6	0	2.204788	4.186211	0.294175	79	7	0	-2.487981	0.748161	3.468201
24	6	0	1.984755	5.119153	1.485385	80	8	0	-2.838091	0.677177	2.197599
25	6	0	-5.148462	3.730387	-1.165968	81	6	0	-1.090326	1.099471	5.304014
26	6	0	-4.452938	4.304049	-2.403666	82	6	0	-1.109342	0.426431	3.922639
27	6	0	-3.002182	3.840656	-2.371140	83	6	0	-2.560286	1.030431	5.782152
28	6	0	-2.383903	4.217769	-1.037477	84	6	0	-0.086925	1.009418	2.939105
29	6	0	-3.159778	3.684900	0.152793	85	6	0	3.346091	1.848405	4.362610
30	6	0	-2.645853	4.190677	1.497930	86	6	0	4.445349	1.008420	3.691684
31	6	0	-7.311218	-1.223103	-1.236999	87	6	0	5.755278	1.050198	4.515993
32	6	0	-7.238209	-0.430199	-2.529834	88	6	0	6.614189	-0.222871	4.350114
33	6	0	-6.079976	0.552508	-2.462517	89	6	0	6.958504	-0.533901	2.882921
34	6	0	-6.201488	1.460033	-1.251209	90	6	0	7.824449	-1.797618	2.723370
35	6	0	-6.243807	0.574576	-0.007426	91	6	0	8.001433	-2.185789	1.240845
36	6	0	-6.506914	1.264366	1.324835	92	6	0	8.835677	-3.469495	1.064995
37	6	0	-4.076601	-5.450468	-0.691227	93	6	0	8.950392	-3.933837	-0.402672
38	6	0	-4.367689	-5.072266	-2.128917	94	6	0	9.786569	-2.988057	-1.286881
39	6	0	-4.836592	-3.630456	-2.137649	95	6	0	9.938275	-3.514726	-2.727144
40	6	0	-6.054085	-3.400099	-1.261606	96	6	0	-1.099308	-1.106055	4.070867
41	6	0	-5.893185	-4.033127	0.129754	97	8	0	-1.250821	-1.643152	5.156563
42	6	0	-7.218705	-4.364686	0.797381	98	6	0	10.778558	-2.567047	-3.604857
43	8	0	-0.825073	-4.249608	-1.705984	99	6	0	1.309224	0.801707	3.497049
44	8	0	-0.320865	-5.863953	1.596589	100	7	0	2.065147	1.882746	3.631927
45	8	0	-3.095710	-4.518686	-0.269885	101	8	0	1.668916	-0.337121	3.837191
46	8	0	-1.019806	-2.727239	0.453583	102	8	0	-3.687427	2.623390	4.272403
47	8	0	4.229119	-2.284906	-3.971867	103	8	0	-5.144375	2.784707	4.325640
48	8	0	1.924834	-3.808577	-2.831048	104	1	0	0.697956	-3.641111	1.214152
49	8	0	0.996449	-2.542841	-0.490763	105	1	0	0.725712	-5.231103	-0.815508
50	8	0	4.619266	-1.961429	-0.352297	106	1	0	-1.362699	-6.425568	-0.137748
51	8	0	3.303998	3.510270	-4.503122	107	1	0	-2.791204	-5.338880	1.634106
52	8	0	3.801196	0.634771	-4.535404	108	1	0	-2.833758	-2.780081	1.320703
53	8	0	4.106737	-0.410044	-1.989026	109	1	0	-0.494453	-3.810874	2.974059
54	8	0	5.471643	2.961926	-1.593298	110	1	0	-2.118687	-3.475979	3.539710
55	8	0	6.262372	2.035517	0.862214	111	1	0	5.799754	-1.616444	-1.956727
56	8	0	0.868580	3.796936	-2.967705	112	1	0	4.449740	-3.643081	-2.482492
57	8	0	1.651340	6.817008	-0.981810	113	1	0	2.106439	-1.750787	-2.484024
58	8	0	3.265123	3.692774	-1.763344	114	1	0	2.615830	-3.882838	-0.452861
59	8	0	0.956467	3.599909	-0.144530	115	1	0	2.857379	-0.928915	0.094625
60	8	0	1.260572	4.416718	2.512762	116	1	0	4.031289	-1.688547	2.130287
61	8	0	-5.152437	3.947625	-3.581251	117	1	0	3.911484	-3.347481	1.594428
62	8	0	-2.234966	4.500087	-3.394350	118	1	0	4.921184	4.626582	-2.595249
63	8	0	-1.060263	3.633675	-1.032286	119	1	0	5.201898	2.829525	-4.262313
64	8	0	-4.503306	4.185857	0.015806	120	1	0	2.881649	1.487049	-2.874062
65	8	0	-1.221574	3.886487	1.640717	121	1	0	5.725372	0.533363	-2.910123
66	8	0	-7.104720	-1.236851	-3.700276	122	1	0	4.122119	1.715459	-0.619194
67	8	0	-6.095251	1.369224	-3.646786	123	1	0	7.071958	1.076229	-0.810837
68	8	0	-5.047341	2.309608	-1.253951	124	1	0	5.884420	0.171501	0.136841
69	8	0	-7.390497	-0.297531	-0.163149	125	1	0	-0.211598	5.319844	-0.192783
70	8	0	-5.350829	1.955162	1.840572	126	1	0	-0.021763	5.593112	-2.623502
71	8	0	-3.228515	-5.209100	-2.979855	127	1	0	2.488940	5.925840	-2.695525
72	8	0	-5.207155	-3.243713	-3.477594	128	1	0	3.763468	5.377061	-0.619638

129	1	0	2.792485	3.345850	0.624050
130	1	0	1.478908	6.023156	1.190940
131	1	0	2.945566	5.388530	1.898751
132	1	0	-6.176493	4.047757	-1.112412
133	1	0	-4.470981	5.381251	-2.336245
134	1	0	-2.973644	2.767101	-2.483014
135	1	0	-2.323910	5.297470	-0.984520
136	1	0	-3.154859	2.608240	0.131696
137	1	0	-3.181436	3.727736	2.304303
138	1	0	-2.761974	5.261760	1.546873
139	1	0	-8.170340	-1.858407	-1.172236
140	1	0	-8.155428	0.128490	-2.639500
141	1	0	-5.150148	0.006471	-2.394370
142	1	0	-7.110737	2.043864	-1.321536
143	1	0	-5.337921	-0.010360	0.046396
144	1	0	-6.838098	0.497374	2.011836
145	1	0	-7.288701	1.999554	1.224535
146	1	0	-3.739638	-6.469391	-0.590227
147	1	0	-5.142329	-5.715148	-2.517137
148	1	0	-4.043176	-3.001393	-1.772580
149	1	0	-6.931902	-3.776321	-1.768273
150	1	0	-5.309629	-3.349947	0.723237
151	1	0	-7.032801	-4.671272	1.818340
152	1	0	-7.660899	-5.194449	0.261841
153	1	0	-1.273762	-3.418778	-1.473578
154	1	0	0.378915	-6.513339	1.449028
155	1	0	3.929836	-1.372914	-4.135573
156	1	0	0.961470	-3.758732	-2.726154
157	1	0	2.469492	3.639612	-4.011269
158	1	0	3.320032	1.095219	-5.238371
159	1	0	6.427507	2.924295	0.516833
160	1	0	1.029915	3.028113	-2.399499
161	1	0	1.359191	7.566897	-1.516086
162	1	0	0.302483	4.366939	2.304602
163	1	0	-5.367920	2.994451	-3.622340
164	1	0	-1.444419	3.978190	-3.596461
165	1	0	-0.922956	3.248155	0.978062
166	1	0	-6.391741	-1.905514	-3.622624
167	1	0	-6.319253	0.813664	-4.408786
168	1	0	-4.540442	1.417814	1.824285
169	1	0	-2.399675	-4.943577	-2.534982
170	1	0	-4.535809	-3.559549	-4.101152
171	1	0	-8.824072	-3.254573	1.279504
172	1	0	-0.885444	-1.331776	2.045815
173	1	0	1.916845	-1.816857	2.848071
174	1	0	-2.804596	1.794119	6.502592
175	1	0	-2.742391	0.047083	6.185573
176	1	0	-0.424798	0.580662	5.973830
177	1	0	-0.785344	2.131708	5.193004
178	1	0	3.666232	2.876743	4.467246
179	1	0	3.162425	1.447852	5.352524
180	1	0	4.641316	1.372376	2.691560
181	1	0	4.079101	-0.005025	3.634227
182	1	0	6.335451	1.918514	4.221092
183	1	0	5.517334	1.161864	5.571070
184	1	0	7.532060	-0.109576	4.920496
185	1	0	6.074210	-1.065765	4.773462
186	1	0	6.037479	-0.686632	2.335400
187	1	0	7.447471	0.321641	2.432146
188	1	0	8.798172	-1.637417	3.178524
189	1	0	7.353356	-2.622986	3.251171
190	1	0	7.021328	-2.328790	0.794163
191	1	0	8.480727	-1.362093	0.720970
192	1	0	9.831564	-3.313693	1.471183
193	1	0	8.374079	-4.262398	1.647147
194	1	0	9.406910	-4.919601	-0.426182
195	1	0	7.953599	-4.033820	-0.824193
196	1	0	9.325907	-2.006149	-1.318769
197	1	0	10.772382	-2.866921	-0.845628
198	1	0	10.406084	-4.494166	-2.701758
199	1	0	8.954364	-3.640293	-3.168920
200	1	0	10.875178	-2.952457	-4.613834
201	1	0	11.774249	-2.446626	-3.190929
202	1	0	10.315114	-1.587462	-3.660659
203	1	0	-0.159802	0.520267	1.977264
204	1	0	-0.318570	2.050509	2.798442
205	1	0	1.751590	2.780149	3.287025
206	1	0	-4.317948	0.689653	4.501760
207	1	0	-5.358678	2.669217	3.363393

(*2R*,5*R*)-4b-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815741	2.496646	-2.807938
2	6	0	-0.686719	4.010839	-2.711344
3	6	0	-1.988742	4.662178	-3.166894
4	6	0	-3.170098	4.092360	-2.403887
5	6	0	-3.201241	2.572836	-2.415410
6	6	0	-3.728820	1.901405	-3.688667
7	6	0	4.373102	1.295006	-3.141239
8	6	0	3.887648	2.707273	-2.905513
9	6	0	2.566406	2.658848	-2.175307
10	6	0	1.547699	1.938934	-3.037539
11	6	0	2.035551	0.528504	-3.360947
12	6	0	1.225396	-0.135268	-4.484263
13	6	0	5.752391	-3.168708	-0.954299
14	6	0	6.560201	-2.046472	-0.280822
15	6	0	5.798133	-0.735810	-0.405590
16	6	0	5.662308	-0.308190	-1.854824
17	6	0	5.390749	-1.542170	-2.747112
18	6	0	6.650584	-1.945790	-3.520341
19	6	0	1.738455	-4.511461	1.296345
20	6	0	3.038088	-4.511549	2.090693
21	6	0	4.048814	-5.400827	1.365179
22	6	0	4.251092	-4.948484	-0.079458
23	6	0	2.948805	-4.723601	-0.837307
24	6	0	2.272699	-5.986752	-1.359655
25	6	0	-1.625873	-2.563067	4.978687
26	6	0	-0.140718	-2.547344	5.265456

27	6	0	0.651686	-2.595680	3.973969	83	6	0	-4.911392	-3.335613	-4.901697
28	6	0	0.221109	-3.782028	3.123144	84	6	0	-3.709333	-1.793516	-1.693447
29	6	0	-1.282190	-3.764209	2.932122	85	6	0	-3.846098	-0.551397	-3.924033
30	6	0	-1.850971	-4.985614	2.240201	86	8	0	-3.367344	-0.578506	-5.044788
31	6	0	-4.607747	1.741405	3.969823	87	6	0	-0.578471	-0.505970	0.003063
32	6	0	-3.662942	1.710892	5.155961	88	6	0	-0.835953	0.509788	1.138171
33	6	0	-2.516837	0.761960	4.884608	89	6	0	0.153587	1.691611	1.160561
34	6	0	-3.060290	-0.601261	4.495815	90	6	0	1.621014	1.317547	1.446422
35	6	0	-3.954633	-0.472270	3.270338	91	6	0	2.507104	2.579955	1.513834
36	6	0	-4.589073	-1.758092	2.759883	92	6	0	4.006988	2.277347	1.695754
37	6	0	-4.174642	4.920663	-0.343689	93	6	0	4.868050	3.545936	1.524829
38	6	0	-3.820991	5.470235	1.028326	94	6	0	6.355423	3.286430	1.831826
39	6	0	-3.378923	4.367110	1.966626	95	6	0	7.263232	4.499345	1.538583
40	6	0	-4.437939	3.286390	2.032518	96	6	0	-2.252160	-1.377842	-1.574888
41	6	0	-4.668907	2.723570	0.642798	97	8	0	-1.543787	-1.222804	-2.572088
42	6	0	-5.764143	1.676682	0.560906	98	7	0	-1.843174	-1.193579	-0.320970
43	8	0	-0.349553	4.417610	-1.377385	99	6	0	7.017083	5.692303	2.483884
44	8	0	-2.265787	4.294943	-4.531918	100	6	0	8.019370	6.849178	2.283691
45	8	0	-2.996846	4.516010	-1.016002	101	6	0	7.856312	7.561824	0.926083
46	8	0	-1.909469	2.064005	-1.999533	102	8	0	-6.367750	-4.195140	-3.128967
47	8	0	4.857318	3.437676	-2.157759	103	8	0	-6.918993	-5.228885	-4.015263
48	8	0	2.236500	4.030435	-1.923520	104	1	0	-0.943164	2.188683	-3.825467
49	8	0	0.330420	1.857302	-2.260957	105	1	0	0.126266	4.345078	-3.337333
50	8	0	3.391023	0.600271	-3.908497	106	1	0	-1.938701	5.733010	-3.023953
51	8	0	6.781893	-2.309754	1.112828	107	1	0	-4.092082	4.492753	-2.799620
52	8	0	6.537008	0.267937	0.299428	108	1	0	-3.875532	2.287710	-1.639166
53	8	0	4.587149	0.647176	-1.898917	109	1	0	-2.987574	1.789961	-4.458662
54	8	0	4.891899	-2.639102	-1.948342	110	1	0	-4.551993	2.480546	-4.089449
55	8	0	6.494001	-3.320248	-3.910591	111	1	0	5.275038	1.293745	-3.734082
56	8	0	3.517910	-3.163189	2.233429	112	1	0	3.726781	3.159980	-3.877501
57	8	0	3.502324	-6.734310	1.314042	113	1	0	2.694216	2.112264	-1.256298
58	8	0	4.938219	-3.688689	0.081305	114	1	0	1.387083	2.486572	-3.956632
59	8	0	2.008837	-3.987785	0.002022	115	1	0	2.040999	-0.049977	-2.450293
60	8	0	1.013904	-5.627814	-1.953891	116	1	0	1.378734	-1.207712	-4.456476
61	8	0	0.167070	-1.332216	5.969875	117	1	0	1.632471	0.241031	-5.410010
62	8	0	2.016560	-2.672471	4.399197	118	1	0	6.368217	-3.944081	-1.380477
63	8	0	0.783759	-3.603163	1.805177	119	1	0	7.535697	-1.940273	-0.725631
64	8	0	-1.914783	-3.751292	4.245604	120	1	0	4.801357	-0.855948	-0.005010
65	8	0	-3.299783	-4.893992	2.282507	121	1	0	6.582062	0.182127	-2.148897
66	8	0	-3.160366	3.044431	5.353964	122	1	0	4.592774	-1.324325	-3.431338
67	8	0	-1.764413	0.712007	6.098875	123	1	0	7.541422	-1.826896	-2.914003
68	8	0	-1.918616	-1.423990	4.201098	124	1	0	6.744952	-1.283514	-4.373965
69	8	0	-5.039778	0.412414	3.680222	125	1	0	1.346020	-5.514991	1.250645
70	8	0	-3.747585	-2.287984	1.715038	126	1	0	2.877655	-4.877444	3.091752
71	8	0	-2.789884	6.442964	0.873894	127	1	0	5.003856	-5.365461	1.868961
72	8	0	-3.194949	4.994467	3.238014	128	1	0	4.877959	-5.656362	-0.605840
73	8	0	-3.885616	2.260110	2.876464	129	1	0	3.144753	-4.052287	-1.653470
74	8	0	-5.085248	3.830148	-0.203192	130	1	0	2.146892	-6.714082	-0.574544
75	8	0	-5.530204	0.898916	-0.639343	131	1	0	2.885986	-6.421324	-2.135327
76	7	0	-4.176954	0.574583	-3.273947	132	1	0	-2.213262	-2.592470	5.881980
77	8	0	-0.154435	0.216277	-4.459767	133	1	0	0.112690	-3.411125	5.863631
78	6	0	-6.123710	-3.066609	-4.018915	134	1	0	0.455091	-1.696084	3.411235
79	7	0	-5.660358	-1.993690	-3.176361	135	1	0	0.546377	-4.706199	3.586158
80	8	0	-6.484537	-1.348692	-2.357426	136	1	0	-1.569586	-2.877196	2.402946
81	6	0	-3.726528	-3.066451	-3.943968	137	1	0	-1.527004	-5.893143	2.733241
82	6	0	-4.178810	-1.835667	-3.143975	138	1	0	-1.565146	-5.003348	1.202826

139	1	0	-5.492756	2.321280	4.174554
140	1	0	-4.197985	1.368502	6.030734
141	1	0	-1.931948	1.148428	4.062818
142	1	0	-3.624527	-1.019847	5.320993
143	1	0	-3.409740	-0.020229	2.463205
144	1	0	-5.566363	-1.514606	2.370498
145	1	0	-4.707030	-2.475663	3.563190
146	1	0	-4.698624	5.656554	-0.931200
147	1	0	-4.721104	5.907106	1.444841
148	1	0	-2.461576	3.924546	1.601530
149	1	0	-5.351714	3.683164	2.458417
150	1	0	-3.743025	2.297057	0.293800
151	1	0	-6.715655	2.188261	0.513501
152	1	0	-5.728351	1.041674	1.431693
153	1	0	-1.150449	4.477352	-0.827696
154	1	0	-1.636445	4.685973	-5.151359
155	1	0	4.402423	4.212850	-1.794951
156	1	0	1.382657	4.148099	-1.457799
157	1	0	6.000552	-2.764764	1.463627
158	1	0	6.795543	-0.098006	1.158770
159	1	0	7.128661	-3.558714	-4.598429
160	1	0	3.522480	-2.741842	1.360892
161	1	0	3.803472	-7.284133	2.047994
162	1	0	0.656577	-4.857155	-1.489156
163	1	0	1.130444	-1.224332	5.981375
164	1	0	2.638772	-2.607038	3.645836
165	1	0	-3.559118	-4.888559	3.216005
166	1	0	-2.436550	3.003809	5.997437
167	1	0	-1.017327	0.082512	6.037460
168	1	0	-3.711699	-3.265128	1.743458
169	1	0	-2.462562	6.674993	1.755857
170	1	0	-3.073107	4.333691	3.948264
171	1	0	-6.253747	0.296125	-0.861030
172	1	0	-4.666919	0.537021	-2.404851
173	1	0	-0.666297	-0.304808	-3.811100
174	1	0	-4.931486	-4.342195	-5.285364
175	1	0	-4.880736	-2.617299	-5.707650
176	1	0	-2.806609	-2.861915	-4.461203
177	1	0	-3.610601	-3.908311	-3.275566
178	1	0	-2.469690	-1.431674	0.427983
179	1	0	-0.269669	0.020835	-0.883828
180	1	0	0.173254	-1.233150	0.285951
181	1	0	-1.823261	0.923508	0.971707
182	1	0	-0.849410	0.002256	2.098010
183	1	0	0.094116	2.198699	0.206579
184	1	0	-0.172441	2.391710	1.927209
185	1	0	1.992618	0.664733	0.661868
186	1	0	1.689886	0.771772	2.385259
187	1	0	2.167221	3.207784	2.333600
188	1	0	2.372266	3.152362	0.603331
189	1	0	4.171716	1.849496	2.682524
190	1	0	4.336137	1.553243	0.960108
191	1	0	4.479903	4.337707	2.157783
192	1	0	4.783285	3.863780	0.491821
193	1	0	6.465320	3.001671	2.876473
194	1	0	6.672770	2.449485	1.223346
195	1	0	7.114593	4.801683	0.507534
196	1	0	8.302142	4.193159	1.636244
197	1	0	-4.298881	-1.093439	-1.121879
198	1	0	-3.850815	-2.769495	-1.245127
199	1	0	7.089448	5.338496	3.509161
200	1	0	6.010417	6.072747	2.346707
201	1	0	7.882165	7.576265	3.078708
202	1	0	9.031435	6.465156	2.373208
203	1	0	6.844571	7.938711	0.816704
204	1	0	8.057443	6.888197	0.102261
205	1	0	8.539610	8.400975	0.847117
206	1	0	-7.040032	-2.823869	-4.523602
207	1	0	-7.460720	-5.721993	-3.378633

(*2S*,5*R*)-4a-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.556010	2.381136	0.199294
2	6	0	-4.802326	3.456461	-0.858698
3	6	0	-4.693949	4.832295	-0.208994
4	6	0	-3.398744	5.013962	0.583560
5	6	0	-3.097150	3.838308	1.512208
6	6	0	-3.886057	3.951312	2.832815
7	6	0	-5.993272	-2.172023	-2.295885
8	6	0	-5.820914	-0.929112	-3.138887
9	6	0	-4.910757	0.022881	-2.392904
10	6	0	-5.471820	0.392575	-1.036554
11	6	0	-5.782985	-0.866951	-0.216687
12	6	0	-6.672766	-0.587374	0.981251
13	6	0	-2.137031	-5.862480	-2.054540
14	6	0	-2.390840	-5.247448	-3.421979
15	6	0	-3.052102	-3.902353	-3.192445
16	6	0	-4.322279	-4.044876	-2.392380
17	6	0	-4.095043	-4.816368	-1.094004
18	6	0	-5.386226	-5.279386	-0.423503
19	6	0	2.508079	-3.611329	-1.211049
20	6	0	1.627234	-4.527810	-2.043940
21	6	0	0.939832	-5.653995	-1.238818
22	6	0	-0.321304	-5.353772	-0.399370
23	6	0	-0.287371	-4.254174	0.667382
24	6	0	0.670650	-4.522614	1.853383
25	6	0	5.232086	0.524446	-0.709771
26	6	0	6.007715	-0.273921	-1.765256
27	6	0	5.157474	-1.358986	-2.431181
28	6	0	4.339710	-2.090686	-1.380532
29	6	0	3.486038	-1.059967	-0.662763
30	6	0	2.384120	-1.652076	0.177430
31	6	0	3.241358	5.377606	-1.502668
32	6	0	3.864038	4.791268	-2.758666
33	6	0	3.890988	3.277114	-2.661854
34	6	0	4.502919	2.815292	-1.357797
35	6	0	3.753538	3.436629	-0.183031
36	6	0	4.266048	3.091296	1.215859
37	6	0	-1.959934	6.368854	-0.881571

38	6	0	-1.528681	6.123183	-2.316928	94	1	0	-3.417604	4.721797	3.429328
39	6	0	-0.266759	5.278816	-2.323359	95	1	0	-6.652475	-2.891962	-2.755976
40	6	0	0.802626	5.892735	-1.448304	96	1	0	-6.783915	-0.466626	-3.293154
41	6	0	0.273175	6.073255	-0.030210	97	1	0	-3.947243	-0.434923	-2.246198
42	6	0	1.246720	6.757684	0.901773	98	1	0	-6.357796	1.002958	-1.167129
43	8	0	-3.869200	3.384523	-1.931446	99	1	0	-4.865199	-1.329045	0.103449
44	8	0	-5.776383	4.968446	0.741027	100	1	0	-7.645749	-0.270113	0.624778
45	8	0	-2.328425	5.097409	-0.373981	101	1	0	-6.221146	0.183611	1.573415
46	8	0	-3.321253	2.581665	0.847707	102	1	0	-1.685331	-6.839165	-2.119884
47	8	0	-5.262452	-1.197523	-4.424992	103	1	0	-3.054379	-5.891959	-3.977895
48	8	0	-4.781255	1.227730	-3.181418	104	1	0	-2.374823	-3.264958	-2.649435
49	8	0	-4.410571	1.085684	-0.360594	105	1	0	-5.076537	-4.522304	-3.006659
50	8	0	-6.560549	-1.819644	-1.035514	106	1	0	-3.519320	-4.214744	-0.413152
51	8	0	-1.210989	-5.075937	-4.199316	107	1	0	-5.125877	-6.006716	0.325418
52	8	0	-3.415602	-3.294144	-4.452445	108	1	0	-6.046493	-5.740420	-1.146950
53	8	0	-4.706477	-2.697482	-2.065938	109	1	0	2.948595	-4.141790	-0.385168
54	8	0	-3.396305	-6.043472	-1.411175	110	1	0	2.285732	-4.999788	-2.757113
55	8	0	-6.056809	-4.202565	0.274104	111	1	0	0.615444	-6.380379	-1.976864
56	8	0	0.687547	-3.748282	-2.797520	112	1	0	-0.617248	-6.296662	0.046104
57	8	0	1.926895	-6.250118	-0.369587	113	1	0	-1.299936	-4.116697	1.026176
58	8	0	-1.328909	-4.933358	-1.363656	114	1	0	1.485360	-5.150890	1.542547
59	8	0	1.702576	-2.535265	-0.749291	115	1	0	0.135866	-5.033925	2.647278
60	8	0	1.267994	-3.303015	2.333958	116	1	0	5.913015	1.061887	-0.073266
61	8	0	6.555970	0.665379	-2.684773	117	1	0	6.836568	-0.775699	-1.293963
62	8	0	6.054270	-2.266888	-3.078087	118	1	0	4.470458	-0.904574	-3.135026
63	8	0	3.528647	-3.076295	-2.056965	119	1	0	4.990973	-2.578089	-0.665989
64	8	0	4.420486	-0.297454	0.137988	120	1	0	3.024239	-0.408000	-1.385875
65	8	0	1.471743	-0.685916	0.607649	121	1	0	2.697964	-2.197869	1.042201
66	8	0	3.158722	5.188054	-3.936042	122	1	0	0.026601	-3.338547	0.208334
67	8	0	4.699147	2.723535	-3.718866	123	1	0	3.323898	6.452361	-1.482930
68	8	0	4.343256	1.388830	-1.390733	124	1	0	4.877698	5.149998	-2.852030
69	8	0	3.902502	4.878174	-0.347546	125	1	0	2.879138	2.902260	-2.714353
70	8	0	3.597504	1.946956	1.763048	126	1	0	5.550883	3.082371	-1.330277
71	8	0	-2.548769	5.489067	-3.081801	127	1	0	2.710684	3.175254	-0.229556
72	8	0	0.276727	5.211719	-3.660025	128	1	0	4.014991	3.920866	1.855304
73	8	0	1.888973	4.955560	-1.485804	129	1	0	5.345547	2.981647	1.216203
74	8	0	-0.892452	6.930104	-0.138352	130	1	0	-2.776062	7.072319	-0.826941
75	8	0	0.657157	6.688449	2.213220	131	1	0	-1.310617	7.072110	-2.784497
76	7	0	-3.891140	2.704839	3.589856	132	1	0	-0.496563	4.290606	-1.953333
77	8	0	-6.780607	-1.727983	1.852470	133	1	0	1.105327	6.845967	-1.864727
78	6	0	-2.497004	-0.425188	4.314131	134	1	0	-0.003572	5.119185	0.384868
79	6	0	-2.769427	-1.591474	5.313549	135	1	0	1.381652	7.783316	0.578055
80	6	0	-3.161995	-2.792498	4.423045	136	1	0	2.192665	6.234212	0.866942
81	6	0	-3.899058	-2.166003	3.240883	137	1	0	-4.035635	2.570633	-2.456758
82	7	0	-3.390771	-0.807860	3.203385	138	1	0	-6.587622	5.280648	0.320739
83	8	0	-4.064631	0.112627	2.523471	139	1	0	-4.570260	-1.895144	-4.404458
84	6	0	-1.030420	-0.564361	3.859606	140	1	0	-4.681973	0.971925	-4.112208
85	8	0	-0.674533	-1.667279	3.429801	141	1	0	-0.522455	-4.577544	-3.702339
86	7	0	-0.218041	0.467917	4.010341	142	1	0	-2.703678	-3.443613	-5.093276
87	6	0	1.190947	0.379480	3.580478	143	1	0	-6.260771	-3.425859	-0.275235
88	1	0	-5.380077	2.412414	0.899954	144	1	0	0.405749	-3.002160	-2.247116
89	1	0	-5.817631	3.346885	-1.229646	145	1	0	2.394792	-6.981431	-0.792074
90	1	0	-4.742786	5.585485	-0.984115	146	1	0	0.599295	-2.687042	2.694016
91	1	0	-3.461393	5.927289	1.160838	147	1	0	5.862117	1.198548	-3.115929
92	1	0	-2.046127	3.836391	1.738981	148	1	0	5.539594	-2.966816	-3.503830
93	1	0	-4.907307	4.230163	2.641141	149	1	0	0.997428	-0.274760	-0.128010

150	1	0	2.189062	5.104114	-3.825235
151	1	0	4.459727	3.138219	-4.560479
152	1	0	3.757931	1.125696	1.270251
153	1	0	-2.939177	4.720450	-2.603658
154	1	0	-0.440823	5.036134	-4.286384
155	1	0	1.268034	7.019614	2.883449
156	1	0	-3.600830	-1.315132	5.951663
157	1	0	-1.908987	-1.802425	5.930644
158	1	0	-3.775358	-3.511100	4.943313
159	1	0	-2.274457	-3.258722	4.036311
160	1	0	-7.186382	-2.480734	1.404184
161	1	0	-0.573670	1.379302	4.236110
162	1	0	1.222331	-0.141836	2.640680
163	1	0	-4.642278	2.073231	3.430321
164	6	0	-2.778735	2.215743	4.153648
165	8	0	-1.710343	2.826240	4.129077
166	6	0	-2.930756	0.913488	4.943945
167	1	0	-2.343084	1.050875	5.842904
168	1	0	-3.965251	0.802270	5.234753
169	1	0	-4.968377	-2.146166	3.328806
170	8	0	-3.586989	-2.814028	1.982923
171	8	0	-4.222760	-4.128237	2.139017
172	1	0	-5.015663	-4.027984	1.557319
173	1	0	1.551016	1.383117	3.409168
174	6	0	2.087188	-0.339827	4.602977
175	1	0	2.144234	0.238499	5.520240
176	1	0	1.654601	-1.306766	4.832175
177	6	0	3.489081	-0.535947	3.995547
178	1	0	3.375530	-1.161411	3.118916
179	1	0	3.871094	0.420825	3.659059
180	6	0	4.492011	-1.199770	4.953861
181	1	0	4.155463	-2.205994	5.188078
182	1	0	4.521110	-0.642448	5.886542
183	6	0	5.919873	-1.259528	4.366557
184	1	0	6.268783	-0.245398	4.201429
185	1	0	6.584354	-1.715523	5.096290
186	6	0	6.004502	-2.062616	3.050573
187	1	0	5.506858	-3.017555	3.199598
188	1	0	5.474437	-1.540202	2.261946
189	6	0	7.454326	-2.325091	2.586618
190	1	0	8.010997	-2.801314	3.389505
191	1	0	7.430483	-3.023295	1.756420
192	6	0	8.193352	-1.044170	2.150259
193	1	0	8.245147	-0.359835	2.989853
194	1	0	7.617635	-0.550573	1.371256
195	6	0	9.624934	-1.303137	1.632767
196	1	0	10.130626	-0.349341	1.508650
197	1	0	10.180189	-1.863316	2.380474
198	6	0	9.670846	-2.057840	0.289566
199	1	0	9.234529	-3.044408	0.401937
200	1	0	9.073798	-1.522095	-0.443278
201	6	0	11.106632	-2.207607	-0.248955
202	1	0	11.543165	-1.222162	-0.379857
203	1	0	11.711215	-2.733317	0.484353
204	6	0	11.143110	-2.967861	-1.588795
205	1	0	10.736172	-3.966764	-1.470776
206	1	0	10.552786	-2.449390	-2.336450
207	1	0	12.158654	-3.057648	-1.959162

