Stability of Cyclic Imine Toxins: Interconversion of Pinnatoxin Amino Ketone and Pinnatoxin A in Aqueous Media

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SUPPORTING INFORMATION

GENERAL PROCEDURES, SPECTRAL DATA, COMPUTATION DATA

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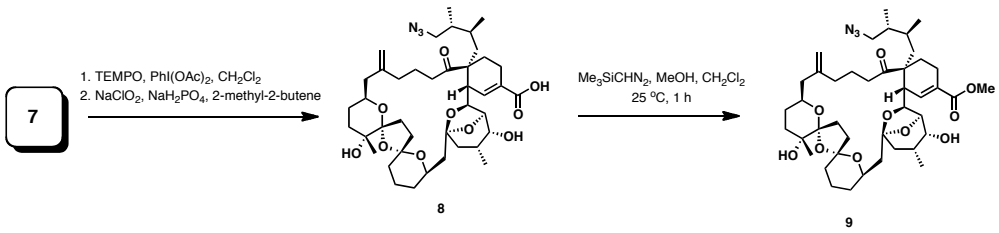
Experimental Information:

All reactions were carried out under an inert atmosphere of dry argon in oven or flame-dried glassware, unless the reaction procedure states otherwise. Tetrahydrofuran (THF) and diethylether (Et_2O) were distilled from sodium-benzophenone in a continuous still under an atmosphere of argon. Dichloromethane, diisopropylamine, pyridine, triethylamine, and chlorotrimethylsilane were distilled from calcium hydride in a continuous still under an atmosphere of argon. Chlorotriethylsilane (Et_3SiCl), and diisopropylethylamine (Hunig's Base) were distilled from calcium hydride under an inert atmosphere of dry argon and stored over calcium hydride. Reaction temperatures were controlled by IKA ETS-D4 fuzzy thermo couples. Room temperature reactions were carried out between 22-24 °C. Analytical thin-layer chromatography (TLC) was performed using pre-coated TLC plates with Silica Gel 60 F_{254} (EMD no. 5715-7) and visualized using combinations of UV, anisaldehyde, ceric ammonium molybdate (CAM), potassium permanganate, and iodine staining. Flash column chromatography was performed using 40-63 mm silica gel (Merck, Geduran, no. 11567-1) as the stationary phase. Proton magnetic resonance spectra were recorded at 200, 400, and 500 MHz on Varian Mercury Vx, Varian Unity Inova, and Varian Unity Inova spectrometers, respectively and at 800 MHz on a Bruker Avance II 800 Ultrashield Plus. Carbon magnetic resonance spectra were recorded at 50 MHz, 100 MHz, and 125 MHz on Varian Mercury Vx, Varian Unity Inova, and Varian Unity Inova spectrometers, respectively and at 200 MHz on a Bruker Avance II 800 Ultrashield Plus. All chemical shifts were reported in d units relative to tetramethylsilane. Optical Rotations were measured on a Roudolph Research Analytical AUTOPOL III polarimeter. High Resolution mass spectral data were obtained by the Mass Spectrometry laboratory at the University of California, Santa Barbara.

Optimization of the azide reduction protocol

Although many methods are available for azide reduction, the complexity of compound **7** and the presence of sensitive functionality, such as the carbonyl group, allylic hydroxy group, and double bonds, required a careful evaluation of these methods. Commonly used reducing agents for the azido group include: trialkyl- and triarylphosphines (Staudinger reduction), hydrogen-Pd/C, hydrogen-$Pd(OH)_2$, hydrogen-5% $Pd/CaCO_3$ (Lindlar's catalyst), 1,3-propaneditiol, and lithium aluminum hydride. The Staudinger reduction and Pd-catalyzed hydrogenolysis are by far the most popular methods for the reduction of azides. Considering the small scale of our intended experiments and the functional group composition of our substrate, we decided to focus our efforts on phosphine-based reagents and hydrogenolysis in the presence of deactivated palladium catalysts, specifically 5% Pd-$CaCO_3$ poisoned with lead and 5% Pd-$BaSO_4$ combinations.