(*2S*,5*R*)-4a-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.247313	-0.627720	1.759351
2	6	0	4.320311	0.169342	3.064722
3	6	0	5.461630	1.179624	2.977114
4	6	0	5.407493	2.001444	1.692856
5	6	0	5.239955	1.157224	0.434442
6	6	0	6.542798	0.470985	-0.007545
7	6	0	0.891118	-4.666266	2.920056
8	6	0	1.007353	-3.524125	3.919976
9	6	0	1.492973	-2.296401	3.175500
10	6	0	2.837731	-2.533772	2.528315
11	6	0	2.746616	-3.761404	1.628976
12	6	0	4.072639	-4.299242	1.127363
13	6	0	-3.670444	-5.325198	0.131756
14	6	0	-3.668114	-5.100615	1.633618
15	6	0	-2.395175	-4.382182	2.038318
16	6	0	-1.154958	-5.121831	1.582997
17	6	0	-1.232162	-5.321157	0.069948
18	6	0	-0.197048	-6.270107	-0.517566
19	6	0	-5.803931	-0.628284	-0.824677
20	6	0	-5.796934	-1.876200	0.027111
21	6	0	-5.964687	-3.198807	-0.749195
22	6	0	-4.767779	-3.812686	-1.508984
23	6	0	-4.064176	-3.063224	-2.642629
24	6	0	-4.951302	-2.774749	-3.882682
25	6	0	-4.802009	4.223833	-1.378285
26	6	0	-5.935287	4.201492	-0.352604
27	6	0	-5.986851	2.857932	0.373113
28	6	0	-5.947481	1.742061	-0.658243
29	6	0	-4.656443	1.845516	-1.463521
30	6	0	-4.469837	0.636250	-2.357642
31	6	0	0.157370	6.098439	-0.636743
32	6	0	-0.922458	6.610318	0.306478
33	6	0	-2.022851	5.572900	0.442185
34	6	0	-2.553061	5.183303	-0.922454
35	6	0	-1.402818	4.619449	-1.755276
36	6	0	-1.692569	4.265418	-3.209088
37	6	0	4.270918	4.157934	2.138268
38	6	0	2.992626	4.423044	2.916750
39	6	0	1.782247	4.315283	1.999858
40	6	0	1.959088	5.171453	0.761882
41	6	0	3.215544	4.680488	0.056303
42	6	0	3.538494	5.329249	-1.266031
43	8	0	3.106132	0.852208	3.364584
44	8	0	6.713433	0.456515	2.951677
45	8	0	4.212401	2.789433	1.807162
46	8	0	4.170604	0.213211	0.628672
47	8	0	-0.196698	-3.167270	4.596098
48	8	0	1.607411	-1.205340	4.116450

49	8	0	3.067606	-1.402151	1.671718	105	1	0	7.200639	1.235861	-0.397713
50	8	0	2.178941	-4.874866	2.374760	106	1	0	0.591462	-5.590057	3.388223
51	8	0	-4.793852	-4.339770	2.076263	107	1	0	1.743122	-3.811129	4.657917
52	8	0	-2.363594	-4.283322	3.481160	108	1	0	0.783118	-2.046925	2.406243
53	8	0	-0.035758	-4.282410	1.911041	109	1	0	3.601995	-2.646520	3.287616
54	8	0	-2.476816	-6.005833	-0.223947	110	1	0	2.117195	-3.508596	0.795265
55	8	0	1.162399	-5.836804	-0.308049	111	1	0	4.644543	-4.648662	1.979028
56	8	0	-4.632244	-1.917555	0.868789	112	1	0	4.603102	-3.524140	0.609600
57	8	0	-7.056422	-3.051268	-1.679533	113	1	0	-4.484553	-5.964414	-0.170964
58	8	0	-3.746596	-4.061456	-0.497534	114	1	0	-3.706778	-6.057889	2.130178
59	8	0	-4.526287	-0.456829	-1.403810	115	1	0	-2.380097	-3.395519	1.602679
60	8	0	-4.888373	-1.395552	-4.308675	116	1	0	-1.086327	-6.076515	2.088665
61	8	0	-5.787963	5.321956	0.504586	117	1	0	-1.208866	-4.357519	-0.416768
62	8	0	-7.227268	2.798413	1.083477	118	1	0	-0.401768	-6.379115	-1.573145
63	8	0	-6.062756	0.485044	0.034834	119	1	0	-0.291962	-7.231704	-0.040757
64	8	0	-4.827841	3.068544	-2.233420	120	1	0	-6.563013	-0.697859	-1.586693
65	8	0	-3.242259	0.515931	-3.011714	121	1	0	-6.640301	-1.783260	0.694296
66	8	0	-0.419238	6.970179	1.592253	122	1	0	-6.206796	-3.938948	0.004179
67	8	0	-3.127119	6.128396	1.181227	123	1	0	-5.128200	-4.764088	-1.885574
68	8	0	-3.580750	4.211864	-0.664804	124	1	0	-3.224017	-3.687233	-2.921934
69	8	0	-0.435165	5.701177	-1.857301	125	1	0	-5.985705	-2.952408	-3.655084
70	8	0	-2.460966	3.058193	-3.335200	126	1	0	-4.657609	-3.427945	-4.696084
71	8	0	2.838924	3.520166	4.008679	127	1	0	-4.882544	5.088637	-2.016590
72	8	0	0.616433	4.774774	2.724439	128	1	0	-6.875823	4.315313	-0.868467
73	8	0	0.803878	4.960978	-0.071594	129	1	0	-5.136033	2.758097	1.034740
74	8	0	4.311313	4.957569	0.967835	130	1	0	-6.781005	1.853392	-1.342129
75	8	0	4.518573	4.452562	-1.865277	131	1	0	-3.798787	1.935470	-0.821304
76	7	0	6.312105	-0.524140	-1.053203	132	1	0	-5.283169	0.522548	-3.051585
77	8	0	3.847587	-5.359580	0.182442	133	1	0	-3.682756	-2.135428	-2.264145
78	6	0	4.436633	-1.918202	-3.654579	134	1	0	0.869434	6.875064	-0.867291
79	6	0	4.656822	-2.998656	-4.754823	135	1	0	-1.347314	7.503341	-0.127054
80	6	0	3.692761	-4.143911	-4.388695	136	1	0	-1.630674	4.697046	0.939501
81	6	0	3.620223	-4.126292	-2.862597	137	1	0	-2.973316	6.054949	-1.409238
82	7	0	3.956742	-2.753084	-2.542369	138	1	0	-0.971895	3.770643	-1.254813
83	8	0	3.996051	-2.306111	-1.291817	139	1	0	-0.745239	4.097243	-3.690772
84	6	0	3.286478	-1.001929	-4.123226	140	1	0	-2.183646	5.097093	-3.701235
85	8	0	2.239136	-1.532212	-4.475874	141	1	0	5.150958	4.398449	2.714229
86	7	0	3.504153	0.313314	-4.149448	142	1	0	3.024692	5.424614	3.319799
87	6	0	2.458619	1.262053	-4.558536	143	1	0	1.646672	3.288428	1.697097
88	6	0	2.215084	2.345336	-3.485515	144	1	0	2.049424	6.212894	1.037256
89	6	0	1.232084	1.933942	-2.365662	145	1	0	3.139328	3.620740	-0.112222
90	6	0	1.603856	0.630688	-1.628067	146	1	0	3.934443	6.322847	-1.098309
91	6	0	0.864148	0.468146	-0.285147	147	1	0	2.644223	5.378447	-1.871952
92	6	0	-0.674768	0.470056	-0.408164	148	1	0	2.414515	0.194663	3.605988
93	6	0	-1.386479	-0.137833	0.821654	149	1	0	7.005995	0.214290	3.839434
94	6	0	-1.095631	0.612097	2.138095	150	1	0	-1.003996	-3.547486	4.186519
95	6	0	-1.717080	-0.052588	3.387775	151	1	0	0.833327	-1.235842	4.701101
96	6	0	-3.257824	-0.014863	3.427624	152	1	0	-4.728850	-3.422935	1.726608
97	6	0	-3.839601	-0.820640	4.610099	153	1	0	-3.254677	-4.084706	3.806962
98	6	0	-3.507397	-0.221493	5.990596	154	1	0	1.321518	-4.947903	-0.665085
99	1	0	5.127769	-1.257138	1.714435	155	1	0	-3.840792	-1.810450	0.322814
100	1	0	4.563423	-0.525154	3.864188	156	1	0	-7.905349	-3.288456	-1.285166
101	1	0	5.399477	1.849789	3.824212	157	1	0	-3.992701	-1.031886	-4.245711
102	1	0	6.287208	2.627048	1.615819	158	1	0	-4.872123	5.430678	0.825700
103	1	0	4.906493	1.796757	-0.363474	159	1	0	-7.298450	1.932758	1.509821
104	1	0	7.028236	-0.011932	0.821000	160	1	0	-2.722060	1.344260	-3.097087

161	1	0	-0.092216	6.184913	2.085715
162	1	0	-2.792400	6.639523	1.932364
163	1	0	-3.409109	3.203820	-3.162133
164	1	0	2.942702	2.584814	3.711617
165	1	0	0.622742	4.381847	3.610361
166	1	0	4.850781	4.803679	-2.700721
167	1	0	5.682664	-3.344265	-4.709949
168	1	0	4.462413	-2.607225	-5.741599
169	1	0	4.008500	-5.101053	-4.771317
170	1	0	2.705325	-3.897332	-4.739695
171	1	0	3.084156	-5.884185	0.469889
172	1	0	4.336433	0.713620	-3.757900
173	1	0	2.768343	1.733669	-5.485439
174	1	0	1.562727	0.693338	-4.751304
175	1	0	1.803584	3.218035	-3.988531
176	1	0	3.158051	2.652085	-3.046598
177	1	0	1.187119	2.748929	-1.648673
178	1	0	0.238736	1.831508	-2.793258
179	1	0	2.663051	0.611049	-1.409558
180	1	0	1.382712	-0.219489	-2.263853
181	1	0	1.205183	-0.451405	0.174011
182	1	0	1.180278	1.266777	0.377127
183	1	0	-1.028736	1.487752	-0.547762
184	1	0	-0.979718	-0.085171	-1.290191
185	1	0	-2.453642	-0.142960	0.629277
186	1	0	-1.065184	-1.172072	0.931137
187	1	0	-0.021870	0.657366	2.282439
188	1	0	-1.454852	1.635257	2.055260
189	1	0	-1.331856	0.455788	4.266997
190	1	0	-1.383897	-1.083857	3.452906
191	1	0	-3.589459	1.018109	3.499564
192	1	0	-3.667878	-0.423833	2.514649
193	1	0	-4.918301	-0.875319	4.500182
194	1	0	-3.459418	-1.837091	4.556709
195	1	0	-3.849102	0.806956	6.046874
196	1	0	-3.994124	-0.782133	6.781698
197	1	0	-2.441263	-0.237515	6.180318
198	1	0	6.234520	-1.479396	-0.785367
199	6	0	5.905151	-0.166171	-2.277119
200	8	0	5.727317	1.013798	-2.584620
201	6	0	5.798552	-1.273150	-3.322458
202	1	0	6.176806	-0.833975	-4.237126
203	1	0	6.460397	-2.079344	-3.039438
204	1	0	4.271711	-4.808679	-2.349277
205	8	0	2.269050	-4.431099	-2.419481
206	8	0	2.153086	-5.855025	-2.772248
207	1	0	2.054656	-6.232030	-1.875103

(*2R*,5*R*)-4a-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.732251	4.630926	-0.014190
2	6	0	0.547673	5.605510	1.142390
3	6	0	-0.858874	6.201661	1.070405
4	6	0	-1.941182	5.148645	0.835058
5	6	0	-1.603433	4.150010	-0.271808
6	6	0	-1.767522	4.710810	-1.702452
7	6	0	5.910970	3.592988	-0.566697
8	6	0	5.514702	4.288863	0.727130
9	6	0	4.055744	3.986667	0.995760
10	6	0	3.194012	4.406009	-0.169703
11	6	0	3.675247	3.750783	-1.458862
12	6	0	2.969272	4.284974	-2.702650
13	6	0	7.692168	-1.430935	-0.993785
14	6	0	8.023339	-0.648794	0.273062
15	6	0	6.977388	0.421781	0.532089
16	6	0	6.716284	1.252403	-0.705268
17	6	0	6.247958	0.318319	-1.814775
18	6	0	5.879439	0.972723	-3.144915
19	6	0	4.001376	-4.533229	0.902487
20	6	0	5.424251	-4.132984	1.249796
21	6	0	6.442006	-4.429714	0.131648
22	6	0	6.432594	-3.581263	-1.150705
23	6	0	5.220477	-3.558412	-2.073496
24	6	0	4.762418	-4.890525	-2.685600
25	6	0	-0.861222	-4.602348	1.889479
26	6	0	-0.271687	-5.563030	2.919880
27	6	0	1.188474	-5.216491	3.187042
28	6	0	1.904492	-5.104834	1.853869
29	6	0	1.255729	-4.021632	1.002946
30	6	0	2.034982	-3.784552	-0.267467
31	6	0	-3.701101	-0.605096	3.899335
32	6	0	-2.946117	-1.440477	4.922106
33	6	0	-1.711232	-2.054235	4.286943
34	6	0	-2.091903	-2.783252	3.017970
35	6	0	-2.724945	-1.790501	2.052709
36	6	0	-3.115131	-2.348517	0.687309
37	6	0	-2.942040	4.577034	3.039934
38	6	0	-2.275141	4.078287	4.312152
39	6	0	-2.022626	2.585951	4.186808
40	6	0	-3.284598	1.844335	3.818308
41	6	0	-3.893995	2.408569	2.549000
42	6	0	-5.255810	1.835784	2.203373
43	8	0	0.759897	4.982462	2.409490
44	8	0	-0.912567	7.089633	-0.070137
45	8	0	-1.970893	4.364560	2.041642
46	8	0	-0.280449	3.656640	-0.039625
47	8	0	6.300391	3.879454	1.846675
48	8	0	3.591743	4.709662	2.160032
49	8	0	1.902679	3.863579	0.127381
50	8	0	5.094404	4.040707	-1.627992
51	8	0	8.105085	-1.517498	1.406275
52	8	0	7.439119	1.311565	1.568727
53	8	0	5.716470	2.202033	-0.339826
54	8	0	7.386782	-0.550234	-2.068707
55	8	0	4.470321	1.264434	-3.211042
56	8	0	5.493610	-2.769473	1.688481
57	8	0	6.301357	-5.810221	-0.262641
58	8	0	6.577534	-2.222365	-0.660445

59	8	0	3.367323	-3.452949	0.223009	115	1	0	5.352684	-5.134102	-3.563107
60	8	0	3.355371	-4.803070	-3.018577	116	1	0	-1.844172	-4.925897	1.591763
61	8	0	-1.107505	-5.510151	4.069094	117	1	0	-0.308326	-6.571004	2.538566
62	8	0	1.764910	-6.279103	3.952186	118	1	0	1.246624	-4.267246	3.703652
63	8	0	3.289372	-4.793328	2.110361	119	1	0	1.836545	-6.051573	1.329410
64	8	0	-0.076608	-4.488031	0.700590	120	1	0	1.208579	-3.098520	1.556704
65	8	0	1.556810	-2.741584	-1.054307	121	1	0	2.096140	-4.642062	-0.911190
66	8	0	-2.566260	-0.663547	6.059833	122	1	0	4.398020	-3.159618	-1.515655
67	8	0	-1.121253	-3.003030	5.200693	123	1	0	-4.656852	-0.284769	4.280523
68	8	0	-0.879373	-3.301519	2.459970	124	1	0	-3.581871	-2.237929	5.275705
69	8	0	-3.946382	-1.343300	2.710377	125	1	0	-1.002804	-1.275536	4.045374
70	8	0	-2.000430	-2.346597	-0.227412	126	1	0	-2.779481	-3.585384	3.246323
71	8	0	-1.046413	4.759025	4.555416	127	1	0	-2.067197	-0.952642	1.894493
72	8	0	-1.593834	2.041297	5.454361	128	1	0	-3.851066	-1.684772	0.267931
73	8	0	-2.856945	0.492303	3.604078	129	1	0	-3.561194	-3.332144	0.784465
74	8	0	-4.122863	3.831194	2.765960	130	1	0	-3.237596	5.612057	3.113272
75	8	0	-5.772482	2.499635	1.039599	131	1	0	-2.923421	4.258367	5.156395
76	7	0	-0.962171	3.966091	-2.667870	132	1	0	-1.280769	2.414574	3.421903
77	8	0	2.890444	3.334688	-3.773032	133	1	0	-3.985100	1.899734	4.642981
78	6	0	-0.311037	0.507502	-3.996713	134	1	0	-3.213169	2.269942	1.727144
79	6	0	0.223187	-0.019327	-5.352076	135	1	0	-5.921371	1.961507	3.050803
80	6	0	0.596949	-1.479361	-5.017325	136	1	0	-5.166555	0.790502	1.959700
81	6	0	1.273396	-1.327734	-3.663448	137	1	0	1.697259	4.705799	2.466337
82	7	0	0.576079	-0.221650	-3.074467	138	1	0	-0.530262	7.953853	0.128957
83	8	0	0.597392	-0.024425	-1.747228	139	1	0	6.605491	2.952758	1.764483
84	6	0	-1.783698	0.073653	-3.935575	140	1	0	4.261680	4.631055	2.856458
85	8	0	-2.522380	0.514966	-4.810759	141	1	0	7.246647	-1.969150	1.537758
86	7	0	-2.159090	-0.829128	-3.027336	142	1	0	7.779171	0.794405	2.313982
87	6	0	-3.576441	-1.205381	-2.927316	143	1	0	3.908061	0.476886	-3.324522
88	1	0	0.738922	5.207785	-0.926084	144	1	0	4.927397	-2.245213	1.103499
89	1	0	1.251136	6.422692	1.012943	145	1	0	6.796704	-6.407226	0.312573
90	1	0	-1.068432	6.722268	1.995558	146	1	0	3.192205	-3.987710	-3.515362
91	1	0	-2.891489	5.632402	0.650838	147	1	0	-0.986460	-4.682596	4.576145
92	1	0	-2.230045	3.286483	-0.168625	148	1	0	2.700795	-6.084414	4.101134
93	1	0	-1.466438	5.742765	-1.741786	149	1	0	1.408048	-1.901123	-0.596542
94	1	0	-2.818283	4.645569	-1.960744	150	1	0	-2.168879	0.192429	5.799234
95	1	0	6.934390	3.801656	-0.835881	151	1	0	-1.096062	-2.619365	6.089827
96	1	0	5.645643	5.353781	0.602895	152	1	0	-1.339169	-3.025941	-0.023597
97	1	0	3.934668	2.925662	1.142341	153	1	0	-0.473037	4.765936	3.756014
98	1	0	3.186807	5.486946	-0.248451	154	1	0	-0.890265	2.596310	5.821187
99	1	0	3.532099	2.689664	-1.376151	155	1	0	-5.736223	3.453768	1.194990
100	1	0	3.491186	5.182763	-3.010055	156	1	0	1.112748	0.532574	-5.628007
101	1	0	1.954696	4.537472	-2.446079	157	1	0	-0.533777	0.079630	-6.110853
102	1	0	8.524910	-2.034542	-1.317690	158	1	0	1.239447	-1.949409	-5.743946
103	1	0	8.983275	-0.169020	0.161068	159	1	0	-0.298406	-2.072931	-4.892268
104	1	0	6.047884	-0.043424	0.828322	160	1	0	3.584105	2.648820	-3.684845
105	1	0	7.627068	1.749256	-1.016076	161	1	0	-1.610668	-1.005534	-2.210626
106	1	0	5.412246	-0.270857	-1.472803	162	1	0	-3.927738	-1.478829	-3.912678
107	1	0	6.178360	0.293291	-3.931232	163	1	0	-0.348755	4.471428	-3.267990
108	1	0	6.383136	1.915796	-3.278474	164	6	0	-1.061471	2.621473	-2.794001
109	1	0	4.001395	-5.417463	0.286482	165	8	0	-1.825664	1.960598	-2.110206
110	1	0	5.700396	-4.743982	2.096216	166	6	0	-0.216322	2.029499	-3.909168
111	1	0	7.418615	-4.251637	0.568718	167	1	0	-0.620093	2.420577	-4.836833
112	1	0	7.320963	-3.863930	-1.705086	168	1	0	0.817111	2.345682	-3.822020
113	1	0	5.446940	-2.853975	-2.864085	169	1	0	-3.616743	-2.069518	-2.282064
114	1	0	4.859708	-5.696856	-1.985242	170	6	0	-4.447362	-0.061586	-2.374138

171	1	0	-4.027254	0.286698	-1.438387
172	1	0	-4.397468	0.761173	-3.074039
173	6	0	-5.910099	-0.499299	-2.174176
174	1	0	-6.277941	-0.946430	-3.092689
175	1	0	-5.958590	-1.264568	-1.401811
176	6	0	-6.813951	0.684471	-1.771583
177	1	0	-6.833873	1.400802	-2.589301
178	1	0	-6.387868	1.191631	-0.913347
179	6	0	-8.260320	0.263525	-1.434260
180	1	0	-8.232936	-0.488375	-0.652168
181	1	0	-8.788423	1.123972	-1.031567
182	6	0	-9.045389	-0.266355	-2.651358
183	1	0	-8.976744	0.469668	-3.447964
184	1	0	-8.588554	-1.178734	-3.020358
185	6	0	-10.536589	-0.537851	-2.353651
186	1	0	-10.982932	0.353805	-1.920773
187	1	0	-11.047243	-0.729331	-3.291344
188	6	0	-10.761253	-1.728993	-1.400604
189	1	0	-10.251628	-1.535160	-0.463433
190	1	0	-10.312736	-2.620625	-1.831084
191	6	0	-12.251410	-2.003220	-1.102164
192	1	0	-12.320435	-2.728793	-0.296053
193	1	0	-12.719855	-1.088457	-0.748576
194	6	0	-13.036993	-2.544048	-2.312864
195	1	0	-13.024471	-1.817992	-3.118420
196	1	0	-12.549470	-3.443251	-2.680291
197	6	0	-14.500991	-2.871482	-1.960619
198	1	0	-14.521073	-3.604474	-1.159756
199	1	0	-14.988003	-1.975114	-1.588397
200	6	0	-15.280852	-3.414021	-3.173960
201	1	0	-15.290334	-2.685042	-3.977504
202	1	0	-14.819950	-4.322395	-3.547603
203	1	0	-16.308274	-3.639727	-2.909614
204	1	0	1.322510	-2.172487	-3.011449
205	8	0	2.685452	-0.877866	-3.885701
206	8	0	3.394577	-2.076505	-4.340459
207	1	0	3.627919	-1.842158	-5.253538

(*2R*,5*R*)-4a-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.784896	1.594396	-1.749374
2	6	0	-3.487182	2.590498	-2.865634
3	6	0	-3.925221	3.986084	-2.427319
4	6	0	-3.420380	4.353277	-1.033485
5	6	0	-3.654177	3.264751	0.011960
6	6	0	-5.102874	3.241791	0.522267
7	6	0	-3.001360	-3.307920	-3.624585
8	6	0	-2.380347	-2.228017	-4.501471
9	6	0	-2.226738	-0.990849	-3.639067
10	6	0	-3.541165	-0.541637	-3.036404
11	6	0	-4.243532	-1.710408	-2.357871
12	6	0	-5.678173	-1.431856	-1.958353
13	6	0	0.035982	-6.202555	-0.252802
14	6	0	0.306537	-6.119556	-1.747591
15	6	0	-0.291163	-4.839136	-2.294086
16	6	0	-1.763578	-4.711786	-1.965909
17	6	0	-1.910363	-4.753290	-0.443666
18	6	0	-3.327314	-4.794061	0.122649
19	6	0	4.483976	-3.641452	0.957975
20	6	0	3.789144	-4.678720	0.104004
21	6	0	3.042739	-5.779578	0.882725
22	6	0	1.654252	-5.501883	1.497255
23	6	0	1.444195	-4.393624	2.530866
24	6	0	2.214519	-4.598546	3.862076
25	6	0	6.498056	0.909799	1.275602
26	6	0	7.454156	0.165160	0.343786
27	6	0	6.768052	-1.035357	-0.307323
28	6	0	6.032035	-1.832700	0.757865
29	6	0	5.003197	-0.929785	1.425314
30	6	0	4.057729	-1.707008	2.315315
31	6	0	3.584256	5.220377	0.065910
32	6	0	4.710014	4.879871	-0.896942
33	6	0	4.994284	3.390351	-0.854971
34	6	0	5.244327	2.939513	0.569614
35	6	0	3.999516	3.246112	1.403563
36	6	0	4.046109	2.927012	2.893833
37	6	0	-1.479654	5.817580	-1.416392
38	6	0	-0.478870	5.663347	-2.551846
39	6	0	0.728656	4.870838	-2.078538
40	6	0	1.291342	5.466732	-0.808386
41	6	0	0.205505	5.480135	0.258477
42	6	0	0.639602	6.042127	1.591571
43	8	0	-2.103274	2.605792	-3.216158
44	8	0	-5.368777	3.984140	-2.343191
45	8	0	-1.996925	4.525904	-1.151229
46	8	0	-3.236133	1.991953	-0.512846
47	8	0	-1.098827	-2.575225	-5.030586
48	8	0	-1.703451	0.120109	-4.407917
49	8	0	-3.147253	0.357754	-1.983608
50	8	0	-4.287284	-2.860197	-3.240646
51	8	0	1.702814	-6.151096	-2.046469
52	8	0	-0.150176	-4.812595	-3.732357
53	8	0	-2.170769	-3.438834	-2.474980
54	8	0	-1.357560	-6.029150	-0.024647
55	8	0	-3.994524	-3.512910	0.106914
56	8	0	2.935783	-4.047979	-0.863190
57	8	0	3.911482	-6.260840	1.930182
58	8	0	0.781256	-5.179639	0.375133
59	8	0	3.526707	-2.697535	1.401296
60	8	0	2.923984	-3.414311	4.290225
61	8	0	7.986767	1.101381	-0.580539
62	8	0	7.789199	-1.850608	-0.889211
63	8	0	5.425097	-2.969217	0.116505
64	8	0	5.815152	0.018164	2.173030
65	8	0	2.947233	-0.996571	2.791728
66	8	0	4.428303	5.285524	-2.233979
67	8	0	6.185068	3.103878	-1.610317
68	8	0	5.519711	1.534808	0.469626
69	8	0	3.862739	4.695394	1.355868

70	8	0	3.918772	1.519149	3.156547	126	1	0	0.377545	-4.366719	2.717323
71	8	0	-1.060348	5.040430	-3.694848	127	1	0	2.969179	-5.353770	3.746204
72	8	0	1.772468	4.933928	-3.075588	128	1	0	1.522928	-4.914872	4.634083
73	8	0	2.397473	4.629323	-0.434016	129	1	0	7.033314	1.622123	1.882191
74	8	0	-0.835696	6.344022	-0.268718	130	1	0	8.279891	-0.219949	0.920835
75	8	0	-0.399337	5.675251	2.523659	131	1	0	6.051397	-0.696788	-1.044829
76	7	0	-5.375397	2.149059	1.454738	132	1	0	6.732918	-2.170863	1.511743
77	8	0	-6.198254	-2.508310	-1.141261	133	1	0	4.413267	-0.406883	0.694626
78	6	0	-4.734347	-0.220716	3.780825	134	1	0	4.568254	-2.213151	3.114926
79	6	0	-5.682017	-1.228941	4.479504	135	1	0	1.735334	-3.455985	2.100436
80	6	0	-6.625229	-1.721961	3.352633	136	1	0	3.475290	6.286977	0.178305
81	6	0	-5.814148	-1.550821	2.054721	137	1	0	5.602824	5.401896	-0.586042
82	7	0	-4.606180	-0.861814	2.454572	138	1	0	4.148062	2.846533	-1.250469
83	8	0	-3.427917	-1.213441	1.927827	139	1	0	6.100324	3.464281	0.975924
84	6	0	-3.372402	-0.225564	4.505176	140	1	0	3.136349	2.774625	0.965467
85	8	0	-2.920887	-1.299266	4.881171	141	1	0	3.201705	3.414174	3.350407
86	7	0	-2.796305	0.956702	4.741165	142	1	0	4.951359	3.329265	3.333718
87	6	0	-1.575380	1.041047	5.557802	143	1	0	-2.263251	6.511400	-1.678499
88	6	0	-0.517958	2.001553	4.988190	144	1	0	-0.143503	6.644730	-2.853016
89	6	0	0.081841	1.552427	3.634176	145	1	0	0.439919	3.846523	-1.892705
90	6	0	-0.715208	2.083603	2.427533	146	1	0	1.632007	6.475557	-1.007027
91	6	0	-0.111486	1.697352	1.063601	147	1	0	-0.180048	4.488234	0.408012
92	6	0	0.020880	0.172639	0.861500	148	1	0	0.738767	7.117496	1.505384
93	6	0	0.177480	-0.200982	-0.626927	149	1	0	1.586259	5.604676	1.876145
94	6	0	1.444667	0.392964	-1.275799	150	1	0	-1.825732	1.736891	-3.579685
95	6	0	1.644555	-0.043611	-2.745709	151	1	0	-5.781088	4.187641	-3.192174
96	6	0	2.106544	-1.507663	-2.875554	152	1	0	-0.703793	-3.341319	-4.564618
97	6	0	2.234892	-1.999424	-4.332782	153	1	0	-0.976905	-0.198442	-4.964081
98	6	0	3.311225	-1.249213	-5.141145	154	1	0	2.138244	-5.342153	-1.692799
99	8	0	-6.492956	-0.679826	1.111131	155	1	0	0.725552	-5.152789	-3.972009
100	8	0	-7.676611	-1.432489	0.683856	156	1	0	-3.569830	-2.839684	0.666404
101	1	0	-4.857598	1.483766	-1.680871	157	1	0	2.432302	-3.341464	-0.432951
102	1	0	-4.088037	2.319849	-3.728795	158	1	0	4.442830	-7.014861	1.645104
103	1	0	-3.556789	4.712392	-3.137799	159	1	0	2.426566	-2.603454	4.110390
104	1	0	-3.892755	5.274547	-0.718345	160	1	0	7.291775	1.637573	-1.008854
105	1	0	-3.002804	3.449606	0.846311	161	1	0	7.377047	-2.633051	-1.281738
106	1	0	-5.800116	3.174757	-0.293533	162	1	0	3.082456	-0.030559	2.902768
107	1	0	-5.273140	4.180019	1.035825	163	1	0	3.513827	5.063288	-2.512028
108	1	0	-3.115428	-4.247490	-4.139937	164	1	0	6.150420	3.577899	-2.454447
109	1	0	-3.053854	-2.033856	-5.323166	165	1	0	4.757599	1.040036	3.023791
110	1	0	-1.555686	-1.223479	-2.834543	166	1	0	-1.376984	4.129006	-3.484960
111	1	0	-4.152064	-0.066491	-3.793273	167	1	0	1.391757	4.788544	-3.953807
112	1	0	-3.662834	-1.958300	-1.495103	168	1	0	-0.232670	6.045736	3.399350
113	1	0	-6.292452	-1.357454	-2.841976	169	1	0	-6.218921	-0.778901	5.303045
114	1	0	-5.722773	-0.515920	-1.391279	170	1	0	-5.068302	-2.036505	4.845201
115	1	0	0.286699	-7.174386	0.141861	171	1	0	-7.523398	-1.130450	3.273691
116	1	0	-0.152146	-6.964744	-2.237512	172	1	0	-6.908330	-2.753547	3.502202
117	1	0	0.222333	-3.995443	-1.860834	173	1	0	-5.466001	-3.035325	-0.759057
118	1	0	-2.325984	-5.517233	-2.420871	174	1	0	-3.153383	1.803994	4.335449
119	1	0	-1.348287	-3.942054	-0.005435	175	1	0	-1.848168	1.363906	6.558357
120	1	0	-3.251477	-5.170465	1.132343	176	1	0	-1.172500	0.043341	5.627400
121	1	0	-3.945089	-5.463552	-0.453030	177	1	0	0.272070	2.060138	5.731901
122	1	0	4.983356	-4.103800	1.793027	178	1	0	-0.938864	2.997802	4.891375
123	1	0	4.572746	-5.163316	-0.458814	179	1	0	1.104583	1.911437	3.562683
124	1	0	2.858354	-6.561719	0.156363	180	1	0	0.130847	0.469565	3.608909
125	1	0	1.339796	-6.447811	1.925969	181	1	0	-0.766935	3.165533	2.500051

182	1	0	-1.727445	1.710027	2.469866
183	1	0	-0.765408	2.084159	0.288816
184	1	0	0.858836	2.172234	0.951140
185	1	0	0.859650	-0.220169	1.426183
186	1	0	-0.882506	-0.298390	1.238262
187	1	0	0.203403	-1.284548	-0.711723
188	1	0	-0.701105	0.146231	-1.157902
189	1	0	1.381046	1.474978	-1.240716
190	1	0	2.318682	0.104835	-0.695637
191	1	0	2.383372	0.604000	-3.206037
192	1	0	0.711703	0.095761	-3.284187
193	1	0	3.057403	-1.636475	-2.367072
194	1	0	1.391863	-2.146830	-2.371333
195	1	0	2.493232	-3.055056	-4.312838
196	1	0	1.271269	-1.917441	-4.820881
197	1	0	4.271655	-1.305758	-4.639158
198	1	0	3.420592	-1.684089	-6.128953
199	1	0	3.055237	-0.203938	-5.265877
200	1	0	-5.565335	-2.468268	1.560453
201	1	0	-7.272985	-1.925246	-0.090128
202	1	0	-5.909069	1.357374	1.150264
203	6	0	-4.881967	2.153626	2.697639
204	8	0	-4.052560	2.979501	3.088069
205	6	0	-5.467090	1.125333	3.651237
206	1	0	-5.501770	1.587340	4.628363
207	1	0	-6.477468	0.913869	3.336034

(*2S*,5*S*)-4b-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.031675	-3.628588	0.069617
2	6	0	-3.103983	-4.688706	-0.118003
3	6	0	-3.923656	-4.769999	1.175328
4	6	0	-4.453562	-3.402757	1.608529
5	6	0	-3.388416	-2.307124	1.586147
6	6	0	-2.404743	-2.277159	2.763552
7	6	0	1.951797	-4.277096	-3.226440
8	6	0	0.660775	-4.355922	-4.028636
9	6	0	-0.451224	-3.762047	-3.180561
10	6	0	-0.487084	-4.352032	-1.769661
11	6	0	0.864661	-4.504659	-1.085877
12	6	0	0.884828	-5.555038	0.016864
13	6	0	4.756649	0.332813	-2.797019
14	6	0	3.990000	0.073070	-4.084818
15	6	0	2.834392	-0.873353	-3.814921
16	6	0	3.315236	-2.156252	-3.172638
17	6	0	4.054814	-1.820325	-1.884863
18	6	0	4.745794	-3.001466	-1.223105
19	6	0	1.696644	3.574686	-0.982458
20	6	0	2.225077	3.479840	-2.406653
21	6	0	3.749579	3.374573	-2.398362
22	6	0	4.271213	2.333137	-1.402749
23	6	0	3.636130	2.454518	-0.019743
24	6	0	4.129897	3.638240	0.829790
25	6	0	-3.474136	4.916057	-1.291925
26	6	0	-2.766509	4.536537	-2.584608
27	6	0	-1.598545	3.645648	-2.232418
28	6	0	-0.620196	4.358357	-1.327160
29	6	0	-1.331638	4.886557	-0.080820
30	6	0	-0.555313	5.927378	0.708753
31	6	0	-7.646399	1.993431	0.353434
32	6	0	-7.582505	2.760835	-0.957868
33	6	0	-6.140170	2.933939	-1.396666
34	6	0	-5.350281	3.616939	-0.297074
35	6	0	-5.450508	2.761527	0.966882
36	6	0	-4.641110	3.307428	2.133665
37	6	0	-6.783192	-3.255350	0.785916
38	6	0	-7.472040	-2.856430	-0.503626
39	6	0	-7.214557	-1.389572	-0.746740
40	6	0	-7.674361	-0.533904	0.417850
41	6	0	-7.146806	-1.039366	1.757913
42	6	0	-7.956118	-0.515691	2.949180
43	8	0	-3.883677	-4.438483	-1.284405
44	8	0	-2.995341	-5.254004	2.167655
45	8	0	-5.406972	-2.995319	0.590637
46	8	0	-2.668373	-2.371832	0.340861
47	8	0	0.837599	-3.692902	-5.276160
48	8	0	-1.721722	-4.031478	-3.791159
49	8	0	-1.294883	-3.357019	-1.086434
50	8	0	1.830600	-5.043235	-2.043199
51	8	0	3.498409	1.276801	-4.679403
52	8	0	2.207445	-1.223891	-5.066518
53	8	0	2.133019	-2.906971	-2.885374
54	8	0	5.148845	-0.908276	-2.243053
55	8	0	5.652855	-2.510474	-0.216649
56	8	0	1.667749	2.367057	-3.107986
57	8	0	4.193703	4.694352	-2.004520
58	8	0	3.904820	1.034291	-1.897508
59	8	0	2.200969	2.543227	-0.147357
60	8	0	3.206224	3.868756	1.914852
61	8	0	-3.563140	3.810314	-3.515477
62	8	0	-0.890698	3.279183	-3.434357
63	8	0	0.303013	3.340818	-0.929127
64	8	0	-2.556107	5.584177	-0.450260
65	8	0	0.632458	5.277417	1.215298
66	8	0	-8.203157	2.018534	-2.034037
67	8	0	-6.106382	3.765063	-2.579547
68	8	0	-3.958589	3.714764	-0.664594
69	8	0	-6.857424	2.701610	1.320183
70	8	0	-3.266657	2.933415	1.920336
71	8	0	-6.888300	-3.642139	-1.544340
72	8	0	-7.930644	-1.029513	-1.937493
73	8	0	-7.062909	0.742242	0.104050
74	8	0	-7.299489	-2.476458	1.857709
75	8	0	-8.360192	0.851028	2.780130
76	7	0	-1.374821	-1.315126	2.383960
77	8	0	2.230053	-5.747676	0.484345
78	6	0	-0.189365	2.592278	3.285379
79	6	0	0.422218	0.267370	2.675962
80	6	0	1.118326	2.249952	3.993847

81	6	0	2.816215	-3.503187	2.959581	137	1	0	-1.185964	6.278330	1.512814
82	6	0	4.344394	-3.329737	2.916696	138	1	0	-0.306388	6.761213	0.065246
83	6	0	4.877528	-2.451310	4.063695	139	1	0	-8.633913	1.912363	0.764540
84	6	0	6.415429	-2.318576	4.054515	140	1	0	-8.039117	3.734002	-0.839550
85	6	0	6.947230	-1.515353	2.851253	141	1	0	-5.715388	1.965298	-1.603781
86	6	0	8.482174	-1.380068	2.872317	142	1	0	-5.756672	4.601437	-0.105051
87	6	0	9.015474	-0.588478	1.662029	143	1	0	-5.093905	1.768127	0.756152
88	6	0	10.551481	-0.460292	1.674642	144	1	0	-4.966851	2.840676	3.048539
89	6	0	11.127426	0.264073	0.438106	145	1	0	-4.760400	4.379692	2.224296
90	6	0	10.790066	1.767880	0.400351	146	1	0	-6.968198	-4.284429	1.044165
91	6	0	11.355119	2.491554	-0.841252	147	1	0	-8.535428	-3.033271	-0.409766
92	6	0	-0.562247	-0.729496	3.291614	148	1	0	-6.152317	-1.250185	-0.866654
93	8	0	-0.640084	-0.957358	4.483618	149	1	0	-8.751963	-0.453495	0.418323
94	6	0	-0.329718	1.537470	2.165195	150	1	0	-6.104813	-0.768060	1.814934
95	7	0	1.288826	0.839640	3.709280	151	1	0	-7.405773	-0.668645	3.868410
96	8	0	2.236062	0.152456	4.339665	152	1	0	-8.863132	-1.094610	2.992847
97	6	0	1.217257	-0.330609	1.503532	153	1	0	-4.620452	-3.832871	-1.108064
98	6	0	1.885370	-1.694597	1.614316	154	1	0	-3.433079	-5.718446	2.892178
99	8	0	2.208256	-2.254970	0.561303	155	1	0	1.189452	-2.790865	-5.154659
100	7	0	2.110644	-2.217526	2.814003	156	1	0	-2.424975	-3.856138	-3.143799
101	6	0	12.893754	2.590804	-0.840727	157	1	0	2.755120	1.641003	-4.141101
102	8	0	1.003425	2.381162	5.433472	158	1	0	2.115180	-0.433350	-5.616805
103	8	0	1.120535	3.826141	5.663224	159	1	0	6.101678	-1.739520	-0.591025
104	1	0	-1.401450	-3.909218	0.895758	160	1	0	0.701957	2.501397	-3.221564
105	1	0	-2.636084	-5.651304	-0.246567	161	1	0	5.073917	4.895278	-2.347059
106	1	0	-4.748504	-5.454632	1.024032	162	1	0	2.303128	3.804223	1.573413
107	1	0	-4.937927	-3.448527	2.575549	163	1	0	-4.508763	3.801692	-3.274252
108	1	0	-3.898800	-1.358728	1.549389	164	1	0	-1.540278	3.002154	-4.099628
109	1	0	-1.992829	-3.253300	2.961954	165	1	0	1.114940	5.832292	1.842650
110	1	0	-2.905045	-1.931113	3.657851	166	1	0	-9.167080	2.094678	-2.029034
111	1	0	2.789848	-4.660751	-3.786911	167	1	0	-6.743832	3.420807	-3.224409
112	1	0	0.436420	-5.388936	-4.240832	168	1	0	-3.063874	3.091742	0.990027
113	1	0	-0.275047	-2.704354	-3.072993	169	1	0	-7.152675	-3.286608	-2.405360
114	1	0	-1.005060	-5.300089	-1.831441	170	1	0	-7.829230	-0.079262	-2.113522
115	1	0	1.215305	-3.558579	-0.723431	171	1	0	-7.621482	1.475060	2.820057
116	1	0	0.480071	-6.483479	-0.372249	172	1	0	-1.264495	-1.182508	1.401878
117	1	0	0.305279	-5.240156	0.868455	173	1	0	2.801480	-5.791924	-0.295149
118	1	0	5.661273	0.892108	-2.986710	174	1	0	-0.985233	2.492984	4.007692
119	1	0	4.662225	-0.387799	-4.792632	175	1	0	1.970507	2.818869	3.669608
120	1	0	2.128151	-0.393802	-3.152805	176	1	0	2.509597	-3.931271	3.905949
121	1	0	3.959310	-2.689035	-3.862385	177	1	0	2.515154	-4.157071	2.156658
122	1	0	3.396021	-1.349830	-1.179696	178	1	0	4.615984	-2.921982	1.953092
123	1	0	5.286614	-3.576263	-1.967769	179	1	0	4.792784	-4.317514	2.989626
124	1	0	4.012807	-3.613884	-0.731717	180	1	0	4.431702	-1.463945	4.008285
125	1	0	1.942859	4.541333	-0.582871	181	1	0	4.568837	-2.887334	5.011243
126	1	0	1.986837	4.403628	-2.918620	182	1	0	6.736111	-1.830738	4.971577
127	1	0	4.081726	3.116834	-3.391217	183	1	0	6.859009	-3.310965	4.046463
128	1	0	5.350173	2.420326	-1.314942	184	1	0	6.642102	-1.989842	1.927907
129	1	0	3.803018	1.529528	0.503979	185	1	0	6.503395	-0.522207	2.871774
130	1	0	4.233578	4.519755	0.221425	186	1	0	8.792602	-0.886061	3.789580
131	1	0	5.085108	3.395476	1.269932	187	1	0	8.927849	-2.371194	2.872479
132	1	0	-4.292672	5.595460	-1.460512	188	1	0	8.708233	-1.091267	0.748653
133	1	0	-2.403057	5.452251	-3.033221	189	1	0	8.560382	0.396677	1.660461
134	1	0	-1.966846	2.764330	-1.732702	190	1	0	10.862205	0.064074	2.574479
135	1	0	-0.141920	5.160039	-1.875838	191	1	0	10.977568	-1.458294	1.724640
136	1	0	-1.546283	4.057468	0.563883	192	1	0	12.204907	0.140334	0.435578

193	1	0	10.747518	-0.210883	-0.462765
194	1	0	9.712678	1.891429	0.413179
195	1	0	11.177744	2.243577	1.297366
196	1	0	11.024551	1.974732	-1.737563
197	1	0	10.942301	3.495400	-0.880517
198	1	0	0.148606	1.890606	1.262241
199	1	0	-1.368773	1.333566	1.966034
200	1	0	-0.175887	3.590301	2.880645
201	1	0	0.576482	-0.409244	0.635667
202	1	0	1.976124	0.386690	1.225912
203	1	0	13.239612	3.092050	0.057388
204	1	0	13.352343	1.610586	-0.880320
205	1	0	13.242326	3.156408	-1.698274
206	1	0	1.983028	-1.648953	3.625530
207	1	0	1.771888	3.828951	6.383213

(*2S*,5*S*)-4b-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.540511	-0.214556	2.637603
2	6	0	-3.117229	-1.201598	3.710847
3	6	0	-3.795860	-2.542350	3.498049
4	6	0	-3.629764	-3.066751	2.072360
5	6	0	-3.938996	-2.017472	1.001156
6	6	0	-5.449622	-1.906674	0.752916
7	6	0	-2.632490	5.018080	2.222696
8	6	0	-2.526439	4.513047	3.648746
9	6	0	-2.193321	3.026982	3.673156
10	6	0	-3.172846	2.234752	2.832158
11	6	0	-3.253669	2.819383	1.430617
12	6	0	-4.360100	2.253605	0.565953
13	6	0	2.141129	6.329102	0.183208
14	6	0	2.152426	5.910844	1.636635
15	6	0	0.909547	5.082978	1.894717
16	6	0	-0.368543	5.832468	1.558904
17	6	0	-0.296281	6.443571	0.152639
18	6	0	-1.266811	7.588538	-0.081865
19	6	0	3.649385	2.443930	-2.263712
20	6	0	4.409381	3.417844	-1.382172
21	6	0	4.101472	4.835749	-1.859086
22	6	0	2.598655	5.104550	-1.919722
23	6	0	1.807011	3.996226	-2.612595
24	6	0	1.829683	4.040936	-4.140101
25	6	0	5.854157	-2.338019	-2.251304
26	6	0	6.624534	-1.249858	-1.507542
27	6	0	5.621879	-0.178992	-1.110691
28	6	0	4.821918	0.288156	-2.316508
29	6	0	4.149166	-0.851315	-3.056406
30	6	0	3.469352	-0.454246	-4.364988
31	6	0	2.852354	-5.967514	0.350804
32	6	0	4.124065	-5.509316	1.045470
33	6	0	4.472332	-4.136492	0.510047
34	6	0	4.646165	-4.168557	-0.992182
35	6	0	3.363688	-4.689139	-1.646575
36	6	0	3.437709	-4.952338	-3.149233
37	6	0	-1.988639	-4.850223	2.359054
38	6	0	-0.785143	-4.776104	3.286316
39	6	0	0.459697	-4.421712	2.492992
40	6	0	0.649341	-5.414235	1.368860
41	6	0	-0.571803	-5.370273	0.455590
42	6	0	-0.499564	-6.380429	-0.667306
43	8	0	-1.696393	-1.377478	3.664974
44	8	0	-5.215105	-2.329768	3.671288
45	8	0	-2.270442	-3.527820	1.914173
46	8	0	-3.357324	-0.727371	1.329393
47	8	0	-1.556335	5.232268	4.418862
48	8	0	-2.290553	2.542967	5.023334
49	8	0	-2.661821	0.888145	2.772028
50	8	0	-3.600639	4.227113	1.551833
51	8	0	3.313498	5.157232	1.990646
52	8	0	0.860512	4.732871	3.295994
53	8	0	-1.386173	4.818502	1.560932
54	8	0	0.982420	7.093646	-0.075496
55	8	0	-2.595640	7.100408	0.169943
56	8	0	4.005651	3.204904	-0.011149
57	8	0	4.570272	4.957532	-3.217503
58	8	0	2.135321	5.115490	-0.550697
59	8	0	2.259038	2.709341	-2.112887
60	8	0	1.041758	2.965330	-4.659431
61	8	0	7.298893	-1.839855	-0.405188
62	8	0	6.296428	0.969452	-0.562353
63	8	0	3.785136	1.132217	-1.770379
64	8	0	5.189059	-1.809614	-3.406198
65	8	0	2.571931	0.665510	-4.153281
66	8	0	4.016923	-5.456189	2.464972
67	8	0	5.704541	-3.666487	1.094643
68	8	0	4.863796	-2.795824	-1.351878
69	8	0	3.071913	-5.986007	-1.051966
70	8	0	3.326264	-3.749943	-3.918486
71	8	0	-0.965813	-3.854978	4.358507
72	8	0	1.610463	-4.499864	3.361389
73	8	0	1.832464	-5.025391	0.656691
74	8	0	-1.709489	-5.725768	1.282930
75	8	0	-1.564159	-6.049488	-1.573499
76	8	0	-4.381203	2.983879	-0.681898
77	6	0	-6.319942	-0.598305	-2.710993
78	6	0	-6.507277	-1.405855	-4.015075
79	6	0	-8.003092	-1.861686	-4.027761
80	6	0	-8.589942	-1.405623	-2.697319
81	7	0	-7.726768	-0.311112	-2.334979
82	8	0	-8.019014	0.436544	-1.255964
83	6	0	-5.581119	0.730544	-2.864969
84	6	0	-1.878296	1.438069	-3.330575
85	6	0	-0.955501	1.161127	-2.133821
86	6	0	-1.276432	-0.178178	-1.442108
87	6	0	-0.176873	-0.647370	-0.467268
88	6	0	0.150636	0.400696	0.614466
89	6	0	1.116580	-0.118183	1.701283
90	6	0	2.447100	-0.634358	1.122192
91	6	0	3.548452	-0.862271	2.180771

92	6	0	4.166997	0.451866	2.701359	148	1	0	0.365176	-3.427815	2.081203
93	6	0	5.451965	0.242553	3.532704	149	1	0	0.766028	-6.408574	1.783587
94	6	0	6.620070	-0.365811	2.726687	150	1	0	-0.702345	-4.383696	0.041951
95	7	0	-5.770977	-1.020361	-0.361497	151	1	0	-0.620669	-7.371548	-0.245118
96	6	0	-5.687352	-1.495274	-1.629172	152	1	0	0.468184	-6.305747	-1.145976
97	8	0	-5.159382	-2.564754	-1.875928	153	1	0	-1.282994	-0.523463	3.467901
98	8	0	-3.867953	-0.363123	-4.139838	154	1	0	-5.483759	-2.403344	4.595815
99	6	0	-4.155434	0.541734	-3.364889	155	1	0	-0.646728	5.042712	4.106925
100	7	0	-3.287134	1.465233	-2.925763	156	1	0	-1.877288	3.195387	5.608292
101	6	0	7.936761	-0.339566	3.526694	157	1	0	3.573347	4.525318	1.291545
102	8	0	-8.368752	-2.396298	-1.646161	158	1	0	1.743432	4.456032	3.584964
103	8	0	-9.096850	-3.601479	-2.047046	159	1	0	-3.263214	7.757094	-0.064286
104	1	0	-4.565466	0.077641	2.806055	160	1	0	3.101131	2.853360	-0.027349
105	1	0	-3.409827	-0.788902	4.668274	161	1	0	5.520212	5.126198	-3.265086
106	1	0	-3.399912	-3.264164	4.197248	162	1	0	1.556817	2.139855	-4.679182
107	1	0	-4.309478	-3.897431	1.940063	163	1	0	6.699608	-2.375896	0.149879
108	1	0	-3.461344	-2.318250	0.085851	164	1	0	5.685182	1.462030	0.003486
109	1	0	-5.956674	-1.562655	1.636959	165	1	0	2.119300	0.602435	-3.301498
110	1	0	-5.813581	-2.897728	0.517108	166	1	0	3.172608	-5.053102	2.766186
111	1	0	-2.945792	6.039535	2.155985	167	1	0	5.727569	-3.930561	2.027261
112	1	0	-3.481213	4.659599	4.130366	168	1	0	4.132710	-3.213291	-3.896178
113	1	0	-1.198351	2.886893	3.276023	169	1	0	-1.134881	-2.940318	4.033784
114	1	0	-4.141196	2.249842	3.316726	170	1	0	1.384564	-4.125912	4.226126
115	1	0	-2.303732	2.722762	0.935368	171	1	0	-1.581533	-6.651114	-2.328174
116	1	0	-5.308700	2.369082	1.077664	172	1	0	-5.823729	-2.234013	-4.015938
117	1	0	-4.180908	1.220499	0.333986	173	1	0	-6.289985	-0.783792	-4.865812
118	1	0	2.984525	6.950224	-0.072792	174	1	0	-8.114288	-2.926852	-4.132447
119	1	0	2.138429	6.791977	2.259293	175	1	0	-8.535456	-1.371800	-4.830936
120	1	0	0.938971	4.191611	1.290861	176	1	0	-4.338047	3.929596	-0.472343
121	1	0	-0.556309	6.584538	2.312457	177	1	0	-1.596538	2.374066	-3.796982
122	1	0	-0.453708	5.646927	-0.554401	178	1	0	-1.782139	0.653006	-4.063948
123	1	0	-1.149696	7.931038	-1.101407	179	1	0	0.067869	1.180485	-2.488658
124	1	0	-1.003498	8.398237	0.586692	180	1	0	-1.050237	1.974334	-1.420355
125	1	0	3.965756	2.522013	-3.285018	181	1	0	-1.429202	-0.940320	-2.200403
126	1	0	5.466788	3.215783	-1.437383	182	1	0	-2.201406	-0.087387	-0.889406
127	1	0	4.571667	5.558959	-1.205678	183	1	0	-0.516258	-1.557001	0.021166
128	1	0	2.411883	6.057153	-2.395636	184	1	0	0.720174	-0.888109	-1.029784
129	1	0	0.783324	4.058384	-2.286286	185	1	0	0.593316	1.273530	0.143518
130	1	0	2.840302	4.039217	-4.516154	186	1	0	-0.776587	0.700046	1.087417
131	1	0	1.360569	4.962015	-4.456674	187	1	0	1.311376	0.685491	2.406112
132	1	0	6.503937	-3.129841	-2.586232	188	1	0	0.635327	-0.920792	2.252885
133	1	0	7.373947	-0.824982	-2.156367	189	1	0	2.257413	-1.572568	0.612098
134	1	0	4.939535	-0.603408	-0.396253	190	1	0	2.807084	0.061769	0.371548
135	1	0	5.471674	0.845662	-2.978973	191	1	0	4.327206	-1.470241	1.740112
136	1	0	3.441188	-1.322465	-2.397237	192	1	0	3.142299	-1.429911	3.014897
137	1	0	2.936041	-1.308915	-4.753638	193	1	0	4.395711	1.097876	1.858415
138	1	0	4.210360	-0.132515	-5.078477	194	1	0	3.437093	0.978942	3.307864
139	1	0	2.568171	-6.965319	0.643809	195	1	0	5.766988	1.204697	3.927920
140	1	0	4.916558	-6.203412	0.809092	196	1	0	5.232488	-0.394478	4.385897
141	1	0	3.671027	-3.458313	0.745877	197	1	0	6.752777	0.169532	1.794209
142	1	0	5.499560	-4.779841	-1.259757	198	1	0	6.393682	-1.390489	2.461375
143	1	0	2.560171	-4.001502	-1.443606	199	1	0	-6.319615	-0.208198	-0.187079
144	1	0	2.590119	-5.566087	-3.405236	200	1	0	-6.115701	1.307429	-3.613058
145	1	0	4.339299	-5.511832	-3.379693	201	1	0	-5.598617	1.300244	-1.950808
146	1	0	-2.839242	-5.272943	2.870554	202	1	0	-3.580442	2.123526	-2.224900
147	1	0	-0.636996	-5.750054	3.729017	203	1	0	8.216343	0.680416	3.770025

204	1	0	8.741517	-0.783784	2.952039
205	1	0	7.834582	-0.892006	4.455838
206	1	0	-9.624671	-1.119808	-2.703698
207	1	0	-8.411040	-4.271757	-1.888319

(*2R*,5*S*)-4b-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.956626	-3.568439	-0.301768
2	6	0	-3.018512	-4.496338	-0.883713
3	6	0	-4.036946	-4.857606	0.200949
4	6	0	-4.612600	-3.614804	0.877544
5	6	0	-3.537704	-2.636404	1.337043
6	6	0	-2.831579	-3.001377	2.645864
7	6	0	1.894236	-3.413148	-3.937401
8	6	0	0.524930	-3.272319	-4.575128
9	6	0	-0.487892	-2.872005	-3.511199
10	6	0	-0.386944	-3.751926	-2.259080
11	6	0	1.033586	-3.957981	-1.755704
12	6	0	1.207639	-5.097165	-0.765878
13	6	0	5.197528	0.632607	-2.737931
14	6	0	4.421891	0.780481	-4.034647
15	6	0	3.155299	-0.053336	-3.941884
16	6	0	3.477238	-1.495462	-3.615986
17	6	0	4.311540	-1.588728	-2.345172
18	6	0	4.868520	-2.981989	-2.074479
19	6	0	2.236514	3.303689	-0.077451
20	6	0	2.930292	3.729699	-1.370969
21	6	0	4.435287	3.478636	-1.324131
22	6	0	4.791792	2.103837	-0.755403
23	6	0	4.041956	1.778520	0.529620
24	6	0	4.512096	2.550946	1.776535
25	6	0	-2.724345	5.288694	-0.267622
26	6	0	-1.815192	5.458424	-1.469421
27	6	0	-0.820069	4.317989	-1.476905
28	6	0	0.008646	4.330012	-0.209636
29	6	0	-0.912281	4.199554	1.002152
30	6	0	-0.263642	4.470379	2.350858
31	6	0	-7.205860	2.330083	-0.329108
32	6	0	-6.817222	3.128083	-1.563216
33	6	0	-5.315028	3.293832	-1.599256
34	6	0	-4.846739	3.989126	-0.336408
35	6	0	-5.266189	3.186298	0.893819
36	6	0	-5.025221	3.881864	2.233162
37	6	0	-6.755091	-3.003796	-0.216637
38	6	0	-7.139238	-2.398677	-1.549597
39	6	0	-6.699646	-0.954205	-1.576609
40	6	0	-7.310201	-0.174051	-0.430273
41	6	0	-7.085076	-0.855962	0.915701
42	6	0	-8.056704	-0.353128	1.994685
43	8	0	-3.620351	-3.929496	-2.048701
44	8	0	-3.296546	-5.635850	1.162553
45	8	0	-5.347149	-2.908401	-0.152961
46	8	0	-2.582410	-2.418265	0.284802
47	8	0	0.615621	-2.339451	-5.651238
48	8	0	-1.796832	-3.012919	-4.070887
49	8	0	-1.141371	-2.991419	-1.285382
50	8	0	1.864635	-4.359148	-2.887442
51	8	0	4.105465	2.147017	-4.298811
52	8	0	2.473210	-0.066507	-5.213071
53	8	0	2.210381	-2.126381	-3.417003
54	8	0	5.489575	-0.739827	-2.520554
55	8	0	5.918819	-2.897067	-1.095609
56	8	0	2.378073	3.048931	-2.500619
57	8	0	4.956721	4.515454	-0.461898
58	8	0	4.355744	1.122151	-1.704312
59	8	0	2.627700	2.008171	0.354015
60	8	0	3.464524	2.450009	2.765664
61	8	0	-2.519681	5.491834	-2.707899
62	8	0	0.075816	4.481219	-2.596703
63	8	0	0.845961	3.175590	-0.296203
64	8	0	-1.945737	5.243467	0.921606
65	8	0	0.793911	3.519954	2.535095
66	8	0	-7.158217	2.419245	-2.778651
67	8	0	-4.940239	4.132713	-2.709219
68	8	0	-3.417078	4.059765	-0.427243
69	8	0	-6.713228	3.021410	0.819432
70	8	0	-3.646950	3.871385	2.607703
71	8	0	-6.444748	-3.140411	-2.555873
72	8	0	-7.134743	-0.438143	-2.841394
73	8	0	-6.575502	1.077018	-0.429562
74	8	0	-7.372872	-2.275214	0.833538
75	8	0	-8.418727	1.024863	1.821032
76	7	0	-1.742519	-2.044856	2.790351
77	8	0	2.614591	-5.361239	-0.584250
78	6	0	-0.606330	1.494914	5.038234
79	6	0	-0.131998	-0.636117	3.871366
80	6	0	0.692374	0.903970	5.552123
81	6	0	2.035584	-4.544810	3.212177
82	6	0	3.464820	-4.575304	2.636956
83	6	0	4.485147	-4.008457	3.642699
84	6	0	5.881799	-3.741209	3.040876
85	6	0	5.926368	-2.457823	2.186556
86	6	0	7.351518	-2.128104	1.703556
87	6	0	7.431450	-0.754337	1.006752
88	6	0	8.849364	-0.455065	0.477498
89	6	0	8.963654	0.875310	-0.299204
90	6	0	8.835128	2.120340	0.601206
91	6	0	8.880619	3.452722	-0.178847
92	6	0	-1.271165	-1.648267	3.989420
93	8	0	-1.753672	-1.997559	5.050520
94	6	0	-0.745555	0.794735	3.666258
95	7	0	0.530097	-0.481271	5.186350
96	8	0	1.443285	-1.355144	5.633293
97	6	0	0.865261	-0.948588	2.730669
98	6	0	1.108266	-2.421734	2.426699
99	8	0	0.880355	-2.861494	1.300212
100	7	0	1.578521	-3.166659	3.429620

101	6	0	10.253728	3.740992	-0.817077
102	8	0	1.818996	1.310734	4.728949
103	8	0	2.065010	2.750871	4.881336
104	1	0	-1.386233	-4.098202	0.441316
105	1	0	-2.547496	-5.420004	-1.179938
106	1	0	-4.835575	-5.430758	-0.253695
107	1	0	-5.269426	-3.871428	1.699823
108	1	0	-4.007558	-1.675796	1.468420
109	1	0	-2.468867	-4.016391	2.621394
110	1	0	-3.506565	-2.890867	3.482477
111	1	0	2.633624	-3.737143	-4.653091
112	1	0	0.223321	-4.218618	-4.994715
113	1	0	-0.287152	-1.858754	-3.197484
114	1	0	-0.855546	-4.701197	-2.483399
115	1	0	1.399293	-3.042255	-1.330512
116	1	0	0.698484	-5.982638	-1.133730
117	1	0	0.827935	-4.800242	0.189736
118	1	0	6.139450	1.158292	-2.769109
119	1	0	5.030193	0.419898	-4.850086
120	1	0	2.521571	0.352513	-3.168168
121	1	0	4.004389	-1.937263	-4.453318
122	1	0	3.740843	-1.229225	-1.506274
123	1	0	5.247609	-3.403449	-3.000218
124	1	0	4.106842	-3.622082	-1.669278
125	1	0	2.443356	4.027957	0.692905
126	1	0	2.799544	4.797884	-1.483552
127	1	0	4.819391	3.557899	-2.330755
128	1	0	5.859995	2.034540	-0.585414
129	1	0	4.118906	0.718820	0.704810
130	1	0	4.704468	3.581119	1.539199
131	1	0	5.404827	2.094149	2.175253
132	1	0	-3.410800	6.113775	-0.161388
133	1	0	-1.283710	6.393381	-1.371621
134	1	0	-1.339823	3.375495	-1.548769
135	1	0	0.580264	5.249082	-0.158185
136	1	0	-1.378331	3.229278	0.989568
137	1	0	-1.027194	4.369253	3.110484
138	1	0	0.105553	5.488598	2.361728
139	1	0	-8.266867	2.236873	-0.193223
140	1	0	-7.288098	4.100961	-1.539593
141	1	0	-4.850508	2.324014	-1.673185
142	1	0	-5.275881	4.983745	-0.297037
143	1	0	-4.775618	2.227545	0.879908
144	1	0	-5.560688	3.329545	2.988600
145	1	0	-5.443706	4.882920	2.195760
146	1	0	-7.093924	-4.021946	-0.117223
147	1	0	-8.212015	-2.455361	-1.677240
148	1	0	-5.625931	-0.918305	-1.479018
149	1	0	-8.359968	-0.000676	-0.617007
150	1	0	-6.051786	-0.700895	1.180794
151	1	0	-7.655540	-0.547605	2.981116
152	1	0	-8.966272	-0.917139	1.876816
153	1	0	-4.449860	-3.460754	-1.862470
154	1	0	-3.863322	-6.229989	1.670777
155	1	0	1.092351	-1.535605	-5.377861
156	1	0	-2.457065	-3.155439	-3.367921
157	1	0	3.425362	2.472352	-3.662235
158	1	0	2.418853	0.834148	-5.562402
159	1	0	6.527923	-2.207124	-1.388962
160	1	0	1.461316	3.367692	-2.638305
161	1	0	5.894396	4.680951	-0.624641
162	1	0	2.625081	2.278631	2.304870
163	1	0	-3.323762	4.931907	-2.700601
164	1	0	-0.443448	4.757340	-3.368284
165	1	0	1.084166	3.441587	3.460906
166	1	0	-8.073904	2.568257	-3.050565
167	1	0	-5.263430	3.747221	-3.536188
168	1	0	-3.124833	4.509957	2.098099
169	1	0	-6.485672	-2.657616	-3.395032
170	1	0	-6.929026	0.509803	-2.915197
171	1	0	-7.696893	1.640453	2.011636
172	1	0	-1.280552	-1.822693	1.933151
173	1	0	2.985638	-5.546772	-1.457411
174	1	0	-1.403389	1.201890	5.706653
175	1	0	1.999860	-5.055907	4.166033
176	1	0	1.353199	-5.031800	2.532839
177	1	0	3.467407	-4.031809	1.702371
178	1	0	3.723198	-5.601177	2.395991
179	1	0	4.107782	-3.078613	4.055539
180	1	0	4.577304	-4.709287	4.468871
181	1	0	6.598873	-3.641439	3.851565
182	1	0	6.191803	-4.589090	2.437065
183	1	0	5.302735	-2.571771	1.310436
184	1	0	5.546328	-1.630376	2.782157
185	1	0	8.038820	-2.138258	2.545741
186	1	0	7.662772	-2.898440	1.006746
187	1	0	6.727126	-0.739661	0.181512
188	1	0	7.129977	0.012264	1.714231
189	1	0	9.550425	-0.447598	1.307617
190	1	0	9.146681	-1.267323	-0.179774
191	1	0	9.921539	0.901371	-0.806745
192	1	0	8.195280	0.902001	-1.068037
193	1	0	7.902472	2.070423	1.152399
194	1	0	9.635554	2.112878	1.335382
195	1	0	8.120938	3.436554	-0.958168
196	1	0	8.633746	4.265142	0.499028
197	1	0	-0.159208	1.343193	2.947033
198	1	0	-1.768484	0.739346	3.326385
199	1	0	-0.569164	2.567720	4.949715
200	1	0	0.510857	-0.515820	1.806767
201	1	0	1.795790	-0.460270	2.985289
202	1	0	11.027577	3.741690	-0.056985
203	1	0	10.507063	2.995142	-1.559812
204	1	0	10.257093	4.710754	-1.302644
205	1	0	1.686130	-2.750028	4.330819
206	1	0	0.917691	1.028973	6.593804
207	1	0	2.865861	2.779824	4.287159