In order to avoid possible difficulties in isolating and purifying small amounts of zwitterionic products, we decided to conduct experiments with the azido ester **9**. TEMPO-catalyzed oxidation of 7 with a stoichiometric amount of $PhI(OAc)_2$ afforded the aldehyde, which was further oxidized with buffered $NaClO_2$ to the carboxylic acid 8. Esterification of the latter with (trimethylsilyl)diazomethane in a mixture of methanol and dichloromethane gave **9** in an overall yield of 86%.

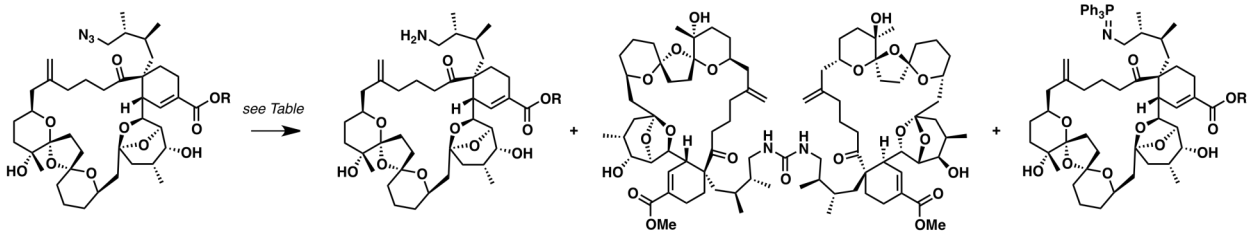


Scheme S1. Substrates for azide reduction.

Reduction of azido ester **9** to amine **10** with triphenylphosphine was accompanied by the unexpected formation of a substantial amount of urea **11** (Table S1, entries 1-3). Presumably, urea formation takes place through the intermediacy of isocyanate formed by a reaction between the initially formed iminophosphorane **12b** and adventitious carbon dioxide. The fraction of **11** in the product mixture could be reduced by performing the Staudinger reduction in the presence of triethylamine (Table 1, entry 2); however, upon scale up to 17 mg (Table S1, entry 3), only the C_2-symmetric urea **11** was formed. Staudinger reductions with trimethylphosphine afforded iminophosphorane **12b** exclusively (entry 4, Me_3P in place of Ph_3P), which was stable to hydrolysis even after heating at 55 °C for 22 h.

In contrast to the results with the phosphine reagents, a hydrogenolysis approach proved to be much more successful in delivering the primary amines (**2** and **10**) selectively (Table S1, entries 5-7). Replacing quinoline with pyridine as an additive improved product isolation.[1] Both the Lindlar catalyst and 5% Pd-$BaSO_4$ are effective hydrogenolysis catalysts. No urea byproducts were observed in any hydrogenation reactions.

Table S1. Reduction of azide to amine: search for optimal conditions.[a]

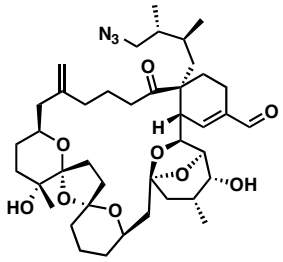


entry	substrate, (R)	reagent	Conditions	products (%)		
				2 or 10	**11**	**12a,b**[c]
1	**9** (**Me**)	Ph_3P (1.5 equiv)	THF-H_2O (3:1), 55 °C, 24 h	50	50	0
2		Ph_3P (2.5 equiv) Et_3N (15 equiv)	THF-H_2O (3:1), 55 °C, 5 h	70	30	0
3[b]		Ph_3P (1.2 equiv) Et_3N (15 equiv)	THF-H_2O (3:1), 55 °C, 5 h	0	100	0
4		Me_3P (15 equiv)	THF-H_2O (3:1), 55 °C, 24 h	0	0	100
5		H_2, Lindlar catalyst quinoline (10 equiv)	EtOH, 20 °C, 20 min.	100	0	0
6		H_2, Lindlar catalyst pyridine (10 equiv)	EtOH, 20 °C, 20 min.	100	0	n/a
7		H_2, 5% Pd-$BaSO_4$ pyridine (10 equiv)	EtOH, 20 °C, 20 min.	100	0	n/a
8	**8** (**H**)	Me_3P (7 equiv)	THF-H_2O (9:1), 20 °C, 60 h	15	0	85
9		Ph_3P (14 equiv)	THF-H_2O (9:1), 55 °C, 60 h	0	0	100
10		Ph_3P (10 equiv)	THF-H_2O-28% aq. NH_3 (28:7:1), 55 °C, 7 h	100	0	0
11		H_2, Lindlar catalyst	EtOH, 20 °C, 36 h	100	0	n/a