(*2R*,5*S*)-4b-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.281020	-0.854927	2.881999
2	6	0	-2.639583	-1.766242	3.913636
3	6	0	-3.108143	-3.197373	3.725643
4	6	0	-2.950296	-3.683565	2.285641
5	6	0	-3.492347	-2.694710	1.249998
6	6	0	-5.014254	-2.832167	1.098713
7	6	0	-3.215784	4.460732	2.505994
8	6	0	-2.953575	3.962938	3.914389
9	6	0	-2.394845	2.546146	3.892214
10	6	0	-3.285607	1.621263	3.088904
11	6	0	-3.532148	2.201580	1.705467
12	6	0	-4.581676	1.479879	0.887777
13	6	0	1.171924	6.512126	0.225810
14	6	0	1.332029	6.092774	1.670168
15	6	0	0.249133	5.080630	1.985528
16	6	0	-1.146778	5.624126	1.732556
17	6	0	-1.251286	6.248067	0.333951
18	6	0	-2.399061	7.229972	0.171795
19	6	0	3.122374	2.926753	-2.361275
20	6	0	3.769889	4.003465	-1.510214
21	6	0	3.214292	5.357167	-1.947955
22	6	0	1.686921	5.384737	-1.917554
23	6	0	1.040051	4.168279	-2.579031
24	6	0	0.963625	4.225154	-4.104503
25	6	0	6.048125	-1.447125	-2.555598
26	6	0	6.681245	-0.257137	-1.838727
27	6	0	5.548580	0.639887	-1.367507
28	6	0	4.614658	0.983878	-2.517090
29	6	0	4.086011	-0.242027	-3.235487
30	6	0	3.273734	0.051951	-4.494849
31	6	0	3.801553	-5.519081	0.151294
32	6	0	5.025552	-4.875041	0.781162
33	6	0	5.126788	-3.461180	0.248961
34	6	0	5.215897	-3.454461	-1.261013
35	6	0	3.993440	-4.162950	-1.850808
36	6	0	4.019569	-4.400854	-3.359265
37	6	0	-1.031486	-5.182319	2.442381
38	6	0	0.197239	-4.924689	3.301608
39	6	0	1.325133	-4.376317	2.446167
40	6	0	1.601161	-5.319443	1.297512
41	6	0	0.337628	-5.455829	0.454132
42	6	0	0.496381	-6.429402	-0.691876
43	8	0	-1.214673	-1.713570	3.778422
44	8	0	-4.529454	-3.215417	3.990111
45	8	0	-1.547334	-3.918436	2.037955
46	8	0	-3.108108	-1.328272	1.557472
47	8	0	-2.064098	4.815158	4.645048
48	8	0	-2.341252	2.037701	5.235875
49	8	0	-2.577569	0.370747	2.974071
50	8	0	-4.085978	3.536515	1.872362
51	8	0	2.614198	5.526526	1.947212
52	8	0	0.334750	4.719037	3.382125
53	8	0	-1.992113	4.463559	1.775698
54	8	0	-0.103734	7.089923	0.044199
55	8	0	-3.619356	6.539991	0.491459
56	8	0	3.486050	3.721652	-0.121731
57	8	0	3.576420	5.558820	-3.329288
58	8	0	1.309981	5.316145	-0.523900
59	8	0	1.719066	2.966756	-2.125729
60	8	0	0.325135	3.042166	-4.594466
61	8	0	7.502815	-0.742411	-0.786245
62	8	0	6.066247	1.876402	-0.840407
63	8	0	3.493034	1.650061	-1.897463
64	8	0	5.241159	-1.020774	-3.661261
65	8	0	2.225923	1.014295	-4.211571
66	8	0	4.992847	-4.848765	2.205169
67	8	0	6.303338	-2.809912	0.771111
68	8	0	5.197018	-2.061541	-1.608427
69	8	0	3.940556	-5.493523	-1.261543
70	8	0	3.678650	-3.224923	-4.101521
71	8	0	-0.063678	-4.048609	4.395002
72	8	0	2.521767	-4.281070	3.248373
73	8	0	2.668722	-4.747372	0.528803
74	8	0	-0.681138	-5.992772	1.337149
75	8	0	-0.652673	-6.242844	-1.533573
76	8	0	-4.775314	2.206894	-0.346635
77	6	0	-6.276082	-1.638455	-2.276345
78	6	0	-6.454499	-2.420014	-3.596642
79	6	0	-7.819200	-3.134838	-3.443497
80	6	0	-8.647898	-2.119168	-2.671560
81	7	0	-7.673302	-1.575537	-1.763835
82	8	0	-8.028611	-0.724473	-0.795085
83	6	0	-5.745990	-0.214346	-2.451916
84	6	0	-2.232374	1.039593	-3.158935
85	6	0	-1.206596	0.905081	-2.022743
86	6	0	-1.288506	-0.460979	-1.314393
87	6	0	-0.078537	-0.757433	-0.404500
88	6	0	0.154408	0.336805	0.655982
89	6	0	1.248727	-0.024755	1.683231
90	6	0	2.607422	-0.331961	1.026274
91	6	0	3.788674	-0.390175	2.019631
92	6	0	4.223490	1.001537	2.524289
93	6	0	5.570390	0.990671	3.280560
94	6	0	6.771948	0.579118	2.402485
95	7	0	-5.548960	-2.009944	0.018187
96	6	0	-5.468116	-2.454005	-1.262556
97	8	0	-4.831083	-3.449335	-1.557098
98	8	0	-3.969560	-1.056128	-3.826884
99	6	0	-4.345446	-0.190945	-3.044684
100	7	0	-3.602282	0.861946	-2.668664
101	6	0	8.111091	0.802563	3.131289
102	8	0	-9.041541	-1.018836	-3.540933
103	8	0	-10.068093	-1.605743	-4.413115
104	1	0	-4.325630	-0.726493	3.120172
105	1	0	-2.933173	-1.408071	4.892498
106	1	0	-2.558701	-3.848918	4.389059
107	1	0	-3.494212	-4.612768	2.184249
108	1	0	-3.030701	-2.911744	0.303045
109	1	0	-5.511368	-2.578542	2.018396

110	1	0	-5.220996	-3.870246	0.873975
111	1	0	-3.685961	5.421972	2.475780
112	1	0	-3.890971	3.954737	4.449432
113	1	0	-1.413736	2.566290	3.440072
114	1	0	-4.216463	1.480487	3.624078
115	1	0	-2.607024	2.259618	1.159779
116	1	0	-5.509769	1.445433	1.446766
117	1	0	-4.259306	0.487579	0.632931
118	1	0	1.893315	7.257458	-0.068633
119	1	0	1.217981	6.957655	2.305212
120	1	0	0.381419	4.208166	1.368032
121	1	0	-1.405616	6.332713	2.506949
122	1	0	-1.324417	5.441079	-0.375077
123	1	0	-2.395993	7.592370	-0.847591
124	1	0	-2.225579	8.066838	0.836228
125	1	0	3.360666	3.060556	-3.397860
126	1	0	4.840843	3.971743	-1.628897
127	1	0	3.602455	6.142389	-1.312506
128	1	0	1.324246	6.297969	-2.368437
129	1	0	0.040843	4.065481	-2.192615
130	1	0	1.937566	4.385598	-4.538685
131	1	0	0.337391	5.062637	-4.378626
132	1	0	6.792780	-2.124312	-2.940671
133	1	0	7.315711	0.285160	-2.521710
134	1	0	4.985015	0.108402	-0.621787
135	1	0	5.127982	1.641698	-3.206726
136	1	0	3.502334	-0.824155	-2.544058
137	1	0	2.858649	-0.873458	-4.865199
138	1	0	3.909952	0.491718	-5.245533
139	1	0	3.691094	-6.550790	0.443838
140	1	0	5.900505	-5.436775	0.490340
141	1	0	4.245480	-2.917130	0.540167
142	1	0	6.136662	-3.923271	-1.586507
143	1	0	3.106473	-3.609849	-1.591952
144	1	0	3.263643	-5.136967	-3.576739
145	1	0	4.981910	-4.811673	-3.649337
146	1	0	-1.772204	-5.739783	2.994153
147	1	0	0.520572	-5.865606	3.721927
148	1	0	1.055332	-3.406223	2.055608
149	1	0	1.891833	-6.287322	1.688690
150	1	0	0.032386	-4.497037	0.068091
151	1	0	0.543030	-7.432923	-0.284535
152	1	0	1.415398	-6.208292	-1.218836
153	1	0	-0.955570	-0.804388	3.565506
154	1	0	-4.722107	-3.332185	4.929068
155	1	0	-1.155844	4.775465	4.278763
156	1	0	-2.000131	2.739197	5.810484
157	1	0	2.928658	4.948152	1.224575
158	1	0	1.264807	4.580598	3.617698
159	1	0	-4.393270	7.084952	0.302256
160	1	0	2.648924	3.231424	-0.091541
161	1	0	4.483538	5.875418	-3.429310
162	1	0	0.961273	2.308179	-4.656052
163	1	0	7.028147	-1.370661	-0.207848
164	1	0	5.420271	2.262366	-0.232018
165	1	0	1.845741	0.878894	-3.333283
166	1	0	4.115154	-4.582864	2.558588
167	1	0	6.420856	-3.074145	1.696528
168	1	0	4.392018	-2.569431	-4.116165
169	1	0	-0.391754	-3.170317	4.092567
170	1	0	2.290905	-3.950550	4.129314
171	1	0	-0.646725	-6.856209	-2.278826
172	1	0	-5.630471	-3.091839	-3.744900
173	1	0	-6.500547	-1.724917	-4.418368
174	1	0	-7.710487	-4.031351	-2.847239
175	1	0	-8.276389	-3.370082	-4.390358
176	1	0	-4.872153	3.145980	-0.125949
177	1	0	-2.118655	2.005296	-3.635787
178	1	0	-2.067724	0.273982	-3.900700
179	1	0	-0.220756	1.066857	-2.441746
180	1	0	-1.371122	1.701906	-1.303627
181	1	0	-1.372292	-1.243180	-2.062887
182	1	0	-2.183574	-0.500938	-0.708877
183	1	0	-0.254273	-1.702063	0.103471
184	1	0	0.810241	-0.870943	-1.017890
185	1	0	0.434841	1.261379	0.159999
186	1	0	-0.777597	0.500068	1.183350
187	1	0	1.357939	0.801388	2.380496
188	1	0	0.928727	-0.890094	2.256631
189	1	0	2.534272	-1.287871	0.519004
190	1	0	2.814225	0.411754	0.263566
191	1	0	4.626547	-0.866293	1.528145
192	1	0	3.523774	-1.019089	2.866534
193	1	0	4.300396	1.680404	1.679624
194	1	0	3.456144	1.404392	3.177942
195	1	0	5.752950	1.987438	3.673368
196	1	0	5.501711	0.320886	4.134145
197	1	0	6.768197	1.137511	1.474120
198	1	0	6.692681	-0.465718	2.131192
199	1	0	-6.193108	-1.279833	0.230184
200	1	0	-6.412170	0.283341	-3.149977
201	1	0	-5.782241	0.338388	-1.528499
202	1	0	-3.948550	1.477899	-1.953982
203	1	0	8.242173	1.851255	3.377884
204	1	0	8.941742	0.494831	2.506384
205	1	0	8.147729	0.231962	4.054336
206	1	0	-9.517929	-2.488564	-2.161867
207	1	0	-10.505194	-0.795420	-4.720415

(*2S*,5*S*)-4a-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.037674	-3.960972	-1.218600
2	6	0	-2.021996	-4.523605	-2.227431
3	6	0	-2.995737	-5.428574	-1.466723
4	6	0	-3.655991	-4.700953	-0.295807
5	6	0	-2.669503	-3.944627	0.588436
6	6	0	-1.875256	-4.775279	1.609544
7	6	0	3.491931	-2.863409	-3.660355
8	6	0	2.314892	-3.255434	-4.558038

9	6	0	1.004185	-2.921628	-3.855018	65	8	0	0.282496	3.539490	2.197258
10	6	0	1.033463	-3.452200	-2.434817	66	8	0	-7.495271	1.658079	-2.850037
11	6	0	2.215771	-2.927736	-1.646725	67	8	0	-5.575579	3.773468	-2.876321
12	6	0	2.271181	-3.438367	-0.211968	68	8	0	-3.725073	3.804162	-0.866725
13	6	0	5.519015	1.986794	-2.870257	69	8	0	-6.456068	1.905785	0.682735
14	6	0	4.898414	1.862218	-4.251947	70	8	0	-3.137736	2.377909	2.010686
15	6	0	3.928618	0.692592	-4.256182	71	8	0	-5.549670	-3.685679	-3.427936
16	6	0	4.554596	-0.585442	-3.740623	72	8	0	-6.621390	-1.010348	-3.284695
17	6	0	5.243315	-0.366812	-2.401254	73	8	0	-6.266593	0.171233	-0.819599
18	6	0	6.128809	-1.517084	-1.952507	74	8	0	-6.596043	-3.375420	0.073877
19	6	0	1.768769	3.892229	-0.497585	75	8	0	-7.820421	-0.352519	1.615749
20	6	0	2.443592	4.399675	-1.768591	76	7	0	-0.929088	-3.873247	2.257868
21	6	0	3.950431	4.529525	-1.556204	77	8	0	1.152846	-2.909049	0.550361
22	6	0	4.552981	3.261924	-0.946044	78	6	0	-3.373039	-0.324615	5.095820
23	6	0	3.750284	2.717633	0.233948	79	7	0	-2.451750	-0.593795	4.009428
24	6	0	3.911094	3.496171	1.544871	80	8	0	-2.718007	-0.438275	2.727714
25	6	0	-3.315199	5.147158	-0.610922	81	6	0	-1.378104	-1.358910	5.964484
26	6	0	-2.507063	5.562451	-1.837070	82	6	0	-1.112092	-0.900809	4.491293
27	6	0	-1.311374	4.630760	-1.933108	83	6	0	-2.924621	-1.350839	6.126579
28	6	0	-0.557095	4.607799	-0.611738	84	8	0	-0.717937	1.424489	3.896954
29	6	0	-1.420892	4.271438	0.582550	85	6	0	-0.289807	0.399591	4.443894
30	6	0	-0.772202	4.495597	1.941403	86	7	0	0.906164	0.338789	5.015518
31	6	0	-7.049599	1.305573	-0.469507	87	6	0	1.813472	1.507145	5.085584
32	6	0	-7.003715	2.258099	-1.650026	88	6	0	3.043195	1.158571	5.933065
33	6	0	-5.587783	2.752924	-1.862495	89	6	0	3.954373	0.113411	5.258681
34	6	0	-5.053744	3.364628	-0.586208	90	6	0	5.208187	-0.188093	6.102594
35	6	0	-5.058663	2.300623	0.507884	91	6	0	6.085774	-1.314144	5.517360
36	6	0	-4.520704	2.758430	1.865702	92	6	0	6.752628	-0.946295	4.177803
37	6	0	-5.892745	-3.908847	-1.025442	93	6	0	7.667070	-2.070029	3.652483
38	6	0	-6.299654	-3.207100	-2.307253	94	6	0	8.323107	-1.709316	2.306303
39	6	0	-6.096636	-1.714743	-2.142020	95	6	0	9.231111	-2.837677	1.776305
40	6	0	-6.802951	-1.158515	-0.921585	96	6	0	9.808208	-2.532699	0.377100
41	6	0	-6.425338	-1.953736	0.326637	97	6	0	10.889922	-1.434429	0.386751
42	6	0	-7.348534	-1.699728	1.526138	98	6	0	11.462659	-1.184380	-1.022655
43	8	0	-2.693187	-3.425260	-2.878751	99	6	0	-0.426531	-1.943194	3.598495
44	8	0	-2.226014	-6.499902	-0.881751	100	6	0	-1.313179	-3.154309	3.330747
45	8	0	-4.494208	-3.688591	-0.896525	101	8	0	-2.297893	-3.432591	4.001556
46	8	0	-1.768325	-3.195546	-0.270754	102	8	0	-3.079977	0.950751	5.685543
47	8	0	2.474765	-2.582717	-5.802707	103	8	0	-3.350090	1.956128	4.661594
48	8	0	-0.080576	-3.567843	-4.538060	104	1	0	-0.481516	-4.756797	-0.755430
49	8	0	-0.181385	-2.995515	-1.796766	105	1	0	-1.506828	-5.071555	-2.998605
50	8	0	3.392260	-3.403830	-2.341138	106	1	0	-3.765440	-5.790962	-2.135249
51	8	0	4.224290	3.063947	-4.628051	107	1	0	-4.240985	-5.394728	0.291977
52	8	0	3.465384	0.396803	-5.585802	108	1	0	-3.217174	-3.186070	1.122190
53	8	0	3.419727	-1.452470	-3.584942	109	1	0	-1.363955	-5.600189	1.144963
54	8	0	6.155281	0.759655	-2.535384	110	1	0	-2.552647	-5.157683	2.357208
55	8	0	6.830703	-1.127613	-0.757903	111	1	0	4.428113	-3.201243	-4.072243
56	8	0	2.156063	3.448478	-2.824820	112	1	0	2.335717	-4.314489	-4.759015
57	8	0	4.185124	5.580171	-0.597835	113	1	0	0.881187	-1.848311	-3.823801
58	8	0	4.454488	2.247245	-1.972948	114	1	0	1.069478	-4.533799	-2.466722
59	8	0	2.363914	2.644848	-0.166471	115	1	0	2.198203	-1.850225	-1.643056
60	8	0	2.968211	3.020174	2.508943	116	1	0	3.188643	-3.110173	0.249658
61	8	0	-3.333500	5.552257	-2.993194	117	1	0	2.243820	-4.519033	-0.203993
62	8	0	-0.398777	5.105127	-2.938902	118	1	0	6.273348	2.756532	-2.835583
63	8	0	0.436712	3.573513	-0.776569	119	1	0	5.678675	1.686425	-4.975578
64	8	0	-2.538165	5.206706	0.568338	120	1	0	3.099886	0.927728	-3.607128

121	1	0	5.240012	-0.974620	-4.482610
122	1	0	4.506151	-0.140202	-1.650415
123	1	0	6.825510	-1.761567	-2.745977
124	1	0	5.529389	-2.377822	-1.711586
125	1	0	1.863895	4.609787	0.297907
126	1	0	2.011035	5.337922	-2.074387
127	1	0	4.436332	4.724752	-2.503012
128	1	0	5.583373	3.440873	-0.669515
129	1	0	4.036149	1.692051	0.397163
130	1	0	3.826348	4.557002	1.378519
131	1	0	4.898918	3.299928	1.938078
132	1	0	-4.169482	5.789541	-0.468523
133	1	0	-2.149917	6.571825	-1.698743
134	1	0	-1.661493	3.633317	-2.150351
135	1	0	-0.089717	5.577263	-0.481876
136	1	0	-1.788020	3.268816	0.516159
137	1	0	-1.549663	4.409705	2.683650
138	1	0	-0.341468	5.485015	1.991476
139	1	0	-8.048121	1.026121	-0.199594
140	1	0	-7.637012	3.106560	-1.439338
141	1	0	-4.953323	1.925731	-2.147827
142	1	0	-5.681528	4.196123	-0.289219
143	1	0	-4.491093	1.446248	0.177414
144	1	0	-5.124233	2.324380	2.648536
145	1	0	-4.539861	3.831362	1.955261
146	1	0	-6.118727	-4.962887	-1.059034
147	1	0	-7.339615	-3.408493	-2.510199
148	1	0	-5.042783	-1.510872	-2.025911
149	1	0	-7.871584	-1.146026	-1.081135
150	1	0	-5.391389	-1.739735	0.549076
151	1	0	-6.854929	-2.022225	2.434688
152	1	0	-8.222450	-2.311720	1.378771
153	1	0	-2.808982	-2.723332	-2.218263
154	1	0	-2.126379	-7.252374	-1.478791
155	1	0	2.631695	-1.631452	-5.665373
156	1	0	-0.927466	-3.170929	-4.281208
157	1	0	3.456393	3.231692	-4.041270
158	1	0	3.187493	1.211971	-6.028632
159	1	0	7.244928	-0.269411	-0.926675
160	1	0	2.028388	2.584598	-2.401804
161	1	0	4.114830	6.457421	-0.996248
162	1	0	2.048803	3.279333	2.290602
163	1	0	-3.985945	4.827955	-2.969542
164	1	0	0.212912	4.395193	-3.185375
165	1	0	-0.071605	2.750295	2.644783
166	1	0	-7.119824	0.766756	-2.998744
167	1	0	-6.124808	3.489839	-3.622249
168	1	0	-3.057361	1.436113	2.215809
169	1	0	-4.589279	-3.607725	-3.270144
170	1	0	-6.340825	-1.448847	-4.101374
171	1	0	-7.122624	0.304602	1.760214
172	1	0	-0.114308	-3.597951	1.733762
173	1	0	0.500444	-2.488969	-0.031487
174	1	0	-3.230456	-1.067534	7.120941
175	1	0	-3.309289	-2.316192	5.847742
176	1	0	-0.984701	-2.348719	6.133967
177	1	0	-0.930487	-0.661277	6.655431
178	1	0	1.201373	-0.500499	5.463267
179	1	0	2.129084	1.796857	4.096543
180	1	0	1.267144	2.329888	5.527755
181	1	0	3.610074	2.071164	6.081061
182	1	0	2.730130	0.808881	6.913248
183	1	0	4.237139	0.489553	4.282927
184	1	0	3.410797	-0.814608	5.100290
185	1	0	5.801211	0.717164	6.198075
186	1	0	4.894705	-0.471371	7.104017
187	1	0	6.863209	-1.561254	6.234734
188	1	0	5.480315	-2.206975	5.383778
189	1	0	5.994674	-0.735279	3.431142
190	1	0	7.338721	-0.040508	4.309780
191	1	0	8.439061	-2.278466	4.388667
192	1	0	7.082382	-2.978537	3.532945
193	1	0	7.557803	-1.509326	1.564851
194	1	0	8.904299	-0.801101	2.435051
195	1	0	10.041518	-3.020685	2.477437
196	1	0	8.643817	-3.750238	1.719616
197	1	0	10.245560	-3.439011	-0.033890
198	1	0	8.991861	-2.234391	-0.270184
199	1	0	10.473852	-0.509896	0.771538
200	1	0	11.693183	-1.728821	1.055793
201	1	0	11.911714	-2.089815	-1.417325
202	1	0	10.676259	-0.874813	-1.703620
203	1	0	12.221601	-0.409473	-1.006688
204	1	0	-0.172351	-1.501204	2.644910
205	1	0	0.496420	-2.274718	4.059243
206	1	0	-4.388440	-0.376147	4.752094
207	1	0	-2.459968	2.058209	4.261874

(*2S*,5S)-4a-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618979	3.223090	2.492468
2	6	0	-0.631138	4.628357	1.910041
3	6	0	0.627408	5.364032	2.383156
4	6	0	1.885173	4.566586	2.079875
5	6	0	1.798412	3.123735	2.571688
6	6	0	1.985380	2.947306	4.085594
7	6	0	-5.586990	1.414496	2.099997
8	6	0	-5.259907	2.570339	1.168007
9	6	0	-3.753878	2.644334	0.990920
10	6	0	-3.029116	2.674934	2.336011
11	6	0	-3.495905	1.600592	3.309884
12	6	0	-3.153101	1.889468	4.776453
13	6	0	-5.755877	-3.236905	-0.630800
14	6	0	-5.742757	-1.932382	-1.444636
15	6	0	-5.058031	-0.879421	-0.589350
16	6	0	-5.934208	-0.519360	0.595064
17	6	0	-6.483276	-1.810406	1.240151
18	6	0	-7.984241	-1.957836	1.005248
19	6	0	-1.192656	-4.959359	-0.661702

20	6	0	-2.090145	-5.089352	-1.884722	76	7	0	2.400041	1.577039	4.389496
21	6	0	-3.387656	-5.783297	-1.484577	77	8	0	-1.813892	2.339798	4.995632
22	6	0	-4.089949	-5.060381	-0.343300	78	6	0	5.365859	-2.105279	3.548431
23	6	0	-3.166184	-4.729815	0.820775	79	7	0	4.392298	-1.049748	3.786725
24	6	0	-2.886866	-5.878518	1.782922	80	8	0	4.805906	0.198296	3.938928
25	6	0	3.438319	-3.724819	-2.998585	81	6	0	3.234922	-2.968437	4.335458
26	6	0	2.265881	-4.136186	-3.876148	82	6	0	2.996757	-1.486751	3.915309
27	6	0	0.977506	-3.896861	-3.095060	83	6	0	4.521122	-3.386634	3.588822
28	6	0	1.029545	-4.629815	-1.753074	84	8	0	2.924991	-1.774782	1.516466
29	6	0	2.296952	-4.324816	-0.971782	85	6	0	2.287057	-1.547436	2.547481
30	6	0	2.558214	-5.269532	0.187089	86	7	0	0.958598	-1.491783	2.609978
31	6	0	5.104739	1.423357	-2.852323	87	6	0	0.041692	-1.854359	1.508756
32	6	0	4.457755	0.846023	-4.096734	88	6	0	2.249870	-0.743916	5.039354
33	6	0	3.491024	-0.255900	-3.730769	89	6	0	1.574425	0.582152	4.691195
34	6	0	4.214839	-1.345353	-2.950494	90	8	0	0.342881	0.654372	4.739341
35	6	0	4.785514	-0.713448	-1.678743	91	6	0	-0.410762	-0.652406	0.663037
36	6	0	5.695107	-1.598282	-0.833969	92	6	0	0.620339	-0.278903	-0.420751
37	6	0	2.827361	5.374603	-0.047156	93	6	0	0.327035	1.084139	-1.072920
38	6	0	2.419498	5.286566	-1.500416	94	6	0	-0.995466	1.140256	-1.859337
39	6	0	2.665710	3.882789	-1.995438	95	6	0	-1.303126	2.570815	-2.352417
40	6	0	4.111824	3.464604	-1.807228	96	6	0	-2.758375	2.718883	-2.837824
41	6	0	4.566473	3.680166	-0.365737	97	6	0	-3.197723	4.186190	-3.021553
42	6	0	6.092069	3.680919	-0.202071	98	6	0	-4.735212	4.309908	-3.044778
43	8	0	-0.797204	4.632690	0.493394	99	6	0	-5.233458	5.756288	-3.241765
44	8	0	0.622141	5.457655	3.820359	100	6	0	-4.978566	6.314854	-4.655398
45	8	0	1.979671	4.476221	0.640467	101	6	0	-5.535745	7.743105	-4.818252
46	8	0	0.573723	2.528983	2.112726	102	1	0	-0.703328	3.288307	3.554213
47	8	0	-5.970799	2.389371	-0.061824	103	1	0	-1.487863	5.149658	2.318660
48	8	0	-3.462377	3.840535	0.263366	104	1	0	0.679379	6.338152	1.912653
49	8	0	-1.650097	2.414286	1.973390	105	1	0	2.755837	5.057167	2.491060
50	8	0	-4.948221	1.585338	3.341731	106	1	0	2.578426	2.575335	2.068995
51	8	0	-5.029441	-2.068708	-2.677877	107	1	0	1.087925	3.177958	4.627223
52	8	0	-4.842449	0.299920	-1.384369	108	1	0	2.764422	3.608875	4.437213
53	8	0	-5.105287	0.189616	1.528496	109	1	0	-6.648467	1.357214	2.289297
54	8	0	-5.762059	-2.970965	0.764466	110	1	0	-5.606829	3.488737	1.614254
55	8	0	-8.350079	-3.280834	1.423291	111	1	0	-3.421915	1.761359	0.468230
56	8	0	-2.328729	-3.774267	-2.430920	112	1	0	-3.152262	3.658262	2.768874
57	8	0	-3.051287	-7.093149	-0.980653	113	1	0	-3.122334	0.648799	2.970519
58	8	0	-4.513497	-3.822634	-0.949902	114	1	0	-3.389144	1.012581	5.367450
59	8	0	-1.895763	-4.201183	0.327145	115	1	0	-3.804467	2.689426	5.091267
60	8	0	-1.951069	-5.423830	2.778414	116	1	0	-6.571717	-3.898704	-0.878451
61	8	0	2.307367	-3.469576	-5.125374	117	1	0	-6.740090	-1.608461	-1.697824
62	8	0	-0.114076	-4.397321	-3.875871	118	1	0	-4.120574	-1.264441	-0.218037
63	8	0	-0.059196	-4.155118	-0.913794	119	1	0	-6.733421	0.120547	0.251555
64	8	0	3.440477	-4.530374	-1.840489	120	1	0	-6.280988	-1.784767	2.295339
65	8	0	3.814181	-4.936359	0.798118	121	1	0	-8.232490	-1.801721	-0.039071
66	8	0	3.664994	1.845831	-4.784749	122	1	0	-8.488236	-1.188885	1.581269
67	8	0	2.969754	-0.828901	-4.941316	123	1	0	-0.919784	-5.937237	-0.297901
68	8	0	3.246624	-2.348368	-2.646919	124	1	0	-1.586186	-5.647150	-2.653689
69	8	0	5.683783	0.357851	-2.107210	125	1	0	-4.060839	-5.828859	-2.328534
70	8	0	4.984663	-2.643660	-0.144834	126	1	0	-4.938789	-5.635053	0.000218
71	8	0	1.016672	5.578708	-1.552993	127	1	0	-3.602954	-3.912074	1.364287
72	8	0	2.284773	3.885792	-3.377556	128	1	0	-2.524179	-6.746823	1.257862
73	8	0	4.094188	2.041523	-2.085649	129	1	0	-3.796819	-6.140453	2.300780
74	8	0	4.189482	5.005677	0.091309	130	1	0	4.381313	-3.865954	-3.501091
75	8	0	6.755893	2.755428	-1.072604	131	1	0	2.351873	-5.192567	-4.078697

132	1	0	0.877427	-2.840443	-2.897568
133	1	0	0.939900	-5.693561	-1.940493
134	1	0	2.288136	-3.307369	-0.625452
135	1	0	2.575208	-6.286277	-0.187285
136	1	0	1.782145	-5.171695	0.930077
137	1	0	5.904816	2.104422	-3.068164
138	1	0	5.216099	0.442769	-4.753456
139	1	0	2.696352	0.147153	-3.123427
140	1	0	5.019572	-1.751548	-3.551954
141	1	0	3.981995	-0.309863	-1.082679
142	1	0	6.204425	-0.965772	-0.123122
143	1	0	6.428356	-2.074891	-1.465685
144	1	0	2.744804	6.376714	0.341084
145	1	0	2.994404	5.991391	-2.085375
146	1	0	2.053116	3.212099	-1.421754
147	1	0	4.751087	3.985881	-2.506565
148	1	0	4.084334	2.925818	0.235610
149	1	0	6.351228	3.520119	0.836542
150	1	0	6.434241	4.660025	-0.492042
151	1	0	0.022921	4.749573	-0.017535
152	1	0	-0.114227	5.986477	4.153931
153	1	0	-5.480202	1.809894	-0.673286
154	1	0	-2.501932	4.001936	0.195606
155	1	0	-4.348592	-2.758039	-2.590502
156	1	0	-4.579545	0.033014	-2.279084
157	1	0	-9.310323	-3.377580	1.462873
158	1	0	-2.308516	-3.136603	-1.701239
159	1	0	-2.926348	-7.735751	-1.690715
160	1	0	-1.272557	-4.895668	2.335247
161	1	0	2.432500	-2.507716	-5.021265
162	1	0	-0.926726	-3.908443	-3.666370
163	1	0	4.388813	-4.544988	0.120796
164	1	0	4.190584	2.382131	-5.393148
165	1	0	2.530005	-0.144234	-5.464251
166	1	0	4.312468	-2.287627	0.475846
167	1	0	0.667526	5.309804	-2.416267
168	1	0	2.555377	3.059891	-3.816272
169	1	0	6.582874	1.828128	-0.855818
170	1	0	3.371906	1.347551	4.302230
171	1	0	-1.141386	1.639233	4.907029
172	1	0	4.284495	-3.724307	2.594728
173	1	0	5.039994	-4.178528	4.106701
174	1	0	3.394001	-2.990783	5.407336
175	1	0	2.387398	-3.592258	4.092277
176	1	0	0.512865	-1.091297	3.408765
177	1	0	0.510622	-2.596159	0.887581
178	1	0	1.465695	-1.381667	5.418523
179	1	0	2.963391	-0.577004	5.835709
180	1	0	-0.816899	-2.318259	1.973609
181	1	0	-0.597802	0.204252	1.297649
182	1	0	-1.348089	-0.926365	0.190688
183	1	0	1.602879	-0.249769	0.032715
184	1	0	0.644609	-1.062541	-1.173215
185	1	0	0.305214	1.832695	-0.289345
186	1	0	1.141505	1.332253	-1.746808
187	1	0	-1.809102	0.828061	-1.215178
188	1	0	-0.960492	0.450093	-2.699868
189	1	0	-0.598116	2.858937	-3.129441
190	1	0	-1.158403	3.241738	-1.515981
191	1	0	-2.902644	2.171067	-3.766530
192	1	0	-3.400059	2.272040	-2.091112
193	1	0	-2.758231	4.592690	-3.926815
194	1	0	-2.835648	4.763691	-2.179259
195	1	0	-5.144078	3.681153	-3.833232
196	1	0	-5.102522	3.936924	-2.094921
197	1	0	-4.755728	6.399217	-2.507529
198	1	0	-6.301981	5.790312	-3.046040
199	1	0	-5.445616	5.659418	-5.384897
200	1	0	-3.914694	6.321428	-4.863365
201	1	0	-6.606070	7.756840	-4.640038
202	1	0	-5.067619	8.416748	-4.107838
203	1	0	-5.353700	8.124724	-5.817539
204	1	0	6.129148	-2.073594	4.307204
205	8	0	5.968644	-1.819929	2.275053
206	8	0	6.669078	-3.042419	1.868700
207	1	0	6.159498	-3.199925	1.040660

(*2R*,5*S*)-4a-OOH (*excluded*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028610	-4.037647	-1.072352
2	6	0	-1.963504	-4.504158	-2.173681
3	6	0	-3.063851	-5.353015	-1.532338
4	6	0	-3.773695	-4.617882	-0.393632
5	6	0	-2.814081	-3.961803	0.598734
6	6	0	-2.163834	-4.886651	1.644457
7	6	0	3.643490	-2.946101	-3.254315
8	6	0	2.517517	-3.364601	-4.202177
9	6	0	1.175453	-3.024017	-3.567372
10	6	0	1.134729	-3.553272	-2.145711
11	6	0	2.274694	-3.019568	-1.303522
12	6	0	2.269833	-3.534219	0.130643
13	6	0	5.577993	1.984504	-2.700603
14	6	0	4.925840	1.775780	-4.058189
15	6	0	3.981225	0.588984	-3.979189
16	6	0	4.648657	-0.646722	-3.418427
17	6	0	5.361828	-0.347811	-2.108958
18	6	0	6.274767	-1.467170	-1.636518
19	6	0	1.839994	4.002796	-0.394229
20	6	0	2.462970	4.396219	-1.729738
21	6	0	3.971580	4.581291	-1.583434
22	6	0	4.625882	3.395483	-0.870702
23	6	0	3.874759	2.955861	0.384183
24	6	0	4.066311	3.868962	1.600984
25	6	0	-3.245507	5.248750	-0.395877
26	6	0	-2.494516	5.539817	-1.695464
27	6	0	-1.308701	4.589304	-1.766341
28	6	0	-0.493276	4.674287	-0.484793
29	6	0	-1.316698	4.447028	0.761622
30	6	0	-0.598595	4.702007	2.077606

31	6	0	-6.953777	1.366056	0.078343	87	6	0	1.689165	1.391877	4.186616
32	6	0	-6.997411	2.329189	-1.092777	88	6	0	2.844920	1.264128	5.182311
33	6	0	-5.601968	2.858426	-1.359398	89	6	0	3.796733	0.097845	4.853360
34	6	0	-5.003684	3.494772	-0.117479	90	6	0	4.981877	0.017918	5.835714
35	6	0	-4.987374	2.462511	1.009273	91	6	0	5.977041	-1.110776	5.489511
36	6	0	-4.601111	2.953385	2.406339	92	6	0	6.787503	-0.824139	4.211161
37	6	0	-5.818448	-3.665129	-1.448380	93	6	0	7.740312	-1.972721	3.828967
38	6	0	-5.999792	-2.653318	-2.559803	94	6	0	8.496946	-1.664757	2.522986
39	6	0	-5.736057	-1.270536	-1.992753	95	6	0	9.379432	-2.836335	2.048942
40	6	0	-6.658219	-0.946515	-0.830579	96	6	0	10.012245	-2.573000	0.664929
41	6	0	-6.605610	-2.067285	0.218073	97	6	0	11.138701	-1.521259	0.696879
42	6	0	-7.792552	-2.088504	1.164052	98	6	0	11.763436	-1.309881	-0.696606
43	8	0	-2.485710	-3.325496	-2.826919	99	6	0	-0.413640	-2.357928	3.798877
44	8	0	-2.428994	-6.500115	-0.930632	100	6	0	-1.365708	-3.515026	3.510692
45	8	0	-4.475645	-3.517992	-1.018986	101	8	0	-2.275048	-3.827077	4.266396
46	8	0	-1.792368	-3.263428	-0.163682	102	8	0	-4.600863	-1.126423	2.867015
47	8	0	2.736551	-2.719663	-5.451818	103	8	0	-5.674137	-0.222304	3.305852
48	8	0	0.119800	-3.655316	-4.306676	104	1	0	-0.541528	-4.873004	-0.599427
49	8	0	-0.100606	-3.089043	-1.561121	105	1	0	-1.428730	-5.063904	-2.922168
50	8	0	3.492504	-3.476909	-1.937930	106	1	0	-3.791625	-5.640666	-2.280036
51	8	0	4.215961	2.941865	-4.479768	107	1	0	-4.459306	-5.282401	0.113236
52	8	0	3.493156	0.220342	-5.282407	108	1	0	-3.337308	-3.174370	1.112835
53	8	0	3.545723	-1.534113	-3.185415	109	1	0	-1.751512	-5.770958	1.188672
54	8	0	6.246887	0.788077	-2.319515	110	1	0	-2.903748	-5.177118	2.374771
55	8	0	7.022987	-1.020079	-0.492879	111	1	0	4.603106	-3.269247	-3.621453
56	8	0	2.169256	3.340028	-2.679111	112	1	0	2.555699	-4.427547	-4.379228
57	8	0	4.207852	5.726995	-0.741160	113	1	0	1.060027	-1.949769	-3.539504
58	8	0	4.535761	2.277196	-1.785186	114	1	0	1.171056	-4.635272	-2.170342
59	8	0	2.475772	2.809904	0.045383	115	1	0	2.243091	-1.942231	-1.300183
60	8	0	3.203788	3.456321	2.665034	116	1	0	3.162305	-3.193328	0.631216
61	8	0	-3.361685	5.441571	-2.815697	117	1	0	2.261618	-4.614724	0.133480
62	8	0	-0.442278	4.966327	-2.851716	118	1	0	6.319125	2.767289	-2.728341
63	8	0	0.504747	3.637257	-0.601930	119	1	0	5.692495	1.577938	-4.790647
64	8	0	-2.389174	5.420045	0.717601	120	1	0	3.162633	0.838879	-3.323128
65	8	0	0.466962	3.740612	2.282889	121	1	0	5.326884	-1.053996	-4.157280
66	8	0	-7.546372	1.749492	-2.278798	122	1	0	4.638030	-0.099644	-1.351809
67	8	0	-5.658581	3.879515	-2.375776	123	1	0	6.940470	-1.748891	-2.444338
68	8	0	-3.679551	3.892771	-0.488603	124	1	0	5.689684	-2.318512	-1.331114
69	8	0	-6.368841	2.027972	1.183319	125	1	0	1.940407	4.798628	0.321489
70	8	0	-3.187078	3.134089	2.591175	126	1	0	1.995671	5.289341	-2.110397
71	8	0	-5.144526	-2.888317	-3.678747	127	1	0	4.422210	4.692925	-2.560137
72	8	0	-5.960736	-0.293366	-3.031050	128	1	0	5.657146	3.630179	-0.643293
73	8	0	-6.119501	0.251455	-0.247514	129	1	0	4.193514	1.959168	0.640052
74	8	0	-6.727831	-3.372860	-0.408576	130	1	0	3.925347	4.903096	1.335285
75	8	0	-7.840232	-0.809117	1.838414	131	1	0	5.082022	3.753763	1.952852
76	7	0	-1.135099	-4.112938	2.325729	132	1	0	-4.083439	5.914636	-0.266317
77	8	0	1.109960	-3.039866	0.852555	133	1	0	-2.118951	6.551593	-1.654688
78	6	0	-3.430198	-0.299606	3.074119	134	1	0	-1.676131	3.580824	-1.881807
79	7	0	-2.242397	-1.062714	2.737132	135	1	0	-0.029878	5.653408	-0.451780
80	8	0	-1.772609	-0.966806	1.458070	136	1	0	-1.723658	3.455924	0.752629
81	6	0	-2.129410	-0.874468	5.049410	137	1	0	-1.335527	4.638001	2.860727
82	6	0	-1.235344	-1.051804	3.802551	138	1	0	-0.145507	5.681376	2.078652
83	6	0	-3.242248	0.073905	4.554396	139	1	0	-7.928947	1.038383	0.379338
84	8	0	-0.826050	1.192595	3.008062	140	1	0	-7.637475	3.155450	-0.822889
85	6	0	-0.388690	0.216832	3.635601	141	1	0	-4.967005	2.045029	-1.678631
86	7	0	0.782454	0.229265	4.260447	142	1	0	-5.598952	4.351867	0.171848

143	1	0	-4.376812	1.625090	0.713343
144	1	0	-5.009363	2.230232	3.095991
145	1	0	-5.053469	3.913449	2.598053
146	1	0	-6.029317	-4.672258	-1.771318
147	1	0	-7.015593	-2.706555	-2.919681
148	1	0	-4.720680	-1.208546	-1.637414
149	1	0	-7.662750	-0.789956	-1.200284
150	1	0	-5.680650	-1.979043	0.761919
151	1	0	-7.662359	-2.896368	1.868986
152	1	0	-8.694319	-2.252957	0.591501
153	1	0	-2.525151	-2.622417	-2.157042
154	1	0	-2.301826	-7.223258	-1.558043
155	1	0	2.828628	-1.755682	-5.343407
156	1	0	-0.730061	-3.230759	-4.110224
157	1	0	3.440702	3.103871	-3.900186
158	1	0	3.193573	1.006833	-5.761206
159	1	0	7.417485	-0.164279	-0.713167
160	1	0	2.076220	2.517521	-2.172873
161	1	0	4.109787	6.558142	-1.223627
162	1	0	2.261542	3.647720	2.475220
163	1	0	-4.072522	4.788522	-2.675182
164	1	0	0.159999	4.234895	-3.054311
165	1	0	0.099370	2.844409	2.389684
166	1	0	-6.969604	1.039742	-2.632354
167	1	0	-6.269612	3.605221	-3.075240
168	1	0	-2.676148	2.317177	2.665707
169	1	0	-4.227103	-3.090198	-3.406344
170	1	0	-5.585925	-0.620100	-3.863199
171	1	0	-8.548218	-0.766205	2.494278
172	1	0	-0.339020	-3.822314	1.788998
173	1	0	0.500575	-2.548167	0.279003
174	1	0	-2.927211	1.104255	4.622175
175	1	0	-4.168493	-0.055952	5.084761
176	1	0	-2.536385	-1.843024	5.293533
177	1	0	-1.573233	-0.475417	5.886063
178	1	0	1.098467	-0.578829	4.746643
179	1	0	2.089870	1.481274	3.190670
180	1	0	1.116136	2.284083	4.387988
181	1	0	3.400719	2.191422	5.118116
182	1	0	2.457699	1.164229	6.192070
183	1	0	4.160823	0.236079	3.842588
184	1	0	3.267414	-0.851732	4.877600
185	1	0	5.506500	0.969139	5.841522
186	1	0	4.593436	-0.139587	6.838165
187	1	0	6.667152	-1.245088	6.317484
188	1	0	5.433504	-2.044718	5.371936
189	1	0	6.114380	-0.650107	3.379226
190	1	0	7.363080	0.086505	4.355078
191	1	0	8.447643	-2.147177	4.635428
192	1	0	7.163154	-2.884944	3.701448
193	1	0	7.784602	-1.438812	1.738304
194	1	0	9.109834	-0.781477	2.676402
195	1	0	10.158330	-3.038900	2.779685
196	1	0	8.759819	-3.726743	1.984642
197	1	0	10.421973	-3.501245	0.275029
198	1	0	9.228981	-2.245858	-0.010160
199	1	0	10.750575	-0.576501	1.060807
200	1	0	11.908233	-1.842871	1.392514
201	1	0	12.184657	-2.237543	-1.069890
202	1	0	11.011728	-0.973387	-1.403406
203	1	0	12.554285	-0.568063	-0.664167
204	1	0	0.360030	-2.315255	3.047996
205	1	0	0.026004	-2.508461	4.777076
206	1	0	-3.511368	0.544984	2.427408
207	1	0	-6.350102	-0.322278	2.599179

(*2R*,5*S*)-4a-OOH (*included*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745469	3.119921	2.550867
2	6	0	-0.868084	4.533659	2.005193
3	6	0	0.369326	5.327302	2.435548
4	6	0	1.647568	4.620572	2.013841
5	6	0	1.677796	3.153293	2.434056
6	6	0	2.018683	2.923305	3.909817
7	6	0	-5.607294	1.006858	2.310170
8	6	0	-5.400945	2.218000	1.413932
9	6	0	-3.911783	2.404130	1.185982
10	6	0	-3.137630	2.442992	2.502281
11	6	0	-3.498594	1.316836	3.463356
12	6	0	-3.128799	1.606373	4.922940
13	6	0	-5.509709	-3.519932	-0.646176
14	6	0	-5.612465	-2.173807	-1.386363
15	6	0	-4.981745	-1.119240	-0.490937
16	6	0	-5.844870	-0.890123	0.735409
17	6	0	-6.257723	-2.258058	1.322648
18	6	0	-7.747451	-2.526029	1.113227
19	6	0	-0.881863	-5.012495	-0.965376
20	6	0	-1.806002	-5.067525	-2.174458
21	6	0	-3.057766	-5.861475	-1.816377
22	6	0	-3.763495	-5.291329	-0.593389
23	6	0	-2.825935	-5.034450	0.577590
24	6	0	-2.468664	-6.256066	1.415429
25	6	0	3.637273	-3.347935	-3.264419
26	6	0	2.460879	-3.746601	-4.144624
27	6	0	1.183528	-3.622624	-3.322044
28	6	0	1.300143	-4.462577	-2.050690
29	6	0	2.565222	-4.149763	-1.266151
30	6	0	2.885974	-5.172308	-0.193513
31	6	0	5.191935	1.801405	-2.727749
32	6	0	4.693156	1.252917	-4.048823
33	6	0	3.723071	0.121399	-3.813235
34	6	0	4.385856	-0.978906	-2.994778
35	6	0	4.815747	-0.378916	-1.652350
36	6	0	5.666588	-1.264112	-0.738709
37	6	0	2.456457	5.575792	-0.095265
38	6	0	2.128233	5.457122	-1.564850
39	6	0	2.522294	4.086436	-2.061460
40	6	0	3.982461	3.776305	-1.780028

41	6	0	4.334861	4.025733	-0.316904	97	6	0	-3.656974	4.192742	-2.802490
42	6	0	5.839783	4.135388	-0.053000	98	6	0	-5.194317	4.281435	-2.707359
43	8	0	-1.077945	4.562487	0.592313	99	6	0	-5.735929	5.722432	-2.801456
44	8	0	0.455427	5.360565	3.872711	100	6	0	-5.586805	6.352726	-4.199946
45	8	0	1.660161	4.609554	0.565568	101	6	0	-6.187957	7.771198	-4.258280
46	8	0	0.451770	2.505926	2.060957	102	8	0	6.127973	-2.068867	4.424589
47	8	0	-6.143602	2.034640	0.203902	103	8	0	7.146385	-3.116714	4.293321
48	8	0	-3.728900	3.639561	0.487855	104	1	0	-0.755039	3.154099	3.617357
49	8	0	-1.762096	2.267186	2.078494	105	1	0	-1.739273	4.996518	2.449387
50	8	0	-4.943120	1.187782	3.537638	106	1	0	0.333664	6.320726	2.006458
51	8	0	-4.927142	-2.185161	-2.642487	107	1	0	2.514080	5.141840	2.393146
52	8	0	-4.876582	0.111492	-1.227676	108	1	0	2.433933	2.672290	1.835780
53	8	0	-5.051366	-0.158653	1.683083	109	1	0	1.182254	3.135022	4.548222
54	8	0	-5.450287	-3.318041	0.760070	110	1	0	2.832740	3.573705	4.199937
55	8	0	-7.972746	-3.915727	1.392655	111	1	0	-6.654368	0.860541	2.529193
56	8	0	-2.124369	-3.719854	-2.583696	112	1	0	-5.794749	3.090141	1.911332
57	8	0	-2.648261	-7.195999	-1.450472	113	1	0	-3.541740	1.563565	0.622110
58	8	0	-4.261440	-4.021835	-1.062313	114	1	0	-3.296024	3.406165	2.966911
59	8	0	-1.595087	-4.399275	0.112591	115	1	0	-3.064755	0.403606	3.091738
60	8	0	-1.540828	-5.850347	2.438950	116	1	0	-3.262370	0.702330	5.505008
61	8	0	2.434024	-2.993257	-5.344154	117	1	0	-3.835395	2.339912	5.277703
62	8	0	0.093663	-4.101967	-4.118834	118	1	0	-6.306192	-4.209877	-0.878391
63	8	0	0.199679	-4.124001	-1.159530	119	1	0	-6.637608	-1.911001	-1.595747
64	8	0	3.704785	-4.219144	-2.161648	120	1	0	-4.007682	-1.451189	-0.166986
65	8	0	4.084126	-4.816908	0.507580	121	1	0	-6.707205	-0.306339	0.449077
66	8	0	3.946202	2.257073	-4.781061	122	1	0	-6.024868	-2.271432	2.371692
67	8	0	3.342458	-0.428434	-5.085403	123	1	0	-8.047502	-2.286623	0.098897
68	8	0	3.405889	-2.001894	-2.826695	124	1	0	-8.300913	-1.874604	1.781306
69	8	0	5.722623	0.728744	-1.960162	125	1	0	-0.546239	-6.005111	-0.710422
70	8	0	4.950349	-2.326780	-0.110348	126	1	0	-1.296112	-5.521101	-3.005471
71	8	0	0.712842	5.633764	-1.684520	127	1	0	-3.750254	-5.857919	-2.645891
72	8	0	2.247161	4.100612	-3.468138	128	1	0	-4.575500	-5.939154	-0.292918
73	8	0	4.086560	2.356353	-2.045294	129	1	0	-3.285281	-4.295823	1.209056
74	8	0	3.836772	5.317866	0.113456	130	1	0	-2.069637	-7.046407	0.801197
75	8	0	6.620014	3.195439	-0.803836	131	1	0	-3.353224	-6.618272	1.916697
76	7	0	2.453884	1.543311	4.122360	132	1	0	4.571945	-3.419455	-3.797105
77	8	0	-1.826618	2.171117	5.097862	133	1	0	2.588126	-4.782420	-4.420855
78	6	0	5.301817	-2.228400	3.236719	134	1	0	1.048005	-2.590666	-3.035829
79	7	0	4.337237	-1.149827	3.320012	135	1	0	1.264486	-5.510463	-2.325502
80	8	0	4.690589	0.094014	3.017419	136	1	0	2.494369	-3.166882	-0.838314
81	6	0	3.203064	-3.023356	4.093461	137	1	0	3.003774	-6.139211	-0.667469
82	6	0	2.963287	-1.549297	3.638965	138	1	0	2.071856	-5.218184	0.514963
83	6	0	4.448373	-3.485802	3.311232	139	1	0	5.985047	2.515015	-2.835160
84	8	0	2.708334	-1.786361	1.261343	140	1	0	5.523462	0.889232	-4.637930
85	6	0	2.141506	-1.598502	2.342461	141	1	0	2.861137	0.489552	-3.278598
86	7	0	0.824138	-1.548480	2.484404	142	1	0	5.253650	-1.354649	-3.523876
87	6	0	-0.134533	-1.873545	1.402762	143	1	0	3.946448	-0.010751	-1.129512
88	6	0	2.340878	-0.769510	4.812024	144	1	0	6.110984	-0.603711	-0.003462
89	6	0	1.652039	0.558399	4.519673	145	1	0	6.464586	-1.709857	-1.312161
90	8	0	0.438382	0.659741	4.710415	146	1	0	2.273710	6.566950	0.285777
91	6	0	-0.606651	-0.642749	0.607880	147	1	0	2.675511	6.209687	-2.116731
92	6	0	0.367401	-0.251672	-0.524121	148	1	0	1.925338	3.352156	-1.548074
93	6	0	0.032380	1.120601	-1.141323	149	1	0	4.619961	4.343900	-2.444535
94	6	0	-1.317807	1.164648	-1.882467	150	1	0	3.875738	3.235345	0.254433
95	6	0	-1.684256	2.597298	-2.331730	151	1	0	6.027996	4.062104	1.010640
96	6	0	-3.180024	2.731558	-2.679892	152	1	0	6.148480	5.112023	-0.386167

153	1	0	-0.252904	4.620770	0.081143
154	1	0	-0.292051	5.819723	4.277460
155	1	0	-5.632173	1.523341	-0.449872
156	1	0	-2.784316	3.845582	0.356164
157	1	0	-4.199404	-2.830556	-2.616758
158	1	0	-4.621273	-0.090677	-2.141547
159	1	0	-8.917566	-4.107162	1.453463
160	1	0	-2.111603	-3.154365	-1.796632
161	1	0	-2.492293	-7.753647	-2.223480
162	1	0	-0.896673	-5.248506	2.039894
163	1	0	2.647101	-2.054746	-5.188873
164	1	0	-0.732108	-3.665356	-3.853864
165	1	0	4.598671	-4.155967	0.008274
166	1	0	4.513753	2.830616	-5.312733
167	1	0	2.947192	0.262642	-5.635053
168	1	0	4.173251	-2.033119	0.409470
169	1	0	0.429452	5.347334	-2.565471
170	1	0	2.638940	3.327456	-3.911133
171	1	0	6.441929	2.272823	-0.571967
172	1	0	3.388649	1.298772	3.860662
173	1	0	-1.102200	1.529387	4.984238
174	1	0	4.195057	-3.832268	2.322731
175	1	0	4.987091	-4.260593	3.832381
176	1	0	3.423691	-3.013154	5.153269
177	1	0	2.330555	-3.634383	3.914769
178	1	0	0.424252	-1.189948	3.326411
179	1	0	0.313896	-2.600111	0.748025
180	1	0	1.589044	-1.388845	5.278312
181	1	0	3.133639	-0.604354	5.530356
182	1	0	-0.977951	-2.346197	1.886529
183	1	0	-0.749094	0.199611	1.270792
184	1	0	-1.573444	-0.887192	0.180419
185	1	0	1.372016	-0.226121	-0.123445
186	1	0	0.353829	-1.025470	-1.286718
187	1	0	0.023198	1.853047	-0.342511
188	1	0	0.820193	1.398748	-1.837714
189	1	0	-2.100689	0.812700	-1.221863
190	1	0	-1.292309	0.496735	-2.740837
191	1	0	-1.062674	2.896960	-3.172475
192	1	0	-1.469553	3.268548	-1.510417
193	1	0	-3.402279	2.191439	-3.597680
194	1	0	-3.743644	2.271469	-1.881784
195	1	0	-3.296003	4.625241	-3.730083
196	1	0	-3.240547	4.762736	-1.979687
197	1	0	-5.646531	3.678339	-3.492077
198	1	0	-5.483048	3.855919	-1.752205
199	1	0	-5.224797	6.342268	-2.069832
200	1	0	-6.789786	5.720526	-2.535544
201	1	0	-6.083840	5.719262	-4.929038
202	1	0	-4.539019	6.398118	-4.474088
203	1	0	-7.244620	7.747353	-4.012370
204	1	0	-5.691505	8.423624	-3.547280
205	1	0	-6.079948	8.203698	-5.247536
206	1	0	5.912161	-2.150592	2.358260
207	1	0	7.919652	-2.649406	4.648774

(*5R*)-4b + borneol (*top*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.756679	-1.074052	0.747426
2	6	0	2.708181	-0.669574	1.820503
3	6	0	3.257336	0.509034	2.626182
4	6	0	3.443505	1.708192	1.690634
5	6	0	4.022839	1.275050	0.336451
6	6	0	5.038008	2.258422	-0.218414
7	6	0	1.094138	-4.514560	-1.861970
8	6	0	2.233918	-4.947006	-0.943141
9	6	0	2.679158	-3.754703	-0.125069
10	6	0	3.190746	-2.667399	-1.051187
11	6	0	2.380126	-2.481468	-2.347048
12	6	0	3.350497	-2.110614	-3.449547
13	6	0	-2.800275	-4.831252	1.789395
14	6	0	-1.617846	-3.960115	2.150639
15	6	0	-0.969519	-3.293481	0.945591
16	6	0	-0.603152	-4.379408	-0.062491
17	6	0	-1.899375	-5.082610	-0.477449
18	6	0	-1.769522	-6.293855	-1.395511
19	6	0	-6.810487	-1.784205	1.524223
20	6	0	-6.113095	-2.519047	2.650260
21	6	0	-6.049870	-4.042466	2.475100
22	6	0	-5.192375	-4.669029	1.363698
23	6	0	-5.664287	-4.647244	-0.087738
24	6	0	-6.969672	-5.398257	-0.345968
25	6	0	-6.904513	2.790870	-0.481079
26	6	0	-7.864742	2.909344	0.702384
27	6	0	-7.522262	1.841186	1.735096
28	6	0	-7.499406	0.488297	1.055619
29	6	0	-6.498676	0.490410	-0.083119
30	6	0	-6.455712	-0.886979	-0.702988
31	6	0	-2.767188	6.082715	0.418179
32	6	0	-3.770402	5.883341	1.545339
33	6	0	-4.393681	4.511394	1.417347
34	6	0	-5.084371	4.376173	0.067758
35	6	0	-4.054430	4.635119	-1.032018
36	6	0	-4.627239	4.746636	-2.430742
37	6	0	1.868285	3.612469	1.711156
38	6	0	0.761253	3.717693	2.778815
39	6	0	-0.576399	3.833633	2.069357
40	6	0	-0.647462	5.164099	1.335142
41	6	0	0.660877	5.385834	0.548958
42	6	0	1.486861	6.522061	1.163136
43	8	0	1.436487	-0.325287	1.243316
44	8	0	4.507555	0.163446	3.243066
45	8	0	2.133758	2.262256	1.427211
46	8	0	4.691655	0.000658	0.536775
47	8	0	1.902152	-5.983732	0.008597
48	8	0	3.791527	-4.131627	0.720797
49	8	0	3.096295	-1.354447	-0.463543
50	8	0	1.706844	-3.675957	-2.825460

51	8	0	-2.067620	-2.978610	3.083838	107	1	0	-0.861209	-4.598216	2.590120
52	8	0	0.179513	-2.651418	1.521229	108	1	0	-1.650776	-2.581903	0.500050
53	8	0	0.081744	-3.755149	-1.178001	109	1	0	0.046650	-5.094603	0.406673
54	8	0	-2.438593	-5.699333	0.724820	110	1	0	-2.599814	-4.363357	-0.878470
55	8	0	-1.309659	-5.983825	-2.723272	111	1	0	-2.732064	-6.786592	-1.419802
56	8	0	-4.861798	-1.947936	2.979854	112	1	0	-1.048795	-6.977212	-0.975649
57	8	0	-7.384864	-4.562129	2.285418	113	1	0	-7.732670	-2.279591	1.255047
58	8	0	-3.891441	-4.009646	1.437525	114	1	0	-6.759689	-2.357975	3.505559
59	8	0	-5.956321	-1.687487	0.403597	115	1	0	-5.629586	-4.409407	3.406497
60	8	0	-6.976776	-5.655197	-1.771682	116	1	0	-5.064311	-5.708923	1.644237
61	8	0	-7.798527	4.247811	1.202928	117	1	0	-4.904975	-5.169663	-0.654895
62	8	0	-8.502897	1.863018	2.775875	118	1	0	-7.822882	-4.811031	-0.048313
63	8	0	-7.123336	-0.477773	2.046076	119	1	0	-6.994538	-6.328555	0.211195
64	8	0	-6.924543	1.487968	-1.032028	120	1	0	-5.543543	3.414043	-3.649607
65	8	0	-5.622843	-1.018694	-1.789242	121	1	0	-8.872861	2.740439	0.359003
66	8	0	-3.098181	5.996857	2.822072	122	1	0	-6.532116	2.026859	2.124393
67	8	0	-5.343950	4.391183	2.512611	123	1	0	-8.487757	0.268304	0.664528
68	8	0	-5.571460	3.033020	-0.002603	124	1	0	-5.512623	0.720572	0.279650
69	8	0	-3.486857	5.954363	-0.793563	125	1	0	-7.447896	-1.228960	-0.965385
70	8	0	-5.083888	3.424675	-2.801119	126	1	0	-5.715130	-3.636197	-0.442483
71	8	0	0.782700	2.557809	3.608579	127	1	0	-2.333409	7.070130	0.438053
72	8	0	-1.621465	3.681253	3.046956	128	1	0	-4.533714	6.643568	1.461107
73	8	0	-1.780233	5.066856	0.439788	129	1	0	-3.627266	3.761716	1.517404
74	8	0	1.408268	4.163600	0.480967	130	1	0	-5.896682	5.083569	0.003110
75	8	0	2.816726	6.386736	0.650038	131	1	0	-3.289057	3.878593	-1.002391
76	7	0	5.399705	1.895161	-1.582099	132	1	0	-3.845937	5.090569	-3.093032
77	8	0	2.686145	-1.646179	-4.647347	133	1	0	-5.439734	5.460902	-2.439687
78	6	0	5.950492	2.313828	-3.913320	134	1	0	2.769718	4.117966	2.018916
79	6	0	4.306895	0.962372	-4.858257	135	1	0	0.919371	4.605558	3.382157
80	6	0	3.969874	2.332536	-5.377644	136	1	0	-0.664134	3.042492	1.343655
81	6	0	9.121969	0.069717	-1.572081	137	1	0	-0.813851	5.965197	2.041967
82	6	0	8.307917	-0.894378	-0.694328	138	1	0	0.421868	5.616787	-0.473640
83	6	0	9.156382	-1.467690	0.458045	139	1	0	1.485884	6.462002	2.246566
84	6	0	8.375883	-2.453359	1.356150	140	1	0	1.025593	7.465109	0.886763
85	6	0	7.256368	-1.758046	2.153200	141	1	0	1.321835	0.639034	1.180184
86	6	0	6.380650	-2.722681	2.983719	142	1	0	5.180925	0.058096	2.557461
87	6	0	7.082132	-3.319850	4.221458	143	1	0	1.870583	-6.853325	-0.411411
88	6	0	7.433309	-2.281367	5.310406	144	1	0	3.516727	-4.880054	1.269088
89	6	0	6.200908	-1.575030	5.912472	145	1	0	-1.342404	-2.355038	3.234359
90	6	0	6.585752	-0.636248	7.072775	146	1	0	0.425197	-1.767785	1.170771
91	6	0	5.364095	0.087775	7.669831	147	1	0	-1.901764	-5.358619	-3.161852
92	1	0	4.337236	-1.910430	1.081632	148	1	0	-4.134135	-2.382496	2.506798
93	1	0	2.541155	-1.517623	2.465037	149	1	0	-7.883824	-4.562488	3.112282
94	1	0	2.567813	0.799386	3.398848	150	1	0	-7.828304	-6.018529	-2.046265
95	1	0	4.068224	2.440101	2.186094	151	1	0	-7.087911	4.344877	1.859280
96	1	0	3.210624	1.136878	-0.356811	152	1	0	-8.361874	1.086148	3.337164
97	1	0	5.910273	2.263228	0.425408	153	1	0	-4.944637	-0.298799	-1.853253
98	1	0	4.612362	3.251741	-0.243056	154	1	0	-3.765424	6.014036	3.524376
99	1	0	0.637078	-5.320187	-2.399888	155	1	0	-5.223937	3.557436	2.985994
100	1	0	3.045317	-5.277308	-1.579208	156	1	0	-7.159842	3.477778	-1.266005
101	1	0	1.859681	-3.390360	0.464536	157	1	0	-0.098733	2.466664	4.004038
102	1	0	4.223298	-2.909253	-1.270203	158	1	0	-2.113793	4.513278	3.157290
103	1	0	1.655918	-1.710484	-2.161593	159	1	0	3.353014	7.168277	0.834898
104	1	0	3.943403	-2.990091	-3.673206	160	1	0	5.521515	0.926539	-1.828766
105	1	0	4.012642	-1.324209	-3.141468	161	1	0	3.736658	0.066097	-5.011679
106	1	0	-3.064332	-5.477373	2.611772	162	1	0	3.074423	2.687775	-4.878524