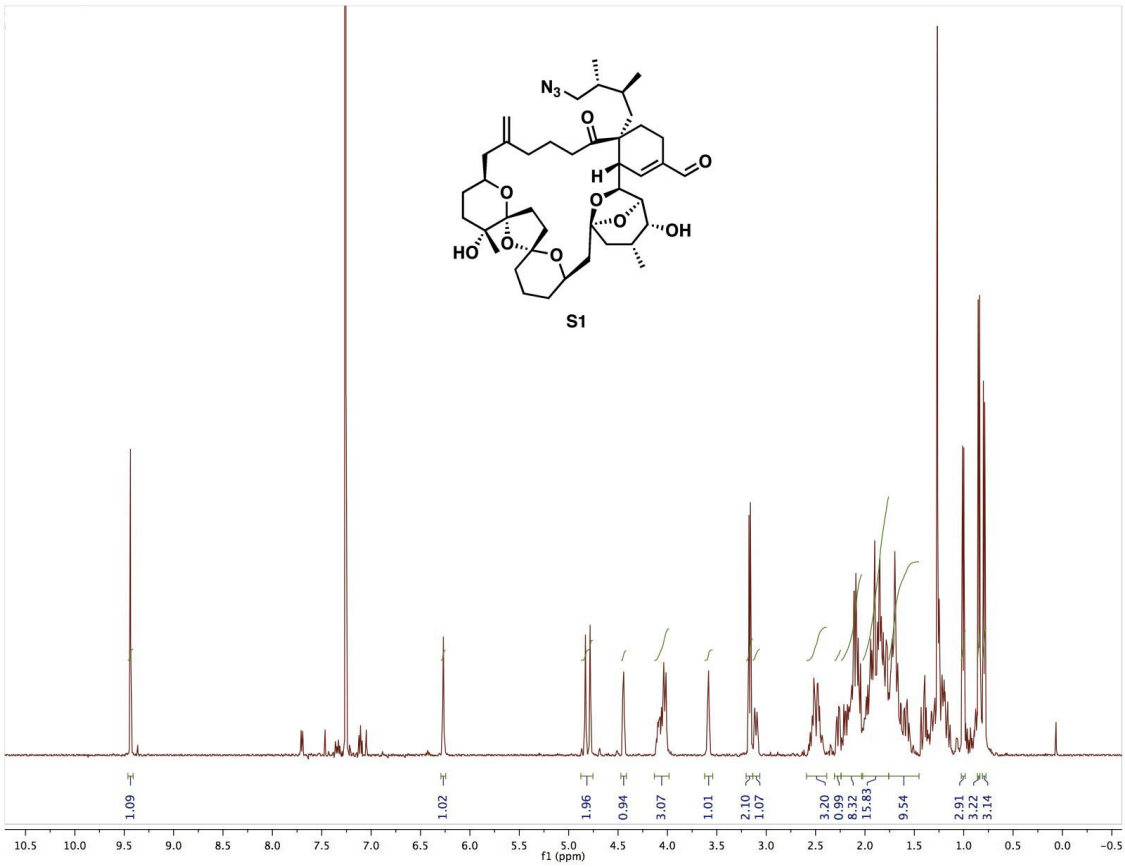
[a] reactions were generally performed on 1-3 mg (1-4 mmol) scale. [b] performed on 17 mg scale. A small amount (0.7 mg) of **12a** was isolated by reverse-phase HPLC and characterized by ^{1}H NMR and mass-spectroscopy only.