163	1	0	2.117893	-2.346069	-4.995577
164	1	0	9.967711	-0.453686	-2.007830
165	1	0	9.509732	0.887988	-0.982098
166	1	0	7.939975	-1.712651	-1.307248
167	1	0	7.444920	-0.365165	-0.312365
168	1	0	10.019481	-1.976568	0.037258
169	1	0	9.533098	-0.651388	1.068840
170	1	0	7.941658	-3.233754	0.737100
171	1	0	9.069284	-2.931272	2.040135
172	1	0	7.697124	-1.006185	2.800707
173	1	0	6.616897	-1.236913	1.453783
174	1	0	6.036586	-3.523271	2.335297
175	1	0	5.498562	-2.186032	3.309092
176	1	0	6.429418	-4.068831	4.662814
177	1	0	7.987326	-3.834611	3.915129
178	1	0	7.967038	-2.789826	6.109449
179	1	0	8.111347	-1.536384	4.907224
180	1	0	5.507790	-2.327680	6.281403
181	1	0	5.682407	-0.999988	5.155008
182	1	0	7.295778	0.104238	6.713277
183	1	0	7.082567	-1.206013	7.853850
184	1	0	4.868325	0.650722	6.885445
185	1	0	4.655100	-0.649866	8.033836
186	6	0	-3.270444	0.802910	-3.396702
187	6	0	-1.971512	-0.014159	-3.212139
188	6	0	-3.116832	-1.175093	-4.802701
189	6	0	-4.079915	-0.010375	-4.457672
190	6	0	-1.718126	-0.506581	-4.672448
191	6	0	-2.367733	-1.330044	-2.492131
192	6	0	-3.148128	-2.134797	-3.585826
193	6	0	-1.474204	0.613533	-5.703774
194	6	0	-0.550146	-1.494972	-4.805904
195	6	0	-0.874335	0.765955	-2.500282
196	8	0	-3.969164	0.964233	-2.135763
197	1	0	-3.037075	1.793764	-3.760118
198	1	0	-5.004032	-0.369691	-4.031593
199	1	0	-4.309021	0.592599	-5.328014
200	1	0	-1.488737	-1.866568	-2.160567
201	1	0	-2.984911	-1.126593	-1.632027
202	1	0	-2.649203	-3.069204	-3.815205
203	1	0	-4.158387	-2.344390	-3.268217
204	1	0	-3.316196	-1.649125	-5.753787
205	1	0	-2.253717	1.361576	-5.722694
206	1	0	-0.532620	1.111468	-5.496362
207	1	0	-1.407742	0.180631	-6.697287
208	1	0	-0.582627	-1.953011	-5.792175
209	1	0	0.395593	-0.979113	-4.710787
210	1	0	-0.562101	-2.284066	-4.068947
211	1	0	-1.235687	1.081478	-1.527260
212	1	0	0.007332	0.153053	-2.353165
213	1	0	-0.589656	1.652108	-3.059713
214	1	0	-4.491877	1.788694	-2.141291
215	6	0	5.755971	1.035119	8.820549
216	1	0	6.448647	1.793350	8.470082
217	1	0	4.884865	1.535745	9.229829
218	1	0	6.236888	0.483630	9.621886
219	6	0	7.474058	2.344978	-4.152131
220	1	0	7.685340	1.756684	-5.038082
221	1	0	7.734004	3.375374	-4.342822
222	6	0	8.419717	1.901951	-3.029379
223	7	0	8.278255	0.636428	-2.624372
224	1	0	7.488450	0.112003	-2.968735
225	8	0	9.272094	2.674274	-2.612713
226	6	0	5.596486	2.833724	-2.512224
227	8	0	5.517635	4.038535	-2.323194
228	6	0	5.222400	3.163208	-4.988196
229	1	0	4.990021	4.132270	-4.581069
230	1	0	5.863255	3.276788	-5.851501
231	1	0	3.785468	2.324557	-6.442820
232	7	0	5.330938	0.966745	-4.115001
233	8	0	5.782868	-0.161592	-3.399340

(*5R*)-4b + borneol (*bottom*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.583439	1.581356	1.778398
2	6	0	-2.466512	0.419531	2.775665
3	6	0	-3.849710	-0.177946	2.985748
4	6	0	-4.436121	-0.724901	1.679658
5	6	0	-3.838782	-0.027079	0.459031
6	6	0	-4.796920	-0.109758	-0.722234
7	6	0	0.706920	4.786377	-0.855196
8	6	0	-0.242363	5.188919	0.264703
9	6	0	-0.564719	4.008372	1.167326
10	6	0	-1.090976	2.848003	0.333098
11	6	0	-0.017249	2.504399	-0.685235
12	6	0	-0.360351	1.396128	-1.645508
13	6	0	6.025912	4.833511	-0.452117
14	6	0	5.284668	5.794256	0.451180
15	6	0	3.880430	5.284793	0.672144
16	6	0	3.174146	5.039796	-0.651373
17	6	0	3.987725	4.143821	-1.584766
18	6	0	3.503836	4.068826	-3.039973
19	6	0	5.520570	-0.121470	-0.210088
20	6	0	5.770989	0.777753	1.002363
21	6	0	7.080894	1.580100	0.915361
22	6	0	7.193323	2.678259	-0.148132
23	6	0	7.168623	2.264098	-1.621200
24	6	0	8.441226	1.566163	-2.094429
25	6	0	3.050392	-3.940331	-2.315808
26	6	0	4.210258	-4.536765	-1.500792
27	6	0	4.381165	-3.634345	-0.280706
28	6	0	4.752196	-2.271069	-0.806877
29	6	0	3.617673	-1.686771	-1.629758
30	6	0	4.113509	-0.365572	-2.205837
31	6	0	-1.356336	-6.311565	-0.373734
32	6	0	-0.034827	-6.607371	0.294892
33	6	0	0.913865	-5.447649	0.090414
34	6	0	1.116697	-5.171667	-1.399158
35	6	0	-0.238866	-4.998375	-2.092795

36	6	0	-0.183326	-5.101841	-3.605422	92	6	0	-4.106597	2.605176	6.475026
37	6	0	-4.972500	-3.156488	1.893804	93	6	0	-4.705709	-0.244664	-5.208296
38	6	0	-4.183209	-4.011046	2.857698	94	6	0	-5.787890	0.703630	-4.678369
39	6	0	-2.881206	-4.385622	2.185174	95	7	0	-5.377079	1.936519	-4.357972
40	6	0	-3.148475	-5.088437	0.864070	96	8	0	-6.950286	0.331153	-4.623878
41	6	0	-4.143792	-4.344608	-0.026892	97	6	0	-4.070815	-0.995779	-2.871995
42	6	0	-4.651681	-5.227393	-1.161180	98	8	0	-4.409632	-2.149365	-2.617954
43	8	0	-1.596814	-0.600019	2.257537	99	6	0	-2.774314	-1.874501	-4.878438
44	8	0	-4.702089	0.880356	3.487005	100	7	0	-2.470687	0.375543	-4.163475
45	8	0	-4.128777	-2.097678	1.467784	101	8	0	-2.741391	1.676965	-3.674075
46	8	0	-3.618380	1.366916	0.819044	102	1	0	-2.817538	2.503697	2.267116
47	8	0	0.363291	6.186156	1.125549	103	1	0	-2.089976	0.806169	3.711595
48	8	0	-1.571660	4.414151	2.114588	104	1	0	-3.831005	-0.972917	3.708378
49	8	0	-1.303712	1.681785	1.147249	105	1	0	-5.510562	-0.579381	1.726524
50	8	0	0.138337	3.682914	-1.527478	106	1	0	-2.903943	-0.509901	0.243044
51	8	0	5.988316	5.908722	1.686683	107	1	0	-5.548031	0.660154	-0.608359
52	8	0	3.208575	6.303959	1.422734	108	1	0	-5.265787	-1.081250	-0.704769
53	8	0	1.931375	4.425993	-0.260784	109	1	0	0.833882	5.572601	-1.583439
54	8	0	5.304962	4.760278	-1.679852	110	1	0	-1.164950	5.557010	-0.160158
55	8	0	2.629702	2.959182	-3.277163	111	1	0	0.336305	3.698038	1.676045
56	8	0	4.660822	1.599104	1.327273	112	1	0	-2.010608	3.119316	-0.163655
57	8	0	8.171808	0.667154	0.671497	113	1	0	0.917244	2.294960	-0.190977
58	8	0	6.076410	3.560555	0.167380	114	1	0	-1.248869	1.644547	-2.198839
59	8	0	4.539309	0.443770	-1.068561	115	1	0	-0.481681	0.465641	-1.116178
60	8	0	8.236425	1.353322	-3.510134	116	1	0	7.016022	5.186888	-0.686773
61	8	0	3.949079	-5.901891	-1.212298	117	1	0	5.223679	6.745115	-0.063002
62	8	0	5.391738	-4.113982	0.641800	118	1	0	3.917210	4.356971	1.222289
63	8	0	5.062497	-1.393831	0.285977	119	1	0	2.991886	5.995850	-1.128471
64	8	0	3.343477	-2.598509	-2.702371	120	1	0	4.060870	3.147870	-1.179062
65	8	0	3.188474	0.357332	-2.941023	121	1	0	4.390667	3.999675	-3.654135
66	8	0	-0.280925	-6.788161	1.704219	122	1	0	2.967257	4.963513	-3.318255
67	8	0	2.153259	-5.831521	0.716816	123	1	0	6.435049	-0.307158	-0.750887
68	8	0	1.877660	-3.943571	-1.495479	124	1	0	5.903882	0.087315	1.822383
69	8	0	-1.095183	-6.124172	-1.757032	125	1	0	7.192525	2.081635	1.868463
70	8	0	0.610286	-4.001564	-4.101911	126	1	0	8.113004	3.215789	0.054597
71	8	0	-3.929470	-3.256001	4.050311	127	1	0	7.052345	3.154431	-2.222269
72	8	0	-2.193872	-5.241888	3.111738	128	1	0	8.597571	0.637731	-1.572474
73	8	0	-1.868135	-5.127150	0.186241	129	1	0	9.301311	2.205101	-1.915631
74	8	0	-5.293417	-3.963960	0.771534	130	1	0	0.810824	-4.110175	-5.040483
75	8	0	-5.599267	-4.581525	-2.007053	131	1	0	5.107255	-4.501007	-2.101096
76	7	0	-4.155019	0.028708	-2.028927	132	1	0	3.453345	-3.573691	0.248916
77	8	0	0.752875	1.242074	-2.566706	133	1	0	5.630359	-2.362935	-1.441409
78	6	0	-3.543207	-0.661173	-4.277020	134	1	0	2.750249	-1.529994	-1.007870
79	6	0	-1.308325	-0.030185	-4.454551	135	1	0	4.961015	-0.553497	-2.846070
80	6	0	-1.278567	-1.444317	-4.944937	136	1	0	6.309744	1.648616	-1.820136
81	6	0	-6.310091	2.927504	-3.818370	137	1	0	-2.048170	-7.133124	-0.289328
82	6	0	-5.562838	3.887364	-2.879376	138	1	0	0.390405	-7.503668	-0.134053
83	6	0	-6.521873	4.850244	-2.155973	139	1	0	0.496469	-4.569877	0.553486
84	6	0	-5.792980	5.916341	-1.309654	140	1	0	1.664671	-5.989135	-1.840486
85	6	0	-4.860444	5.311043	-0.241384	141	1	0	-0.685132	-4.071142	-1.776538
86	6	0	-4.273359	6.362705	0.727235	142	1	0	-1.194115	-5.064795	-3.987544
87	6	0	-5.275836	6.879337	1.785328	143	1	0	0.251656	-6.057290	-3.868930
88	6	0	-5.679831	5.823636	2.838773	144	1	0	-5.895591	-2.793413	2.315514
89	6	0	-4.521552	5.415907	3.770134	145	1	0	-4.749513	-4.905594	3.076717
90	6	0	-4.915408	4.286813	4.740722	146	1	0	-2.325983	-3.481694	1.994774
91	6	0	-3.748704	3.858239	5.652063	147	1	0	-3.493279	-6.095309	1.069480

148	1	0	-3.669611	-3.462697	-0.418016
149	1	0	-5.156482	-6.080626	-0.731554
150	1	0	-3.784841	-5.575033	-1.716589
151	1	0	-0.892791	-0.160599	1.758593
152	1	0	-4.956247	1.466791	2.761186
153	1	0	0.165588	7.087636	0.839365
154	1	0	-1.213936	5.112217	2.681092
155	1	0	5.415109	6.365607	2.319732
156	1	0	2.253993	6.118374	1.484859
157	1	0	3.110843	2.108257	-3.300045
158	1	0	4.761792	2.436997	0.857295
159	1	0	8.487614	0.260696	1.488401
160	1	0	9.011724	0.939400	-3.910610
161	1	0	3.383362	-6.001927	-0.414622
162	1	0	5.945911	-3.367441	0.912551
163	1	0	2.259857	0.396396	-2.607145
164	1	0	0.546159	-7.030303	2.142778
165	1	0	2.462775	-5.243190	1.456386
166	1	0	2.881405	-4.482274	-3.225145
167	1	0	-3.214508	-3.692686	4.536105
168	1	0	-1.471206	-5.729291	2.673707
169	1	0	-5.280471	-3.706497	-2.278775
170	1	0	-3.781589	0.912861	-2.337160
171	1	0	-0.457839	0.594561	-4.287098
172	1	0	-0.625917	-2.068304	-4.348306
173	1	0	1.119507	2.120871	-2.819615
174	1	0	-6.779319	3.484600	-4.622286
175	1	0	-7.091517	2.403163	-3.284902
176	1	0	-4.834346	4.455458	-3.450917
177	1	0	-5.018605	3.295627	-2.153962
178	1	0	-7.147021	5.351016	-2.890055
179	1	0	-7.181462	4.275133	-1.512148
180	1	0	-5.208622	6.556054	-1.965852
181	1	0	-6.537185	6.543492	-0.830798
182	1	0	-5.392792	4.549969	0.318140
183	1	0	-4.039138	4.807978	-0.740510
184	1	0	-3.916242	7.208032	0.142131
185	1	0	-3.415227	5.929782	1.224601
186	1	0	-4.835897	7.728792	2.301628
187	1	0	-6.167233	7.245408	1.286781
188	1	0	-6.489083	6.224019	3.442955
189	1	0	-6.068376	4.940237	2.343498
190	1	0	-4.198408	6.286005	4.337178
191	1	0	-3.679759	5.075413	3.181941
192	1	0	-5.233662	3.420465	4.170802
193	1	0	-5.757117	4.598502	5.352783
194	1	0	-2.881216	3.643893	5.033180
195	1	0	-3.480720	4.679010	6.311092
196	1	0	-4.350357	1.791582	5.803462
197	1	0	-3.279638	2.303228	7.109526
198	1	0	-4.964899	2.799214	7.110408
199	1	0	-4.272901	0.180507	-6.106742
200	1	0	-5.234186	-1.150476	-5.464853
201	1	0	-4.386978	2.109721	-4.296649
202	1	0	-2.930029	-2.736236	-4.252382
203	1	0	-3.148795	-2.091392	-5.867302
204	1	0	-0.904682	-1.461211	-5.962844
205	6	0	3.978512	-2.203196	3.627966
206	6	0	2.872863	-1.148179	3.916614
207	6	0	1.722880	-3.111355	3.808598
208	6	0	3.192338	-3.551066	3.643093
209	6	0	1.874626	-1.930957	4.819036
210	6	0	2.088462	-0.998699	2.594092
211	6	0	1.334657	-2.369420	2.499307
212	6	0	0.554202	-1.184878	5.087094
213	6	0	2.467733	-2.310172	6.190375
214	6	0	0.797661	-4.265916	4.168370
215	8	0	3.344552	-4.343522	2.440910
216	1	0	4.425144	-2.030346	2.659253
217	1	0	4.756890	-2.196862	4.380423
218	1	0	3.492152	-4.168515	4.477907
219	1	0	1.390847	-0.172536	2.643763
220	1	0	2.760127	-0.821352	1.765396
221	1	0	0.265672	-2.223971	2.448382
222	1	0	1.640796	-2.937274	1.637644
223	1	0	3.244467	-0.219261	4.324100
224	1	0	-0.068391	-1.772619	5.754341
225	1	0	0.764417	-0.240334	5.580880
226	1	0	-0.018787	-0.988794	4.194336
227	1	0	2.573937	-1.413918	6.793507
228	1	0	1.800131	-2.984192	6.716298
229	1	0	3.439538	-2.778972	6.126831
230	1	0	0.865849	-5.037644	3.410903
231	1	0	1.074333	-4.706604	5.121070
232	1	0	-0.239097	-3.962455	4.209964
233	1	0	4.247436	-4.365703	2.071493

(*5R*)-4a + borneol (*top*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.896036	3.013229	-0.823364
2	6	0	1.215322	2.319899	-2.129066
3	6	0	2.724963	2.475970	-2.369207
4	6	0	3.542250	1.933837	-1.196265
5	6	0	3.059336	2.432276	0.162015
6	6	0	3.526641	3.852273	0.525092
7	6	0	-3.022845	4.681863	2.259879
8	6	0	-1.948432	5.570583	1.657439
9	6	0	-1.383100	4.948909	0.391983
10	6	0	-0.877863	3.556967	0.688536
11	6	0	-2.001083	2.706728	1.255320
12	6	0	-1.511206	1.342670	1.675486
13	6	0	-7.583146	2.530653	1.011636
14	6	0	-7.680930	4.009279	0.715089
15	6	0	-6.268881	4.506190	0.503762
16	6	0	-5.438619	4.318552	1.762434
17	6	0	-5.505572	2.873726	2.296922
18	6	0	-5.188741	2.762318	3.781434
19	6	0	-5.680769	-0.393464	-2.588858
20	6	0	-7.123048	0.060756	-2.515996

21	6	0	-7.655076	-0.106045	-1.103717	77	8	0	-2.656924	0.485896	1.891428
22	6	0	-6.748257	0.483987	-0.027036	78	6	0	8.324130	4.572206	-3.144735
23	6	0	-5.277978	0.123001	-0.235585	79	6	0	7.798766	3.500310	-1.006081
24	6	0	-4.908431	-1.265779	0.279890	80	6	0	9.522042	4.430192	-2.240385
25	6	0	-1.906747	-2.494691	-4.757534	81	8	0	6.641786	1.519959	-1.658162
26	6	0	-1.616322	-1.093289	-4.225604	82	6	0	7.688836	1.975411	-1.171961
27	6	0	-2.818823	-0.562903	-3.463307	83	7	0	8.721562	1.293408	-0.736772
28	6	0	-4.032860	-0.616056	-4.386736	84	6	0	8.809583	-0.178035	-0.714252
29	6	0	-4.277679	-2.063767	-4.797868	85	6	0	9.131109	-0.662184	0.709518
30	6	0	-5.465875	-2.266505	-5.712146	86	6	0	7.994680	-0.366713	1.703994
31	6	0	1.352613	-4.756831	-1.813919	87	6	0	8.377554	-0.733415	3.151948
32	6	0	1.212492	-5.165738	-3.262700	88	6	0	7.407782	-0.146391	4.201920
33	6	0	0.198229	-4.249640	-3.934639	89	6	0	5.922491	-0.496849	3.977347
34	6	0	-1.142383	-4.336818	-3.220820	90	6	0	5.631471	-2.008735	4.021264
35	6	0	-0.937255	-4.004223	-1.740003	91	6	0	4.139869	-2.309435	3.775866
36	6	0	-2.155760	-4.248364	-0.878895	92	6	0	3.774290	-3.802059	3.930356
37	6	0	4.079510	-0.355583	-0.355133	93	6	0	4.417171	-4.708610	2.861444
38	6	0	4.813157	-1.445198	-1.130361	94	6	0	4.002672	-6.191001	2.986814
39	6	0	3.790449	-2.219069	-1.927059	95	6	0	2.525071	-6.445338	2.626990
40	6	0	2.779111	-2.860157	-1.010330	96	6	0	7.343702	3.886339	0.411759
41	6	0	2.112125	-1.807644	-0.137746	97	6	0	5.951957	3.357992	0.723157
42	6	0	1.277493	-2.385577	0.990299	98	8	0	5.775673	2.307804	1.329992
43	8	0	0.887973	0.928901	-2.114861	99	6	0	7.142016	4.261701	-2.177247
44	8	0	3.087962	3.874194	-2.439004	100	7	0	9.235644	3.880664	-1.139675
45	8	0	3.384447	0.483239	-1.281959	101	8	0	10.119746	3.528371	-0.115128
46	8	0	1.620649	2.383886	0.248850	102	1	0	1.167096	4.048612	-0.892210
47	8	0	-2.467017	6.875558	1.350104	103	1	0	0.642040	2.782097	-2.918123
48	8	0	-0.274366	5.749938	-0.063667	104	1	0	3.012734	1.939504	-3.262433
49	8	0	-0.469439	2.898859	-0.526444	105	1	0	4.575789	2.167700	-1.346983
50	8	0	-2.513677	3.374195	2.445098	106	1	0	3.407316	1.760829	0.923148
51	8	0	-8.485646	4.214655	-0.438692	107	1	0	3.310758	4.004390	1.574641
52	8	0	-6.390129	5.904826	0.167601	108	1	0	2.976058	4.572461	-0.050141
53	8	0	-4.100964	4.708131	1.336683	109	1	0	-3.338216	5.034479	3.228360
54	8	0	-6.888698	2.403442	2.253839	110	1	0	-1.149820	5.701584	2.370325
55	8	0	-6.036876	3.661464	4.520624	111	1	0	-2.156441	4.891353	-0.361826
56	8	0	-7.225311	1.436029	-2.875688	112	1	0	-0.052942	3.603949	1.382256
57	8	0	-7.673142	-1.540604	-0.895131	113	1	0	-2.780972	2.611396	0.517731
58	8	0	-6.854184	1.923594	-0.031468	114	1	0	-0.949991	1.448798	2.593916
59	8	0	-4.886505	0.299491	-1.610925	115	1	0	-0.870050	0.941569	0.907566
60	8	0	-3.476002	-1.423156	0.219441	116	1	0	-8.549955	2.075883	1.153896
61	8	0	-0.464856	-1.172569	-3.386638	117	1	0	-8.105349	4.497227	1.584201
62	8	0	-2.524686	0.792963	-3.103829	118	1	0	-5.827902	3.950650	-0.306832
63	8	0	-5.204520	0.021066	-3.842860	119	1	0	-5.780917	4.990005	2.535653
64	8	0	-3.099212	-2.448966	-5.541723	120	1	0	-4.863655	2.231160	1.728518
65	8	0	-6.627032	-2.291475	-4.848539	121	1	0	-4.169292	3.023752	3.982410
66	8	0	2.455205	-5.080436	-3.972026	122	1	0	-5.353006	1.734642	4.078495
67	8	0	0.044731	-4.679199	-5.303499	123	1	0	-5.615881	-1.455594	-2.451767
68	8	0	-2.124317	-3.369397	-3.657422	124	1	0	-7.682845	-0.576286	-3.182379
69	8	0	0.109852	-4.843383	-1.167486	125	1	0	-8.639752	0.336195	-1.043102
70	8	0	-1.972681	-3.635846	0.413232	126	1	0	-7.057881	0.109207	0.941202
71	8	0	5.794267	-0.989088	-2.063446	127	1	0	-4.685895	0.830632	0.313536
72	8	0	4.416197	-3.279993	-2.670966	128	1	0	-5.356193	-2.046104	-0.305134
73	8	0	1.793693	-3.407570	-1.876305	129	1	0	-5.256731	-1.360144	1.300537
74	8	0	3.142366	-0.992593	0.513181	130	1	0	-1.138763	-2.865635	-5.404373
75	8	0	0.780874	-1.288378	1.797963	131	1	0	-1.443731	-0.440162	-5.073566
76	7	0	4.943221	4.115768	0.260721	132	1	0	-2.969445	-1.165165	-2.580049

133	1	0	-3.812964	-0.045915	-5.276792
134	1	0	-4.391329	-2.711662	-3.945245
135	1	0	-5.335624	-3.210492	-6.224259
136	1	0	-5.528553	-1.471127	-6.444291
137	1	0	2.053740	-5.372184	-1.271400
138	1	0	0.868611	-6.187038	-3.321240
139	1	0	0.551235	-3.233388	-3.882357
140	1	0	-1.553532	-5.326877	-3.361287
141	1	0	-0.648537	-2.969291	-1.702112
142	1	0	-2.277472	-5.312744	-0.744447
143	1	0	-3.022640	-3.841725	-1.378867
144	1	0	4.745027	0.226417	0.259043
145	1	0	5.275364	-2.095971	-0.399784
146	1	0	3.281655	-1.541247	-2.593924
147	1	0	3.260506	-3.626153	-0.414502
148	1	0	1.488943	-1.185598	-0.752988
149	1	0	1.886702	-3.041007	1.595714
150	1	0	0.418124	-2.918384	0.619718
151	1	0	1.620370	0.447247	-1.705080
152	1	0	2.682107	4.300691	-3.205689
153	1	0	-3.374619	6.762400	1.033312
154	1	0	-0.558075	6.676240	-0.084480
155	1	0	-8.269854	5.081759	-0.810204
156	1	0	-5.576852	6.214656	-0.248038
157	1	0	-6.954011	3.404909	4.349255
158	1	0	-6.530650	1.625544	-3.522692
159	1	0	-8.352560	-1.810121	-0.264854
160	1	0	-3.055048	-0.678418	0.707237
161	1	0	-0.247493	-0.307292	-2.987276
162	1	0	-3.191956	1.061358	-2.452372
163	1	0	-7.434686	-2.429377	-5.358392
164	1	0	3.035485	-4.394425	-3.591420
165	1	0	0.934126	-4.842453	-5.654332
166	1	0	-2.495512	-2.805789	0.442866
167	1	0	6.031884	-0.043604	-1.979490
168	1	0	1.503741	-0.669179	1.971478
169	1	0	5.146480	4.935439	-0.264588
170	1	0	-2.394820	-0.226075	2.535359
171	1	0	8.386724	3.847889	-3.949676
172	1	0	10.529015	4.706316	-2.461663
173	1	0	9.492177	1.837694	-0.358938
174	1	0	7.876756	-0.584339	-1.068169
175	1	0	9.594914	-0.481470	-1.396503
176	1	0	9.321775	-1.730349	0.673930
177	1	0	10.045840	-0.182304	1.044929
178	1	0	7.119093	-0.935518	1.407067
179	1	0	7.716839	0.677538	1.656053
180	1	0	8.431940	-1.812303	3.251619
181	1	0	9.372130	-0.348359	3.360935
182	1	0	7.708636	-0.489077	5.188135
183	1	0	7.509410	0.934942	4.192309
184	1	0	5.335577	-0.009678	4.751416
185	1	0	5.593709	-0.081199	3.031428
186	1	0	6.229561	-2.515669	3.273845
187	1	0	5.924711	-2.401602	4.991563
188	1	0	3.551887	-1.735440	4.487707
189	1	0	3.867651	-1.965125	2.783303
190	1	0	4.080619	-4.145124	4.915016
191	1	0	2.695268	-3.899144	3.880855
192	1	0	4.145633	-4.347039	1.872788
193	1	0	5.496717	-4.642023	2.939094
194	1	0	4.628991	-6.786311	2.329445
195	1	0	4.194485	-6.529430	4.000767
196	1	0	1.854933	-5.928467	3.302390
197	1	0	2.312321	-6.107104	1.618021
198	1	0	2.295410	-7.503986	2.678556
199	1	0	8.050317	3.455256	1.100715
200	1	0	7.376359	4.963698	0.504781
201	1	0	5.195953	-2.920104	-3.119980
202	1	0	6.738537	5.198298	-1.819331
203	1	0	6.356166	3.682339	-2.629106
204	1	0	8.255462	5.560187	-3.576954
205	6	0	-1.523905	-2.360934	4.226126
206	6	0	-2.937055	-2.475707	4.834861
207	6	0	-2.418579	-4.628524	4.306530
208	6	0	-1.201767	-3.820134	3.774541
209	1	0	-0.827568	-2.024911	4.984050
210	1	0	-1.156206	-3.872867	2.696153
211	1	0	-0.264046	-4.165283	4.192646
212	6	0	-2.829442	-3.841757	5.584745
213	6	0	-3.888592	-2.818649	3.656064
214	1	0	-4.922496	-2.681938	3.949524
215	1	0	-3.684707	-2.186526	2.809266
216	6	0	-3.573495	-4.316502	3.326041
217	1	0	-4.431875	-4.952594	3.500951
218	1	0	-3.251798	-4.429690	2.302209
219	1	0	-2.222738	-5.681559	4.452446
220	6	0	-1.767518	-3.895776	6.700975
221	1	0	-0.771596	-3.658101	6.356891
222	1	0	-2.024022	-3.209135	7.501382
223	1	0	-1.739754	-4.896763	7.120427
224	6	0	-4.156652	-4.311742	6.205534
225	1	0	-4.062200	-5.343540	6.530453
226	1	0	-4.395000	-3.710314	7.077205
227	1	0	-4.987195	-4.251137	5.518645
228	6	0	-3.353078	-1.242417	5.627490
229	1	0	-3.351667	-0.372017	4.979530
230	1	0	-4.351102	-1.359666	6.036032
231	1	0	-2.667112	-1.051525	6.446668
232	8	0	-1.508622	-1.402491	3.151838
233	1	0	-0.658732	-1.410320	2.654468

(*5R*)-4a + borneol (*bottom*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.613552	5.200072	1.360632
2	6	0	-2.354846	5.429785	2.861801
3	6	0	-3.197247	4.449004	3.693299
4	6	0	-3.200282	3.052486	3.078715
5	6	0	-3.780429	3.113601	1.653048

6	6	0	-5.225778	2.626668	1.572911	62	8	0	7.503436	-3.553612	-0.930974
7	6	0	0.823094	5.545640	-2.429901	63	8	0	5.408446	-3.140892	-2.929274
8	6	0	0.503740	6.620983	-1.379201	64	8	0	4.345006	-5.999939	-0.844115
9	6	0	0.102137	5.961135	-0.066515	65	8	0	2.241929	-6.085291	-2.568729
10	6	0	-0.975285	4.926101	-0.382553	66	8	0	2.320278	-1.584634	4.196058
11	6	0	-0.358792	3.819577	-1.213712	67	8	0	4.302474	-3.184638	3.140074
12	6	0	-1.219111	2.583858	-1.464496	68	8	0	3.798020	-4.382962	0.732773
13	6	0	4.916600	2.358793	-3.350196	69	8	0	0.386331	-3.853089	1.987999
14	6	0	5.426095	3.729360	-2.903713	70	8	0	1.971610	-6.632633	0.328084
15	6	0	4.313395	4.446527	-2.151373	71	8	0	0.690240	3.132799	3.439250
16	6	0	3.058665	4.608909	-2.992518	72	8	0	1.831404	0.682151	2.567286
17	6	0	2.658071	3.274468	-3.606839	73	8	0	0.256914	-1.525911	2.294832
18	6	0	1.616270	3.257150	-4.714649	74	8	0	-1.856504	0.733755	4.406496
19	6	0	4.357728	-2.212285	-2.801049	75	8	0	-2.167702	-2.778042	3.631012
20	6	0	4.498174	-1.241823	-3.944724	76	7	0	-5.274304	1.174176	1.719213
21	6	0	3.479791	-0.134349	-3.823149	77	8	0	-1.005870	1.570096	-0.451657
22	6	0	3.455741	0.536576	-2.437956	78	6	0	-1.894528	-1.853382	-0.622068
23	6	0	3.538248	-0.468694	-1.288787	79	6	0	-4.214204	-1.758878	0.042265
24	6	0	2.186551	-1.125915	-0.961335	80	6	0	-2.199342	-2.769244	0.536052
25	6	0	4.653796	-5.486042	0.444451	81	8	0	-4.402453	-3.648223	-1.446916
26	6	0	6.062416	-4.918941	0.390866	82	6	0	-4.816792	-2.548097	-1.124015
27	6	0	6.113428	-3.847369	-0.693888	83	7	0	-5.748188	-1.856590	-1.799945
28	6	0	5.494310	-4.289168	-2.026534	84	6	0	-6.380521	-2.429998	-2.993299
29	6	0	4.149060	-4.969842	-1.829941	85	6	0	-7.418152	-3.509680	-2.643745
30	6	0	3.564546	-5.689865	-3.019255	86	6	0	-8.588377	-2.959623	-1.810971
31	6	0	0.555228	-2.807201	2.925182	87	6	0	-9.615985	-4.054868	-1.464525
32	6	0	1.967197	-2.801634	3.517602	88	6	0	-10.765229	-3.559169	-0.561694
33	6	0	3.027987	-3.076672	2.480906	89	6	0	-11.712777	-2.562393	-1.257820
34	6	0	2.793425	-4.378299	1.757500	90	6	0	-12.888350	-2.146291	-0.352377
35	6	0	1.414848	-4.370747	1.100148	91	6	0	-13.840136	-1.149580	-1.041994
36	6	0	0.915297	-5.784493	0.767730	92	6	0	-15.013344	-0.738308	-0.130635
37	6	0	-1.279106	1.998524	4.130086	93	6	0	-15.948115	0.314186	-0.763076
38	6	0	0.204384	1.852451	3.852919	94	6	0	-16.762134	-0.219467	-1.958097
39	6	0	0.399134	0.815988	2.770019	95	6	0	-17.728508	0.845945	-2.512082
40	6	0	-0.173750	-0.510702	3.256021	96	6	0	-5.274421	-1.113337	0.955673
41	6	0	-1.684656	-0.364964	3.460748	97	6	0	-5.416914	0.356874	0.662707
42	6	0	-2.366789	-1.506575	4.223723	98	8	0	-5.620651	0.761559	-0.481057
43	8	0	-0.957975	5.419168	3.146237	99	1	0	-2.721810	6.127030	0.831400
44	8	0	-4.561987	4.902035	3.772641	100	1	0	-2.702376	6.416721	3.125515
45	8	0	-1.840561	2.577666	2.974306	101	1	0	-2.814692	4.437038	4.700272
46	8	0	-3.845111	4.494622	1.206987	102	1	0	-3.770242	2.376194	3.699509
47	8	0	1.638116	7.475695	-1.282225	103	1	0	-3.130549	2.553706	1.004408
48	8	0	-0.426413	6.945152	0.823073	104	1	0	-5.624699	2.875866	0.604210
49	8	0	-1.546931	4.433082	0.828795	105	1	0	-5.812962	3.099261	2.346150
50	8	0	-0.126128	4.480410	-2.494217	106	1	0	0.872117	5.976016	-3.417092
51	8	0	6.627644	3.785214	-2.152268	107	1	0	-0.323759	7.228164	-1.710238
52	8	0	4.734565	5.769381	-1.796293	108	1	0	0.961409	5.460611	0.363950
53	8	0	2.076586	5.025202	-2.028508	109	1	0	-1.750631	5.382983	-0.985688
54	8	0	3.818579	2.655530	-4.217330	110	1	0	0.586946	3.510419	-0.794923
55	8	0	1.491644	1.884651	-5.193104	111	1	0	-0.980462	2.204865	-2.450205
56	8	0	5.780719	-0.607509	-3.895520	112	1	0	-2.267557	2.826276	-1.428871
57	8	0	2.176379	-0.715709	-4.028730	113	1	0	5.626631	1.791234	-3.919542
58	8	0	4.468171	1.562957	-2.230541	114	1	0	5.618174	4.262140	-3.823336
59	8	0	4.505212	-1.509413	-1.557209	115	1	0	4.055591	3.872064	-1.273079
60	8	0	1.440391	-0.301314	-0.008275	116	1	0	3.222569	5.378767	-3.735108
61	8	0	6.447768	-4.391007	1.656964	117	1	0	2.295231	2.673819	-2.798136

118	1	0	1.916918	3.906703	-5.526043	174	1	0	-7.798995	-3.929063	-3.570914
119	1	0	0.657757	3.545732	-4.330193	175	1	0	-6.913636	-4.302668	-2.105575
120	1	0	3.389610	-2.679893	-2.846357	176	1	0	-9.071655	-2.159042	-2.361937
121	1	0	4.341937	-1.773237	-4.872425	177	1	0	-8.200580	-2.534952	-0.891249
122	1	0	3.684854	0.603278	-4.568163	178	1	0	-10.032037	-4.463037	-2.381740
123	1	0	2.492717	1.004729	-2.352049	179	1	0	-9.097438	-4.865342	-0.960496
124	1	0	3.891059	0.034204	-0.405739	180	1	0	-11.346847	-4.415874	-0.233060
125	1	0	2.418029	-2.077439	-0.514299	181	1	0	-10.347321	-3.097374	0.328862
126	1	0	1.599910	-1.262697	-1.852230	182	1	0	-11.164780	-1.673846	-1.552699
127	1	0	4.527580	-6.283216	1.152093	183	1	0	-12.103717	-3.017613	-2.163989
128	1	0	6.753069	-5.707199	0.139720	184	1	0	-13.446848	-3.031740	-0.061202
129	1	0	5.584858	-2.986487	-0.339019	185	1	0	-12.498379	-1.698156	0.557572
130	1	0	6.188023	-4.960952	-2.507423	186	1	0	-13.282520	-0.260999	-1.326151
131	1	0	3.420771	-4.273964	-1.461891	187	1	0	-14.219067	-1.598985	-1.953591
132	1	0	4.176054	-6.550140	-3.251142	188	1	0	-15.591957	-1.620091	0.131234
133	1	0	3.499566	-5.039658	-3.881319	189	1	0	-14.607489	-0.336955	0.793851
134	1	0	-0.204287	-2.983496	3.653469	190	1	0	-16.641887	0.668789	-0.005797
135	1	0	2.012711	-3.582186	4.261970	191	1	0	-15.360311	1.170472	-1.082929
136	1	0	3.043877	-2.272578	1.756842	192	1	0	-16.092753	-0.538384	-2.748700
137	1	0	2.913482	-5.213353	2.431473	193	1	0	-17.327410	-1.090977	-1.641395
138	1	0	1.478762	-3.754308	0.218550	194	1	0	-18.428731	1.161377	-1.745740
139	1	0	0.099730	-5.725961	0.057239	195	1	0	-17.180118	1.719576	-2.848735
140	1	0	0.535029	-6.197074	1.688046	196	1	0	-18.296514	0.459251	-3.351138
141	1	0	-1.456880	2.597601	5.007281	197	1	0	-6.227603	-1.596993	0.790908
142	1	0	0.703807	1.520302	4.753850	198	1	0	-4.988743	-1.313402	1.972173
143	1	0	-0.085885	1.153798	1.865594	199	6	0	7.576912	1.195370	0.142268
144	1	0	0.267007	-0.743934	4.210288	200	6	0	7.653142	1.171441	1.690481
145	1	0	-2.171297	-0.141857	2.523359	201	6	0	7.558681	-1.032926	1.110503
146	1	0	-3.417651	-1.255233	4.318980	202	6	0	7.528434	-0.310268	-0.258686
147	1	0	-1.944554	-1.506558	5.218354	203	6	0	8.501143	-0.115870	1.941439
148	1	0	-0.554648	4.538223	3.020065	204	6	0	6.248916	0.738662	2.168360
149	1	0	-4.849309	5.155069	2.884147	205	6	0	6.174442	-0.768097	1.757025
150	1	0	2.443552	6.939126	-1.199008	206	6	0	9.942564	-0.050234	1.398211
151	1	0	-0.388814	6.610438	1.739804	207	6	0	8.600258	-0.527543	3.420687
152	1	0	6.617311	3.176417	-1.372405	208	6	0	8.131636	2.489680	2.284351
153	1	0	5.668473	5.728649	-1.537487	209	8	0	6.432607	1.967703	-0.314196
154	1	0	2.195046	1.724092	-5.834755	210	1	0	8.444574	1.685809	-0.270835
155	1	0	6.458796	-1.278708	-3.736570	211	1	0	6.636704	-0.547476	-0.824436
156	1	0	1.590461	-0.026898	-4.392396	212	1	0	8.390713	-0.565266	-0.862204
157	1	0	0.950174	-0.853885	0.637180	213	1	0	6.154716	0.862116	3.239273
158	1	0	5.717073	-3.908292	2.085245	214	1	0	2.007696	0.517415	1.624642
159	1	0	7.579201	-2.721094	-1.411495	215	1	0	6.008407	-1.413133	2.603877
160	1	0	1.849994	-6.755718	-3.142377	216	1	0	5.382766	-0.962252	1.045735
161	1	0	2.293916	-0.807809	3.598429	217	1	0	7.814022	-2.078332	1.054187
162	1	0	4.350323	-2.528233	3.851225	218	1	0	10.003890	0.277291	0.370251
163	1	0	2.200763	-6.500736	-0.607527	219	1	0	10.535973	0.630225	1.999744
164	1	0	1.620349	3.061083	3.183579	220	1	0	10.396776	-1.033550	1.461798
165	1	0	5.495629	1.347261	1.693616	221	1	0	9.095161	-1.490381	3.493684
166	1	0	-2.940920	-3.081584	3.069213	222	1	0	9.191533	0.195474	3.973083
167	1	0	-5.160528	0.780285	2.627487	223	1	0	7.637328	-0.612893	3.901440
168	1	0	-0.137415	1.143561	-0.532341	224	1	0	7.459055	3.287722	1.987712
169	1	0	-1.897297	-2.426348	-1.541804	225	1	0	8.149907	2.444852	3.367801
170	1	0	-1.503105	-3.386272	1.058860	226	1	0	9.127842	2.739949	1.934380
171	1	0	-5.940442	-0.905801	-1.539140	227	1	0	5.778261	1.461330	-0.819729
172	1	0	-6.852214	-1.617056	-3.529566	228	6	0	-3.093129	-0.866507	-0.562303
173	1	0	-5.611232	-2.860504	-3.621266	229	1	0	-2.836745	-0.047256	0.090744

230	1	0	-3.372746	-0.466260	-1.521448
231	1	0	-0.951326	-1.346913	-0.503102
232	7	0	-3.411573	-2.685709	0.879851
233	8	0	-4.034777	-3.330485	1.958440

(*5S*)-4b + borneol (*top*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.813237	-3.991161	2.405304
2	6	0	-4.082040	-2.708064	3.239587
3	6	0	-3.110018	-2.621557	4.407972
4	6	0	-1.671991	-2.701404	3.906201
5	6	0	-1.463488	-3.854223	2.909381
6	6	0	-0.295469	-4.782266	3.276013
7	6	0	-5.236489	-3.196767	-2.339460
8	6	0	-6.163232	-4.115745	-1.559045
9	6	0	-5.747561	-4.103175	-0.111400
10	6	0	-4.279465	-4.484551	0.068994
11	6	0	-3.386603	-4.421091	-1.182937
12	6	0	-3.006791	-5.827115	-1.636710
13	6	0	-6.916800	1.805284	-1.331578
14	6	0	-7.006283	0.840652	-0.174446
15	6	0	-5.922974	-0.218560	-0.288356
16	6	0	-6.134291	-0.990627	-1.591021
17	6	0	-6.121257	-0.006699	-2.772844
18	6	0	-6.655614	-0.525944	-4.109000
19	6	0	-2.769386	4.936149	0.035111
20	6	0	-3.743070	3.958580	0.694631
21	6	0	-5.202010	4.174820	0.289273
22	6	0	-5.658372	3.906784	-1.147819
23	6	0	-4.896306	4.528606	-2.324545
24	6	0	-5.054431	6.058834	-2.427296
25	6	0	2.124748	5.847130	0.246894
26	6	0	1.553703	6.868504	1.224038
27	6	0	0.200151	6.369055	1.714035
28	6	0	-0.674623	6.017316	0.528253
29	6	0	-0.010494	5.059415	-0.444000
30	6	0	-0.943540	4.846535	-1.623481
31	6	0	3.898990	1.104959	2.184288
32	6	0	3.876146	2.264766	3.184720
33	6	0	2.974111	3.391266	2.725428
34	6	0	3.302834	3.832800	1.314935
35	6	0	3.324474	2.614068	0.404941
36	6	0	3.685241	2.892858	-1.049212
37	6	0	-1.058689	-0.330392	3.801834
38	6	0	-0.979574	0.765843	2.747947
39	6	0	0.278660	0.642400	1.887509
40	6	0	1.499519	0.461829	2.793419
41	6	0	1.285342	-0.823997	3.576860
42	6	0	2.433816	-1.306449	4.439831
43	8	0	-4.068175	-1.497719	2.476164
44	8	0	-3.432806	-3.713778	5.277672
45	8	0	-1.420278	-1.513319	3.114062
46	8	0	-2.642334	-4.682278	2.821693
47	8	0	-7.546511	-3.697687	-1.575919
48	8	0	-6.517212	-5.064282	0.644003
49	8	0	-3.692338	-3.605039	1.050400
50	8	0	-3.979748	-3.844362	-2.391742
51	8	0	-6.879345	1.558126	1.058075
52	8	0	-6.103073	-1.051903	0.862919
53	8	0	-5.037285	-1.931178	-1.701021
54	8	0	-7.080307	1.054485	-2.522466
55	8	0	-5.877589	-1.573026	-4.719335
56	8	0	-3.318845	2.599495	0.509920
57	8	0	-5.500742	5.571896	0.546404
58	8	0	-5.664099	2.469430	-1.333868
59	8	0	-2.094609	4.209446	-0.999181
60	8	0	-3.735597	6.663203	-2.270400
61	8	0	2.510128	7.039175	2.266209
62	8	0	-0.424855	7.418853	2.465440
63	8	0	-1.842583	5.351214	1.049254
64	8	0	1.263881	5.612829	-0.873442
65	8	0	-0.447826	4.006079	-2.607632
66	8	0	3.424747	1.910728	4.505999
67	8	0	3.145245	4.536466	3.583161
68	8	0	2.173984	4.636742	0.975427
69	8	0	4.311331	1.695036	0.948885
70	8	0	2.495861	3.209428	-1.810823
71	8	0	-2.167847	0.637913	1.971971
72	8	0	0.388185	1.852277	1.122123
73	8	0	2.703527	0.360108	1.978146
74	8	0	0.176711	-0.519471	4.467674
75	8	0	2.224352	-2.673704	4.833525
76	7	0	0.394358	-5.207915	2.045776
77	8	0	-2.210362	-5.752766	-2.838262
78	6	0	1.826236	-4.712749	0.132937
79	6	0	2.418651	-6.104540	-0.209132
80	6	0	1.695261	-6.499567	-1.532476
81	6	0	0.481102	-5.604055	-1.534263
82	7	0	0.567023	-4.700271	-0.650822
83	8	0	-0.318372	-3.643408	-0.385672
84	6	0	5.728031	-1.974328	1.263003
85	6	0	6.472921	-0.966340	0.370151
86	6	0	7.891123	-0.687798	0.903806
87	6	0	8.662782	0.367399	0.081671
88	6	0	9.058806	-0.128209	-1.322939
89	6	0	9.781810	0.942179	-2.169289
90	6	0	11.133116	1.426503	-1.597339
91	6	0	12.191679	0.319581	-1.405453
92	6	0	12.609837	-0.369964	-2.718576
93	6	0	13.749044	-1.385384	-2.504940
94	6	0	14.170899	-2.084762	-3.811062
95	1	0	-4.618359	-4.692983	2.535990
96	1	0	-5.076081	-2.786148	3.648655
97	1	0	-3.270055	-1.670869	4.900067
98	1	0	-0.966166	-2.733639	4.725207
99	1	0	-1.274692	-3.411746	1.945205
100	1	0	-0.684897	-5.642708	3.797320
101	1	0	0.423784	-4.269330	3.890506

102	1	0	-5.550756	-3.046878	-3.352126	158	1	0	2.956779	4.288008	4.499171
103	1	0	-6.068844	-5.112286	-1.971799	159	1	0	3.086413	6.152615	-0.131426
104	1	0	-5.890418	-3.110056	0.269932	160	1	0	-2.494307	1.457331	1.541941
105	1	0	-4.274074	-5.499140	0.446113	161	1	0	0.233572	1.710947	0.161405
106	1	0	-2.496785	-3.870629	-0.940629	162	1	0	2.337207	-3.235034	4.047168
107	1	0	-3.896831	-6.418643	-1.816959	163	1	0	-0.168553	-5.708508	1.391144
108	1	0	-2.406835	-6.314241	-0.883595	164	1	0	2.156454	-6.808521	0.569147
109	1	0	-7.726209	2.517993	-1.310890	165	1	0	3.487452	-6.035412	-0.293790
110	1	0	-7.968303	0.347017	-0.226274	166	1	0	1.423831	-7.545598	-1.562095
111	1	0	-4.956240	0.264265	-0.287000	167	1	0	-0.377331	-5.662873	-2.178437
112	1	0	-7.069710	-1.520313	-1.536637	168	1	0	2.306048	-6.284393	-2.402781
113	1	0	-5.127801	0.403183	-2.869926	169	1	0	-2.606099	-5.071294	-3.403255
114	1	0	-6.746085	0.325995	-4.769002	170	1	0	5.690170	-1.617138	2.286307
115	1	0	-7.640370	-0.934553	-3.949837	171	1	0	6.232902	-2.926983	1.259174
116	1	0	-3.250190	5.793909	-0.384491	172	1	0	5.911257	-0.040671	0.322159
117	1	0	-3.684097	4.158346	1.752960	173	1	0	6.519761	-1.379320	-0.630110
118	1	0	-5.806488	3.514633	0.891742	174	1	0	7.814563	-0.338966	1.931221
119	1	0	-6.681836	4.264359	-1.180223	175	1	0	8.460969	-1.612878	0.925307
120	1	0	-5.296550	4.056439	-3.212783	176	1	0	8.053182	1.262403	-0.010852
121	1	0	-5.711118	6.426921	-1.655554	177	1	0	9.558235	0.642587	0.628167
122	1	0	-5.454934	6.327081	-3.397208	178	1	0	9.683725	-1.009949	-1.226528
123	1	0	2.147438	4.112768	-1.677772	179	1	0	8.166558	-0.432500	-1.859068
124	1	0	1.425898	7.823545	0.741736	180	1	0	9.125155	1.802370	-2.270837
125	1	0	0.340120	5.480941	2.310217	181	1	0	9.937121	0.551291	-3.169138
126	1	0	-0.954645	6.934256	0.020985	182	1	0	11.538825	2.177360	-2.270153
127	1	0	0.150003	4.120602	0.053977	183	1	0	10.964874	1.920889	-0.646523
128	1	0	-1.250151	5.768847	-2.082954	184	1	0	13.073679	0.765960	-0.954089
129	1	0	-3.848841	4.292383	-2.269890	185	1	0	11.827043	-0.427339	-0.708004
130	1	0	4.679720	0.412585	2.442591	186	1	0	12.932299	0.384566	-3.431337
131	1	0	4.889695	2.645048	3.216467	187	1	0	11.759013	-0.883291	-3.154028
132	1	0	1.944819	3.081442	2.705067	188	1	0	13.431032	-2.135362	-1.785613
133	1	0	4.229902	4.390981	1.289187	189	1	0	14.609081	-0.875688	-2.079231
134	1	0	2.356042	2.158581	0.454236	190	1	0	13.312536	-2.596233	-4.235982
135	1	0	4.087248	1.988008	-1.473057	191	1	0	14.488271	-1.336245	-4.530768
136	1	0	4.423801	3.678991	-1.144252	192	6	0	0.359736	0.435615	-2.337133
137	1	0	-1.777334	-0.080014	4.564062	193	6	0	-1.081907	-0.088732	-2.534572
138	1	0	-0.920805	1.723456	3.251918	194	6	0	-0.266001	0.119218	-4.660718
139	1	0	0.179474	-0.220978	1.245786	195	6	0	0.904689	0.631461	-3.786643
140	1	0	1.588020	1.263576	3.495627	196	6	0	-0.867632	-1.015411	-3.778840
141	1	0	1.012585	-1.618380	2.903557	197	6	0	-1.915192	1.064633	-3.141319
142	1	0	2.477397	-0.708975	5.335476	198	6	0	-1.354891	1.222639	-4.593818
143	1	0	3.357613	-1.206490	3.884696	199	6	0	0.089532	-2.200310	-3.525935
144	1	0	-3.177307	-1.160774	2.259496	200	6	0	-2.169699	-1.604633	-4.345507
145	1	0	-2.908318	-3.685871	6.088641	201	6	0	-1.695143	-0.710624	-1.285117
146	1	0	-7.962288	-3.893857	-2.426116	202	8	0	0.396034	1.673120	-1.563825
147	1	0	-7.450147	-4.812535	0.596642	203	1	0	0.940497	-0.296245	-1.793809
148	1	0	-6.655457	0.904218	1.738502	204	1	0	1.121620	1.674511	-3.973405
149	1	0	-5.271009	-1.229860	1.370479	205	1	0	1.812964	0.065313	-3.944340
150	1	0	-4.990145	-1.266480	-4.943579	206	1	0	-2.960030	0.788738	-3.149364
151	1	0	-2.989801	2.499703	-0.395104	207	1	0	-1.827899	1.975139	-2.577423
152	1	0	-5.803935	5.707282	1.452905	208	1	0	-2.125784	1.071029	-5.338437
153	1	0	-3.803670	7.626449	-2.312405	209	1	0	-0.933682	2.207789	-4.742368
154	1	0	2.630576	6.218003	2.777966	210	1	0	0.021342	-0.169650	-5.661929
155	1	0	-1.290755	7.108387	2.765589	211	1	0	1.105293	-1.886467	-3.326698
156	1	0	-0.258836	3.113358	-2.253509	212	1	0	-0.251136	-2.779803	-2.676744
157	1	0	4.096539	1.433992	5.010348	213	1	0	0.115780	-2.839630	-4.403568

214	1	0	-1.953651	-2.123146	-5.275637
215	1	0	-2.607557	-2.308890	-3.650528
216	1	0	-2.902249	-0.838659	-4.557375
217	1	0	-1.783724	0.018848	-0.488044
218	1	0	-2.687931	-1.094220	-1.488781
219	1	0	-1.090356	-1.530328	-0.918497
220	1	0	1.266204	2.140290	-1.679158
221	6	0	15.311290	-3.095939	-3.583855
222	1	0	15.004621	-3.864870	-2.882575
223	1	0	15.595985	-3.578833	-4.512232
224	1	0	16.186381	-2.598713	-3.178763
225	6	0	2.634861	-3.499619	-0.332276
226	1	0	2.789436	-3.595864	-1.401504
227	1	0	2.038404	-2.620839	-0.153524
228	6	0	4.013461	-3.417474	0.296520
229	7	0	4.364819	-2.216165	0.780357
230	1	0	3.678392	-1.500988	0.917180
231	8	0	4.776544	-4.379229	0.267169
232	6	0	1.449673	-4.524384	1.595905
233	8	0	2.123857	-3.768374	2.295243

(*5S*)-4b + borneol (*bottom*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.754901	-5.069840	1.400197
2	6	0	-1.413021	-5.118681	2.805177
3	6	0	-0.509870	-4.549409	3.895698
4	6	0	0.215435	-3.318393	3.394140
5	6	0	1.057573	-3.665177	2.156836
6	6	0	2.518781	-3.896709	2.504849
7	6	0	-4.528944	-3.849644	-2.054176
8	6	0	-4.357207	-5.121621	-1.239329
9	6	0	-3.493740	-4.810053	-0.038183
10	6	0	-2.123010	-4.335578	-0.494354
11	6	0	-2.341924	-3.073499	-1.326342
12	6	0	-1.109930	-2.491632	-1.974072
13	6	0	-8.332342	-0.776730	0.053157
14	6	0	-8.090657	-2.086378	0.765756
15	6	0	-6.690209	-2.548570	0.434857
16	6	0	-6.499892	-2.700574	-1.068520
17	6	0	-6.964518	-1.455641	-1.821261
18	6	0	-7.146328	-1.672886	-3.318346
19	6	0	-4.787972	2.441596	-1.077422
20	6	0	-4.939303	2.077060	0.406363
21	6	0	-6.352537	2.174998	1.007915
22	6	0	-7.567123	1.549048	0.303612
23	6	0	-7.910544	1.924582	-1.151745
24	6	0	-8.359345	3.371919	-1.380078
25	6	0	-0.681402	2.201124	-3.869130
26	6	0	-0.886106	3.702472	-3.754090
27	6	0	-1.741891	3.975089	-2.518198
28	6	0	-2.992668	3.119038	-2.528701
29	6	0	-2.728714	1.661061	-2.841036
30	6	0	-4.054656	0.962625	-3.034982
31	6	0	2.499042	0.705823	0.203159
32	6	0	2.387756	2.204483	0.000034
33	6	0	1.170470	2.488682	-0.855724
34	6	0	1.183874	1.744080	-2.194715
35	6	0	1.547680	0.278142	-1.967818
36	6	0	1.892752	-0.523414	-3.208016
37	6	0	-0.966089	-1.158130	3.722955
38	6	0	-1.708345	-0.208538	2.809226
39	6	0	-0.883295	0.043269	1.550296
40	6	0	0.557476	0.451838	1.859736
41	6	0	1.194264	-0.391076	2.958544
42	6	0	2.495929	0.169233	3.549407
43	8	0	-2.680595	-4.449671	2.815215
44	8	0	0.466549	-5.547473	4.257482
45	8	0	-0.792985	-2.364725	2.982183
46	8	0	0.639288	-4.905371	1.541557
47	8	0	-5.634802	-5.602926	-0.760140
48	8	0	-3.441918	-5.998510	0.774422
49	8	0	-1.306030	-3.992472	0.642517
50	8	0	-3.220229	-3.434949	-2.425680
51	8	0	-8.233166	-1.904593	2.174966
52	8	0	-6.454734	-3.775285	1.150058
53	8	0	-5.070668	-2.828480	-1.234549
54	8	0	-8.279497	-1.061168	-1.345537
55	8	0	-5.957636	-2.180800	-3.931219
56	8	0	-4.328433	0.782964	0.636282
57	8	0	-6.666320	3.574825	1.188112
58	8	0	-7.306964	0.129240	0.417094
59	8	0	-4.787053	1.185283	-1.782994
60	8	0	-7.296320	4.330395	-1.230203
61	8	0	0.401542	4.320464	-3.693924
62	8	0	-2.097239	5.368800	-2.527404
63	8	0	-3.538363	3.130140	-1.188869
64	8	0	-1.941502	1.556468	-4.038025
65	8	0	-3.957518	-0.405706	-3.240179
66	8	0	2.187821	2.947278	1.227360
67	8	0	1.141647	3.912131	-1.128434
68	8	0	-0.179944	1.728678	-2.622988
69	8	0	2.731656	0.213283	-1.124375
70	8	0	0.690987	-0.530079	-4.029464
71	8	0	-2.949041	-0.849425	2.495997
72	8	0	-1.445233	1.139225	0.792283
73	8	0	1.290206	0.118283	0.641720
74	8	0	0.285835	-0.588805	4.069634
75	8	0	3.494845	-0.849308	3.712065
76	7	0	3.276793	-4.065283	1.262950
77	8	0	-1.510732	-1.195777	-2.490633
78	6	0	4.584719	-3.369030	-0.653927
79	6	0	5.706483	-4.437198	-0.560833
80	6	0	5.400479	-5.421462	-1.732436
81	6	0	3.969637	-5.092415	-2.074292
82	7	0	3.560601	-4.037836	-1.505890
83	8	0	2.331239	-3.408259	-1.641014
84	6	0	6.796111	1.002785	-0.206569
85	6	0	8.014302	1.164887	-1.131205
86	6	0	9.029299	2.169302	-0.554917

87	6	0	10.254962	2.395243	-1.466906	143	1	0	2.715847	-0.063844	-3.740846
88	6	0	11.183678	1.167854	-1.547286	144	1	0	-1.496559	-1.333020	4.643224
89	6	0	12.373621	1.362482	-2.511887	145	1	0	-1.849248	0.728442	3.335642
90	6	0	13.350920	2.495230	-2.125305	146	1	0	-0.871257	-0.870688	0.980400
91	6	0	14.011368	2.338629	-0.738973	147	1	0	0.602360	1.505758	2.061186
92	6	0	14.889573	1.078817	-0.611523	148	1	0	1.420898	-1.328147	2.500349
93	6	0	15.623695	1.016207	0.741859	149	1	0	2.270152	0.547505	4.532430
94	6	0	16.500351	-0.242739	0.881750	150	1	0	2.858567	0.990863	2.944916
95	6	0	17.229704	-0.292283	2.238282	151	1	0	-2.551624	-3.511917	2.580711
96	6	0	4.943047	-2.079435	-1.373893	152	1	0	0.662083	-5.515731	5.202624
97	6	0	6.016186	-1.266988	-0.679019	153	1	0	-5.442741	-6.359988	-0.182705
98	7	0	5.811151	0.060955	-0.745596	154	1	0	-3.452660	-5.685019	1.697438
99	8	0	7.017481	-1.765289	-0.179235	155	1	0	-7.774647	-2.638303	2.611744
100	6	0	3.931794	-3.056961	0.690644	156	1	0	-6.277882	-4.502201	0.527922
101	8	0	4.082653	-1.947377	1.204855	157	1	0	-5.204527	-1.572625	-3.778072
102	1	0	-0.902890	-6.001229	0.885542	158	1	0	-4.599075	0.205268	-0.097198
103	1	0	-1.600106	-6.148481	3.060983	159	1	0	-5.971188	4.047028	1.689374
104	1	0	-1.150683	-4.295790	4.729568	160	1	0	-7.040649	4.312243	-0.286539
105	1	0	0.834359	-2.883385	4.164564	161	1	0	0.700062	4.402544	-2.770502
106	1	0	0.950714	-2.882486	1.426887	162	1	0	-2.587015	5.576030	-1.721133
107	1	0	2.575250	-4.799955	3.090047	163	1	0	-3.098980	-0.810661	-2.944319
108	1	0	2.923876	-3.064805	3.054311	164	1	0	3.023457	3.166752	1.658920
109	1	0	-5.095494	-3.966315	-2.955145	165	1	0	1.081806	4.395002	-0.293723
110	1	0	-3.890135	-5.873051	-1.860723	166	1	0	-0.049136	1.922831	-4.690728
111	1	0	-3.972471	-4.023197	0.518355	167	1	0	-3.556156	-0.264751	2.007216
112	1	0	-1.635532	-5.102063	-1.085575	168	1	0	-2.380946	0.995687	0.564487
113	1	0	-2.806975	-2.324252	-0.708808	169	1	0	3.831975	-1.155521	2.850627
114	1	0	-0.789902	-3.144084	-2.774426	170	1	0	3.005208	-4.855472	0.715981
115	1	0	-0.314730	-2.391502	-1.251737	171	1	0	5.627260	-4.961900	0.379954
116	1	0	-9.309649	-0.371684	0.260597	172	1	0	6.668194	-3.961947	-0.622922
117	1	0	-8.808774	-2.802536	0.384621	173	1	0	5.518577	-6.456023	-1.440851
118	1	0	-5.999674	-1.803739	0.790294	174	1	0	3.332626	-5.628239	-2.742649
119	1	0	-7.012145	-3.583845	-1.423283	175	1	0	6.036988	-5.236274	-2.590821
120	1	0	-6.253215	-0.673540	-1.641532	176	1	0	-0.836441	-0.810715	-3.085355
121	1	0	-7.466793	-0.736251	-3.761204	177	1	0	6.302049	1.957495	-0.071321
122	1	0	-7.928053	-2.401245	-3.473161	178	1	0	7.124466	0.642886	0.759271
123	1	0	-5.569347	3.083242	-1.433222	179	1	0	7.677641	1.502261	-2.106528
124	1	0	-4.340033	2.789443	0.943243	180	1	0	8.467227	0.189918	-1.245148
125	1	0	-6.301612	1.678453	1.966871	181	1	0	8.529767	3.122417	-0.398963
126	1	0	-8.416807	1.800111	0.929803	182	1	0	9.367966	1.822223	0.417577
127	1	0	-8.725914	1.280678	-1.451823	183	1	0	9.914778	2.656277	-2.465638
128	1	0	-9.186064	3.608811	-0.716067	184	1	0	10.814576	3.242915	-1.087225
129	1	0	-8.713817	3.466727	-2.395805	185	1	0	11.546419	0.930260	-0.552760
130	1	0	0.798096	-1.081064	-4.815042	186	1	0	10.613680	0.309719	-1.885890
131	1	0	-1.399459	4.067459	-4.629148	187	1	0	11.982315	1.571998	-3.504044
132	1	0	-1.178249	3.727989	-1.639324	188	1	0	12.920534	0.428593	-2.585052
133	1	0	-3.697759	3.549948	-3.230909	189	1	0	14.134895	2.540622	-2.876544
134	1	0	-2.209763	1.212329	-2.016701	190	1	0	12.831224	3.446731	-2.162077
135	1	0	-4.614718	1.401581	-3.842925	191	1	0	14.631966	3.211807	-0.556461
136	1	0	-7.083203	1.674035	-1.793359	192	1	0	13.252018	2.326699	0.035991
137	1	0	3.343857	0.393032	0.786807	193	1	0	15.620729	1.070252	-1.415688
138	1	0	3.276575	2.548955	-0.510922	194	1	0	14.278265	0.189225	-0.720831
139	1	0	0.279350	2.184485	-0.333770	195	1	0	14.893990	1.033691	1.547002
140	1	0	1.831810	2.242597	-2.900385	196	1	0	16.246979	1.899248	0.853363
141	1	0	0.721472	-0.178472	-1.462342	197	1	0	15.877823	-1.125643	0.772693
142	1	0	2.147422	-1.526380	-2.898769	198	1	0	17.229468	-0.261588	0.077370

199	1	0	16.515484	-0.295789	3.054965
200	1	0	17.841880	-1.183696	2.320410
201	1	0	17.873865	0.572711	2.356408
202	1	0	5.320131	-2.333466	-2.359974
203	1	0	4.041901	-1.504247	-1.471967
204	1	0	4.944898	0.391981	-1.114654
205	6	0	-3.002683	4.507979	3.661729
206	6	0	-1.479333	4.768296	3.511686
207	6	0	-2.419940	6.350597	2.172344
208	6	0	-3.639092	5.633928	2.802459
209	6	0	-1.413820	6.316637	3.367514
210	6	0	-1.092970	4.281228	2.096332
211	6	0	-1.793731	5.337468	1.175236
212	6	0	-1.873674	7.071329	4.631091
213	6	0	-0.015532	6.849905	3.011469
214	6	0	-2.747823	7.710105	1.562059
215	8	0	-4.539843	5.053422	1.815014
216	1	0	-3.281577	3.543840	3.262202
217	1	0	-3.331711	4.563019	4.690202
218	1	0	-4.214781	6.322826	3.403806
219	1	0	-0.019456	4.276802	1.962252
220	1	0	-1.088138	5.834141	0.520166
221	1	0	-2.547615	4.868370	0.562265
222	1	0	-0.881544	4.353507	4.310769
223	1	0	-1.142146	6.926717	5.419535
224	1	0	-1.937690	8.135936	4.432641
225	1	0	-2.830133	6.740756	5.009104
226	1	0	-0.041209	7.929922	2.912244
227	1	0	0.679274	6.607674	3.809590
228	1	0	0.371675	6.438336	2.091930
229	1	0	-1.855696	8.176233	1.160596
230	1	0	-3.453812	7.609215	0.740932
231	1	0	-3.184640	8.378091	2.296696
232	1	0	-4.735011	5.687415	1.110871
233	1	0	-1.441882	3.281529	1.887970

(*5S*)-4a + borneol (*top*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.442585	-3.448915	-0.788386
2	6	0	-5.024814	-4.922484	-0.508982
3	6	0	-4.294840	-5.501936	-1.732993
4	6	0	-3.176050	-4.580908	-2.234172
5	6	0	-3.739910	-3.155890	-2.431114
6	6	0	-3.637280	-2.583120	-3.835916
7	6	0	-5.086132	0.196206	3.062484
8	6	0	-5.524671	-1.220913	3.404476
9	6	0	-4.989533	-2.178568	2.350576
10	6	0	-5.372936	-1.693805	0.952815
11	6	0	-4.932052	-0.268861	0.672619
12	6	0	-5.555597	0.394285	-0.555826
13	6	0	-0.317462	2.433232	4.071266
14	6	0	-0.998649	1.757500	5.251519
15	6	0	-1.947292	0.697994	4.719365
16	6	0	-2.977030	1.305491	3.799109
17	6	0	-2.325001	2.113113	2.684366
18	6	0	-3.299133	3.051644	1.995351
19	6	0	3.878711	1.859028	2.391732
20	6	0	2.972909	3.042522	2.655729
21	6	0	1.688896	2.801285	1.872220
22	6	0	1.045155	1.438576	2.187435
23	6	0	2.054028	0.288750	2.226525
24	6	0	2.355120	-0.307093	0.849683
25	6	0	7.234167	-1.193366	1.477584
26	6	0	7.115157	-1.173224	2.992587
27	6	0	5.925200	-0.291305	3.338001
28	6	0	6.190737	1.111780	2.787627
29	6	0	6.533524	1.126128	1.294878
30	6	0	7.182846	2.429873	0.877114
31	6	0	3.845316	-4.746777	-0.842874
32	6	0	4.188144	-4.855159	0.631288
33	6	0	4.511039	-3.475286	1.173016
34	6	0	5.739971	-2.936658	0.466987
35	6	0	5.443039	-2.854960	-1.035910
36	6	0	6.706419	-2.669752	-1.886840
37	6	0	-1.324957	-5.577674	-0.969424
38	6	0	-0.609483	-5.254926	0.343794
39	6	0	0.435348	-4.187390	0.092392
40	6	0	1.396053	-4.774908	-0.933015
41	6	0	0.618622	-4.810856	-2.244220
42	6	0	1.434033	-5.215145	-3.460794
43	8	0	-4.289776	-5.064932	0.703955
44	8	0	-5.208277	-5.724275	-2.817528
45	8	0	-2.131490	-4.455586	-1.241884
46	8	0	-5.163731	-3.181772	-2.166039
47	8	0	-5.098239	-1.523691	4.729741
48	8	0	-5.592468	-3.454986	2.553519
49	8	0	-4.702579	-2.581732	0.029870
50	8	0	-5.445807	0.570084	1.746467
51	8	0	-0.033704	1.124830	6.104714
52	8	0	-2.678680	0.072191	5.786608
53	8	0	-3.669181	0.197490	3.204664
54	8	0	-1.294099	2.996955	3.207084
55	8	0	-2.611374	3.807140	0.979924
56	8	0	2.646589	3.151565	4.042840
57	8	0	2.159627	2.804027	0.516043
58	8	0	0.393800	1.361476	3.468786
59	8	0	3.257831	0.682589	2.914210
60	8	0	1.426029	-1.393299	0.628599
61	8	0	7.034401	-2.506708	3.468915
62	8	0	5.790339	-0.199442	4.760386
63	8	0	5.101633	2.041941	3.064902
64	8	0	7.521830	0.105912	0.986212
65	8	0	7.521996	2.388851	-0.520929
66	8	0	3.147822	-5.458839	1.395349
67	8	0	4.758955	-3.584829	2.584621
68	8	0	5.966834	-1.585661	0.901137
69	8	0	4.859234	-4.084414	-1.563129

70	8	0	7.698040	-1.847171	-1.263313	126	1	0	0.313521	1.229289	1.417342
71	8	0	-1.599949	-4.799249	1.265157	127	1	0	1.625032	-0.495324	2.823902
72	8	0	1.071767	-3.847999	1.335202	128	1	0	3.356900	-0.706415	0.861217
73	8	0	2.618184	-4.009927	-1.015505	129	1	0	2.260957	0.421725	0.063272
74	8	0	-0.394765	-5.825686	-2.031064	130	1	0	8.015302	-1.844808	1.137851
75	8	0	2.312170	-4.129458	-3.842415	131	1	0	8.018095	-0.743543	3.398100
76	7	0	-2.287890	-2.075340	-4.119886	132	1	0	5.045023	-0.713713	2.898990
77	8	0	-5.245794	-0.216054	-1.809631	133	1	0	7.017478	1.513665	3.354374
78	6	0	1.879754	-1.467911	-2.517144	134	1	0	5.667917	0.933416	0.687208
79	7	0	0.756162	-0.920055	-2.341258	135	1	0	8.063436	2.595723	1.485376
80	8	0	-0.219800	-1.231404	-1.372705	136	1	0	6.498494	3.247953	1.008970
81	6	0	1.797496	0.418703	-3.971514	137	1	0	3.741611	-5.724887	-1.284999
82	6	0	0.421990	0.171909	-3.274722	138	1	0	5.058462	-5.487206	0.728724
83	6	0	2.609148	-0.880015	-3.689739	139	1	0	3.673371	-2.821327	0.993596
84	8	0	0.953273	1.756562	-1.595162	140	1	0	6.595562	-3.562202	0.677750
85	6	0	0.080505	1.386906	-2.389594	141	1	0	4.746598	-2.039772	-1.165987
86	7	0	-1.054954	2.012963	-2.600298	142	1	0	6.431940	-2.303991	-2.869028
87	6	0	-1.359129	3.318250	-1.976509	143	1	0	7.154453	-3.642491	-1.999888
88	6	0	-2.499193	3.987154	-2.759662	144	1	0	-1.899433	-6.481661	-0.884092
89	6	0	-3.864516	3.322906	-2.485854	145	1	0	-0.123214	-6.149154	0.713965
90	6	0	-4.958587	3.804376	-3.457912	146	1	0	-0.038304	-3.309628	-0.314697
91	6	0	-6.326367	3.133483	-3.198643	147	1	0	1.647606	-5.790829	-0.664316
92	6	0	-7.064595	3.726075	-1.981389	148	1	0	0.152846	-3.854389	-2.428084
93	6	0	-8.444920	3.077240	-1.762309	149	1	0	0.767514	-5.388724	-4.290053
94	6	0	-9.183555	3.659992	-0.541807	150	1	0	1.978667	-6.131010	-3.268210
95	6	0	-10.566572	3.011762	-0.333743	151	1	0	-3.384657	-4.701104	0.676716
96	6	0	-11.304411	3.518335	0.923413	152	1	0	-5.650270	-4.884307	-3.007744
97	6	0	-11.752484	4.989888	0.827189	153	1	0	-4.218326	-1.151919	4.909310
98	6	0	-12.542462	5.429143	2.075772	154	1	0	-5.118696	-4.140915	2.043510
99	6	0	-0.610102	-0.328479	-4.293488	155	1	0	0.674935	0.774638	5.543570
100	6	0	-1.936830	-0.841299	-3.752604	156	1	0	-2.064250	-0.192971	6.486779
101	8	0	-2.698290	-0.098224	-3.126912	157	1	0	-1.880095	4.276661	1.405716
102	1	0	-6.501891	-3.299148	-0.668738	158	1	0	3.439479	3.002653	4.576703
103	1	0	-5.918176	-5.513625	-0.383220	159	1	0	1.521255	2.568426	-0.185743
104	1	0	-3.910464	-6.470442	-1.463671	160	1	0	0.722622	-1.217779	-0.058002
105	1	0	-2.767062	-4.991902	-3.146744	161	1	0	6.152698	-2.892382	3.309530
106	1	0	-3.259885	-2.506714	-1.723984	162	1	0	4.919174	0.174221	4.953376
107	1	0	-4.333300	-1.761312	-3.883810	163	1	0	8.169676	1.684903	-0.663217
108	1	0	-3.897500	-3.320308	-4.581969	164	1	0	2.358973	-4.864449	1.475472
109	1	0	-5.537536	0.915833	3.726520	165	1	0	4.206357	-4.289112	2.956464
110	1	0	-6.602071	-1.277980	3.392731	166	1	0	7.372760	-0.965406	-1.036821
111	1	0	-3.909868	-2.212964	2.415987	167	1	0	-1.169444	-4.422192	2.045635
112	1	0	-6.446348	-1.782157	0.844417	168	1	0	1.285155	-2.873704	1.284237
113	1	0	-3.853152	-0.230137	0.649973	169	1	0	3.107838	-4.123269	-3.293443
114	1	0	-5.268145	1.436505	-0.533377	170	1	0	-1.640317	-2.662803	-4.597041
115	1	0	-6.627548	0.348025	-0.445758	171	1	0	-4.316075	-0.123722	-2.066335
116	1	0	0.354858	3.218323	4.355113	172	1	0	2.206999	-2.274519	-1.898765
117	1	0	-1.536047	2.481994	5.842787	173	1	0	3.643034	-0.666561	-3.457938
118	1	0	-1.378521	-0.031640	4.166262	174	1	0	2.575923	-1.602904	-4.496281
119	1	0	-3.655835	1.912807	4.385816	175	1	0	1.686630	0.620976	-5.025723
120	1	0	-1.893732	1.426476	1.974051	176	1	0	2.284414	1.246794	-3.485305
121	1	0	-3.722332	3.716123	2.739592	177	1	0	-1.821059	1.491616	-2.989114
122	1	0	-4.086780	2.496151	1.521156	178	1	0	-1.649711	3.198073	-0.943606
123	1	0	4.012152	1.768595	1.333397	179	1	0	-0.458668	3.915214	-2.022801
124	1	0	3.444978	3.937560	2.278414	180	1	0	-2.552500	5.030865	-2.469823
125	1	0	0.975119	3.591085	2.054583	181	1	0	-2.265292	3.952429	-3.819334

182	1	0	-4.136022	3.538621	-1.459223
183	1	0	-3.786316	2.245896	-2.582129
184	1	0	-5.063551	4.884032	-3.392568
185	1	0	-4.637481	3.575539	-4.470765
186	1	0	-6.955768	3.262126	-4.074810
187	1	0	-6.181700	2.066280	-3.055796
188	1	0	-6.466459	3.596310	-1.085629
189	1	0	-7.193273	4.794882	-2.130574
190	1	0	-9.052604	3.221634	-2.651669
191	1	0	-8.320012	2.006715	-1.629095
192	1	0	-8.580241	3.503168	0.348438
193	1	0	-9.292688	4.731070	-0.674833
194	1	0	-11.184498	3.192804	-1.209218
195	1	0	-10.434483	1.936377	-0.253387
196	1	0	-12.183623	2.901522	1.087931
197	1	0	-10.661642	3.394728	1.790875
198	1	0	-10.887849	5.632692	0.708524
199	1	0	-12.372405	5.114991	-0.055719
200	1	0	-13.429962	4.817679	2.200407
201	1	0	-11.933430	5.325784	2.967774
202	1	0	-12.853438	6.465171	1.996780
203	1	0	-0.848594	0.496626	-4.955638
204	1	0	-0.129798	-1.094912	-4.885675
205	6	0	6.602181	5.311798	-2.235500
206	6	0	5.175183	5.700203	-1.760316
207	6	0	4.852812	4.950504	-3.883498
208	6	0	6.371662	4.743207	-3.676549
209	6	0	4.279877	4.637568	-2.470421
210	6	0	4.806819	6.980771	-2.538249
211	6	0	4.641248	6.482713	-4.008008
212	6	0	2.761897	4.878692	-2.349748
213	6	0	4.538069	3.189892	-2.008025
214	6	0	5.047735	5.875825	-0.253674
215	8	0	5.851334	7.958090	-2.355457
216	1	0	7.230697	6.186898	-2.238217
217	1	0	7.038968	4.560946	-1.593680
218	1	0	6.948069	5.273667	-4.424021
219	1	0	6.638022	3.695347	-3.726803
220	1	0	3.876082	7.386926	-2.161203
221	1	0	3.665552	6.729581	-4.407298
222	1	0	5.398153	6.934448	-4.636095
223	1	0	4.424467	4.376270	-4.694175
224	1	0	2.233447	4.138834	-2.943681
225	1	0	2.452051	4.740972	-1.320500
226	1	0	2.450072	5.858480	-2.683487
227	1	0	3.974892	2.994895	-1.103601
228	1	0	4.174268	2.504822	-2.771335
229	1	0	5.577933	2.972302	-1.820431
230	1	0	5.342369	4.973059	0.266883
231	1	0	5.693105	6.686107	0.066490
232	1	0	4.027995	6.117199	0.029774
233	1	0	5.617621	8.789614	-2.788139

(*5S*)-4a + borneol (*bottom*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.268424	3.528305	2.188101
2	6	0	2.044601	4.146982	2.933225
3	6	0	1.484217	5.335401	2.134717
4	6	0	1.283860	5.100065	0.623791
5	6	0	2.306606	4.090779	0.101800
6	6	0	2.841250	4.317279	-1.304858
7	6	0	4.281401	-1.650893	2.863194
8	6	0	3.739661	-0.804120	4.015008
9	6	0	2.981556	0.382835	3.446821
10	6	0	3.839481	1.130296	2.430877
11	6	0	4.269520	0.219120	1.296555
12	6	0	5.269454	0.810992	0.303995
13	6	0	1.271034	-5.020706	0.064099
14	6	0	1.453768	-5.440999	1.516054
15	6	0	1.862599	-4.200296	2.293509
16	6	0	3.105691	-3.551919	1.726546
17	6	0	3.067176	-3.391500	0.210100
18	6	0	4.456175	-3.263613	-0.388765
19	6	0	-3.106877	-3.913404	-0.832060
20	6	0	-2.094936	-4.849939	-1.458390
21	6	0	-0.915973	-4.024577	-1.945089
22	6	0	-0.299789	-3.190373	-0.823773
23	6	0	-1.338297	-2.408901	-0.020206
24	6	0	-1.668618	-1.037384	-0.596565
25	6	0	-7.049526	-1.818763	0.282706
26	6	0	-6.469392	-2.378046	1.576886
27	6	0	-5.165375	-3.072532	1.208250
28	6	0	-5.388916	-4.124692	0.115087
29	6	0	-6.115819	-3.532305	-1.084152
30	6	0	-6.554909	-4.526047	-2.127786
31	6	0	-5.229225	2.823991	-1.647614
32	6	0	-6.248280	2.709579	-0.516793
33	6	0	-6.075067	1.352272	0.133677
34	6	0	-6.346096	0.270659	-0.877440
35	6	0	-5.390194	0.398416	-2.049690
36	6	0	-5.772370	-0.527724	-3.221538
37	6	0	-1.069596	5.593775	0.238686
38	6	0	-2.190911	5.183330	1.169376
39	6	0	-2.723359	3.836110	0.722643
40	6	0	-3.312448	4.014510	-0.673338
41	6	0	-2.196833	4.468666	-1.621997
42	6	0	-2.684510	4.978610	-2.968229
43	8	0	1.088553	3.168703	3.321711
44	8	0	2.427971	6.421738	2.271219
45	8	0	-0.041050	4.625296	0.302165
46	8	0	3.461455	4.246860	0.969557
47	8	0	2.914944	-1.623933	4.851036
48	8	0	2.656570	1.267159	4.521701
49	8	0	3.001185	2.176577	1.906263
50	8	0	4.995651	-0.887794	1.904653
51	8	0	0.219429	-5.937028	2.051050
52	8	0	2.169279	-4.491055	3.670298
53	8	0	3.121314	-2.225687	2.283433

54	8	0	2.505800	-4.555059	-0.454190	110	1	0	4.557182	-0.430648	4.612870
55	8	0	4.355078	-3.198280	-1.824386	111	1	0	2.098877	0.034036	2.934681
56	8	0	-1.658044	-5.814963	-0.491737	112	1	0	4.707139	1.550401	2.924499
57	8	0	-1.529417	-3.153674	-2.905191	113	1	0	3.389885	-0.146270	0.787355
58	8	0	0.312224	-3.990493	0.197794	114	1	0	5.641499	-0.001400	-0.310240
59	8	0	-2.505220	-3.216326	0.260989	115	1	0	6.104556	1.218653	0.852826
60	8	0	-0.557292	-0.208911	-0.191016	116	1	0	0.926770	-5.819023	-0.566483
61	8	0	-6.216845	-1.323904	2.510467	117	1	0	2.201836	-6.214303	1.597702
62	8	0	-4.614647	-3.727769	2.353414	118	1	0	1.060409	-3.490294	2.234802
63	8	0	-4.139629	-4.733652	-0.323266	119	1	0	3.970717	-4.117461	2.050952
64	8	0	-7.316528	-2.883269	-0.617034	120	1	0	2.469222	-2.525026	-0.014907
65	8	0	-6.907812	-3.723053	-3.286843	121	1	0	5.043908	-4.124572	-0.092388
66	8	0	-6.143913	3.755501	0.449658	122	1	0	4.935939	-2.366938	-0.042002
67	8	0	-7.006525	1.162824	1.221611	123	1	0	-3.459270	-3.219192	-1.569924
68	8	0	-6.033077	-0.980352	-0.253997	124	1	0	-2.554988	-5.328728	-2.311169
69	8	0	-5.399367	1.763313	-2.562663	125	1	0	-0.168989	-4.667385	-2.393863
70	8	0	-7.136449	-0.947954	-3.137147	126	1	0	0.417743	-2.490971	-1.229923
71	8	0	-1.663952	5.154760	2.494110	127	1	0	-0.897325	-2.226772	0.936741
72	8	0	-3.782225	3.457457	1.642888	128	1	0	-2.599507	-0.689782	-0.168026
73	8	0	-3.896574	2.761706	-1.098617	129	1	0	-1.751639	-1.075097	-1.670028
74	8	0	-1.598044	5.679234	-1.078146	130	1	0	-7.967975	-1.278519	0.431831
75	8	0	-3.275363	3.888186	-3.707908	131	1	0	-7.163553	-3.087345	2.003200
76	7	0	1.897851	3.881615	-2.341293	132	1	0	-4.507295	-2.308962	0.850939
77	8	0	4.730961	1.871669	-0.484919	133	1	0	-5.952535	-4.940259	0.541778
78	6	0	-2.089313	1.440762	-3.344037	134	1	0	-5.489876	-2.802088	-1.558092
79	7	0	-0.871813	1.543947	-3.024812	135	1	0	-7.408258	-5.077839	-1.760147
80	8	0	-0.334182	1.906898	-1.773884	136	1	0	-5.745319	-5.200620	-2.365825
81	6	0	-0.834959	1.289017	-5.361662	137	1	0	-5.353725	3.733323	-2.205072
82	6	0	0.096980	1.297740	-4.105656	138	1	0	-7.235279	2.779011	-0.948731
83	6	0	-2.255533	1.036309	-4.778356	139	1	0	-5.064086	1.263391	0.500026
84	8	0	-0.243168	-1.036791	-3.915670	140	1	0	-7.365955	0.295652	-1.219402
85	6	0	0.615457	-0.143283	-3.936449	141	1	0	-4.398578	0.168252	-1.692591
86	7	0	1.914212	-0.340346	-3.929974	142	1	0	-5.105002	-1.378961	-3.230468
87	6	0	2.511938	-1.684025	-4.030047	143	1	0	-5.617844	0.038781	-4.128742
88	6	0	3.772802	-1.630717	-4.908422	144	1	0	-0.704588	6.577461	0.484709
89	6	0	4.934044	-0.886888	-4.217896	145	1	0	-2.983637	5.916694	1.084670
90	6	0	6.192419	-0.828706	-5.104890	146	1	0	-1.934092	3.100175	0.734107
91	6	0	7.344948	-0.023423	-4.468281	147	1	0	-4.084702	4.770203	-0.624365
92	6	0	7.924521	-0.677853	-3.199023	148	1	0	-1.459663	3.687482	-1.699786
93	6	0	9.112312	0.117939	-2.624540	149	1	0	-1.839422	5.396640	-3.499513
94	6	0	9.686049	-0.522784	-1.345772	150	1	0	-3.398744	5.772683	-2.791910
95	6	0	10.874528	0.276819	-0.776376	151	1	0	0.676508	2.628027	2.612022
96	6	0	11.427622	-0.295088	0.545937	152	1	0	3.249811	6.153286	1.834966
97	6	0	12.125233	-1.660098	0.386054	153	1	0	2.594278	-2.400063	4.364733
98	6	0	12.718828	-2.157612	1.718751	154	1	0	2.035620	1.956733	4.211102
99	6	0	1.084866	2.467202	-4.139633	155	1	0	-0.509718	-5.556034	1.535579
100	6	0	1.981304	2.686265	-2.923976	156	1	0	1.422983	-4.959771	4.072055
101	8	0	2.844938	1.847294	-2.632158	157	1	0	3.871265	-3.984585	-2.115320
102	1	0	4.181644	3.642388	2.747927	158	1	0	-2.442632	-6.172292	-0.048935
103	1	0	2.396077	4.581307	3.855187	159	1	0	-0.929147	-2.506453	-3.325848
104	1	0	0.555441	5.638960	2.579305	160	1	0	-0.444105	0.586879	-0.773947
105	1	0	1.436802	6.067177	0.159555	161	1	0	-6.446441	-0.454376	2.139467
106	1	0	1.915904	3.093022	0.189571	162	1	0	-3.663524	-3.823326	2.203760
107	1	0	3.744097	3.737351	-1.382213	163	1	0	-7.407819	-4.224392	-3.942062
108	1	0	3.071739	5.362697	-1.460858	164	1	0	-5.318103	3.672558	0.975801
109	1	0	4.957165	-2.415835	3.212186	165	1	0	-7.164742	2.008821	1.666950

166	1	0	-7.201331	-1.920734	-3.101470	200	1	0	13.450259	-1.451628	2.097854
167	1	0	-2.363748	4.988700	3.138229	201	1	0	11.939098	-2.269158	2.464925
168	1	0	-3.552680	2.670100	2.151783	202	1	0	13.207779	-3.117706	1.594404
169	1	0	-3.819983	4.210590	-4.436754	203	1	0	1.753987	2.322586	-4.980805
170	1	0	1.069533	4.423601	-2.464894	204	1	0	0.506235	3.359159	-4.327983
171	1	0	4.076095	1.580275	-1.138509	205	6	0	-0.519913	0.589178	3.563327
172	1	0	-2.866670	1.652138	-2.646772	206	6	0	-1.891937	0.925417	4.187738
173	1	0	-2.506341	-0.014108	-4.825266	207	6	0	-1.797632	-1.345302	4.301852
174	1	0	-3.020429	1.628489	-5.253177	208	6	0	-0.460776	-0.970177	3.613343
175	1	0	-0.805753	2.261118	-5.834593	209	6	0	-2.001072	-0.167090	5.296122
176	1	0	-0.545650	0.535963	-6.076078	210	6	0	-2.945408	0.459045	3.154416
177	1	0	2.510008	0.417968	-3.632530	211	6	0	-2.907405	-1.103027	3.249975
178	1	0	2.782386	-2.048289	-3.050485	212	6	0	-0.912082	-0.091775	6.386177
179	1	0	1.765682	-2.333840	-4.463042	213	6	0	-3.363879	-0.197238	6.009109
180	1	0	4.087010	-2.649779	-5.111975	214	6	0	-1.995463	2.386179	4.608037
181	1	0	3.526757	-1.163478	-5.856593	215	8	0	-0.344012	1.199729	2.254353
182	1	0	5.146880	-1.410727	-3.296378	216	1	0	0.260505	0.997472	4.171868
183	1	0	4.635229	0.127271	-3.968916	217	1	0	-0.398686	-1.389510	2.621230
184	1	0	6.533509	-1.839511	-5.312245	218	1	0	0.407767	-1.293182	4.169321
185	1	0	5.932154	-0.375975	-6.058409	219	1	0	-3.936492	0.826445	3.398459
186	1	0	8.142751	0.086256	-5.197810	220	1	0	-2.668096	0.808917	2.168146
187	1	0	6.991810	0.975228	-4.226129	221	1	0	-3.867700	-1.501744	3.531811
188	1	0	7.153911	-0.754739	-2.440463	222	1	0	-2.646706	-1.554870	2.304872
189	1	0	8.248726	-1.688134	-3.434224	223	1	0	-1.811325	-2.330435	4.746399
190	1	0	9.896135	0.185459	-3.374410	224	1	0	0.098018	-0.070857	6.003005
191	1	0	8.789073	1.131162	-2.402411	225	1	0	-1.057726	0.792543	6.998011
192	1	0	8.903602	-0.579644	-0.593718	226	1	0	-1.000166	-0.957190	7.035750
193	1	0	9.995250	-1.538313	-1.569027	227	1	0	-3.408380	-1.057337	6.669868
194	1	0	11.672331	0.310588	-1.513644	228	1	0	-3.485472	0.693693	6.617305
195	1	0	10.551672	1.300410	-0.608072	229	1	0	-4.198309	-0.261779	5.326399
196	1	0	12.142455	0.409356	0.962340	230	1	0	-1.718524	3.028983	3.782606
197	1	0	10.616836	-0.388222	1.263409	231	1	0	-3.000615	2.629494	4.942247
198	1	0	11.419872	-2.394372	0.014375	232	1	0	-1.304160	2.601706	5.414403
199	1	0	12.917248	-1.569657	-0.351559	233	1	0	-0.406253	0.586497	1.494534

General. All reagents were used as purchased without further purification. All solvents were distilled and dried according to standard procedures. TLC analyses were performed on pre-coated silica gel 60F254 sheets and detection was achieved by exposure to UV light (254 nm). Flash chromatography column was carried out using silica gel (200-400 mesh).

Infrared spectra of the compounds were recorded as pressed solids using an attenuated total reflectance (ATR)-IR spectrometer. Semi-preparative HPLC was performed using C18 5 micron, 150mm × 22 mm column with a flow rate of 10 mL/min using UV detection at 254 nm. ^{1}H and ^{13}C NMR, HSQC, HMBC, TOCY, TOCSY-HSQC and ROESY spectra were recorded using 400 MHz and 600 MHz spectrometers, respectively. Circular dichroism (CD) spectra were recorded on a circular dichroism spectropolarimeter at room temperature in water.

High resolution mass spectrometry was performed on a mass spectrometer equipped with an orthogonal nanospray source operated in positive ion mode. MS/MS of Glu-fibrino peptide was used for mass calibration for a calibration range of m/z 100 - 2000. Samples were prepared in a solution containing acetonitrile and formic acid and infused into the nanospray source at a rate of 0.5 - 1 μl min^{-1}. Optimal conditions were: capillary voltage 3000 V, source temperature 110 ^{o}C and a cone voltage of 60 V. Q1 was set to optimally pass ions from m/z 100 – 2000 and all ions transmitted into the pusher region of the TOF analyzer were scanned over the expected m/z range with a 1 s integration time. Data was acquired in continuum mode until acceptable averaged data was obtained.

Matrix assisted laser desorption/ionization time-of- flight (MALDI- TOF) was performed on a mass spectrometer operated in reflectron, positive ion mode with a N_2 laser. Laser power was used at the threshold level required to generate signal. Accelerating voltage was set to 28 kV.

Complete References

(3) Kagan, V. E. ; Tyurina, Y. Y.; Tyurin, V. A.; Konduru, N. V.;Potapovich, A. I.; Osipov, A. N.; Kisin, E. R.; Schwegler-Berry, D.; Mercer, R.; Castranova, V.; Shvedova, A. A.; *Toxicol. Lett.* **2006**, *165*, 88-100
(23) Bardelang, D. ; Charles, L.; Finet, J.-P.; Jicsinszky, L.; Karoui, H.; Marque, S. R. A.;Monnier, V.; Rockenbauer, A.; Rosas, R.;Tordo, P. *Chem. Eur. J.* **2007**, *13*, 9344-9354
(33) Asanuma, T. Asanuma, T; Yasui, H.; Inanami, O.; Waki, K.;Takahashi, M.; Iizuka, D.; Uemura, T.; Durand, G.; Polidori, A.; Kon, Y.; Pucci, B.; Kuwabara, M.; *Chem. Biodivers.* **2007**, *4*, 2253-2267
(61) Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. (2003) Gaussian 03 B.04 ed.; Gaussian, Inc.: Pittsburgh PA, 2003.