Azide reductions of carboxylic acid substrate **8** were investigated next (Table 2, entries 8-11). Formation of rather stable iminophosphorane products **12a** with trimethyl- or triphenylphospine was surprising; the iminophosphorane derived from Ph_3P was isolated in 68% yield after reverse-phase HPLC purification. Addition of ammonia accelerated hydrolysis of intermediate iminophosphorane providing amino acid **2** as a sole identifiable product. Hydrogenolysis of carboxylic acid **8** with Lindlar catalyst delivered amino acid **2** directly and required 36 h to reach completion.[2] However, the product could only be isolated in 35% yield after reverse-phase HPLC purification. Ultimately, we determined that the optimal procedure for the synthesis of PnTX AK (**2**) involved a two-step approach. Azido methyl ester **9** was subjected to hydrogenolysis in the presence of 5% Pd-$BaSO_4$ and pyridine, which was followed by saponification of the amino methyl ester **10** with lithium hydroxide in aqueous THF and purification by reverse-phase HPLC. This protocol afforded 5.1 mg of pure amino acid **2** from 6.3 mg of **9** (85% isolated yield).

Structure of **S1:**



S1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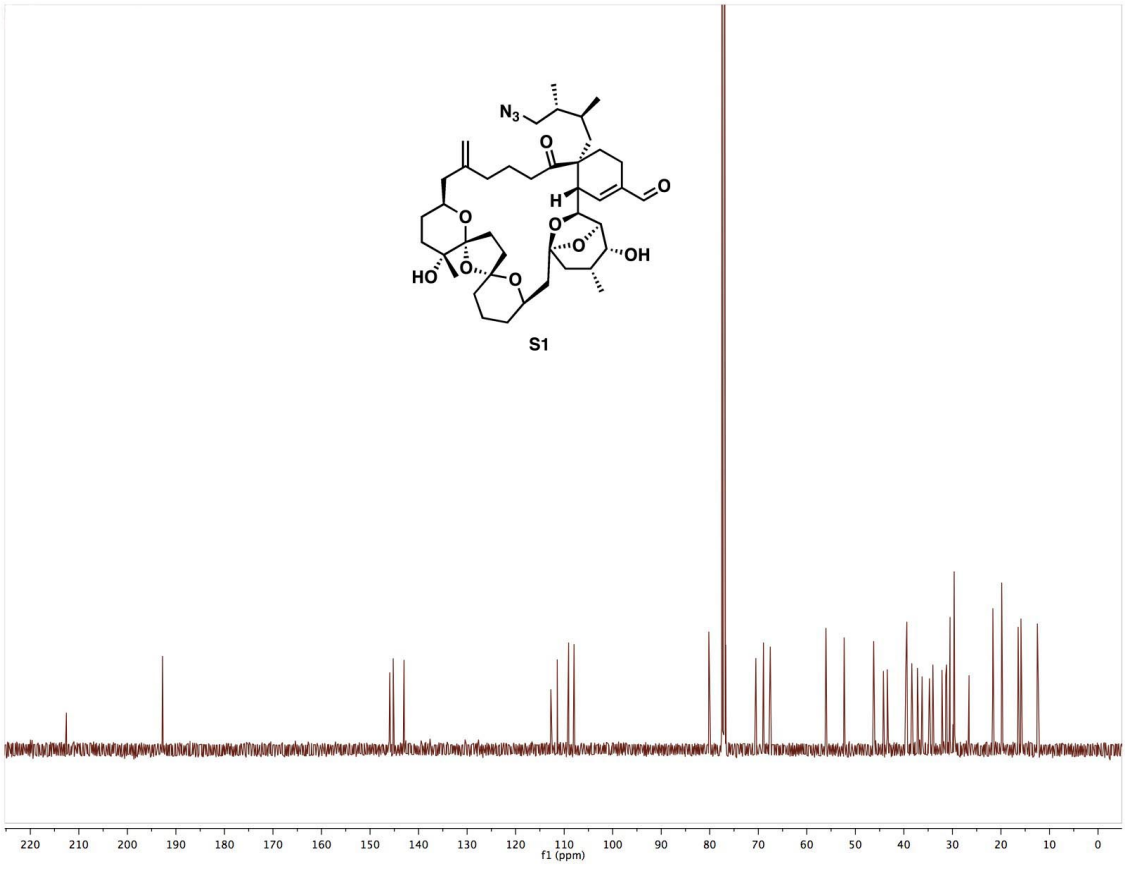
O
H
O
O
O
OH
HO
O
S1
1.09
1.02
1.96
0.94
3.07
1.01
2.10
1.07
3.20
0.99
8.32
15.83
9.54
2.91
3.22
3.14
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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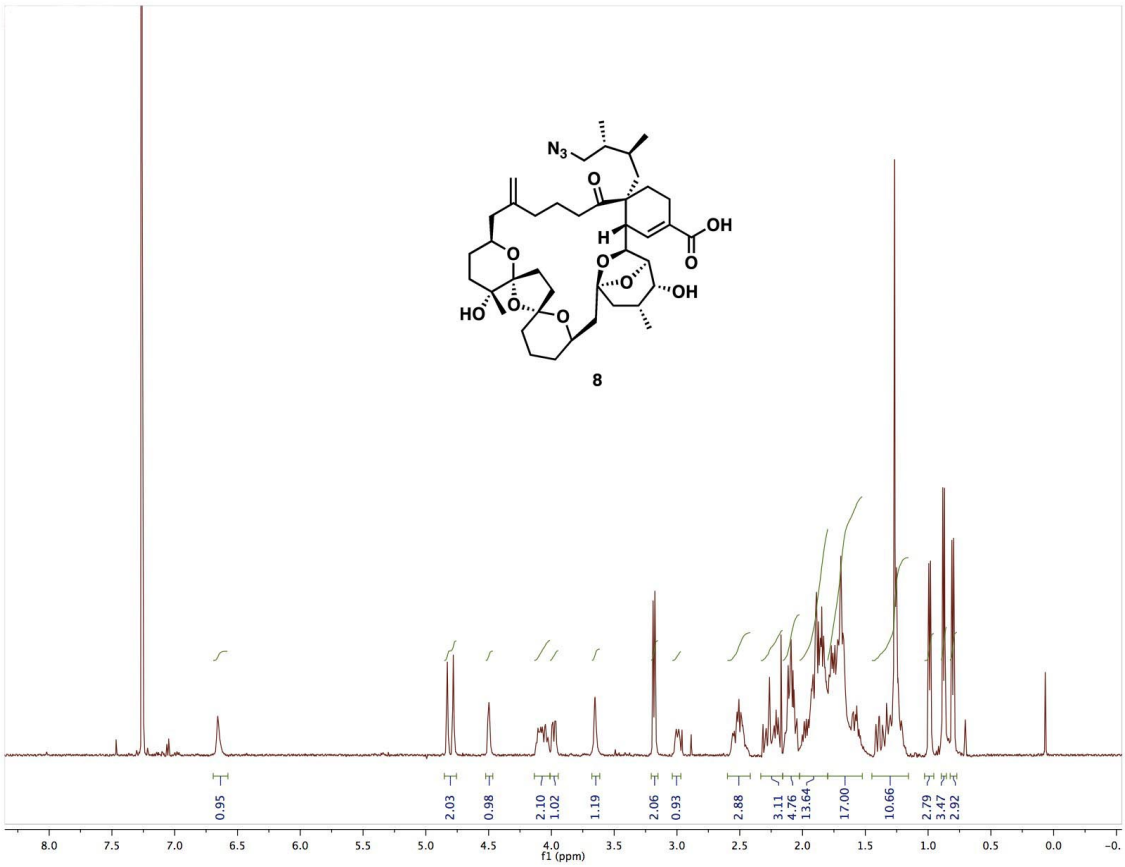
O
O
H
O
O
O
OH
HO
O
S1
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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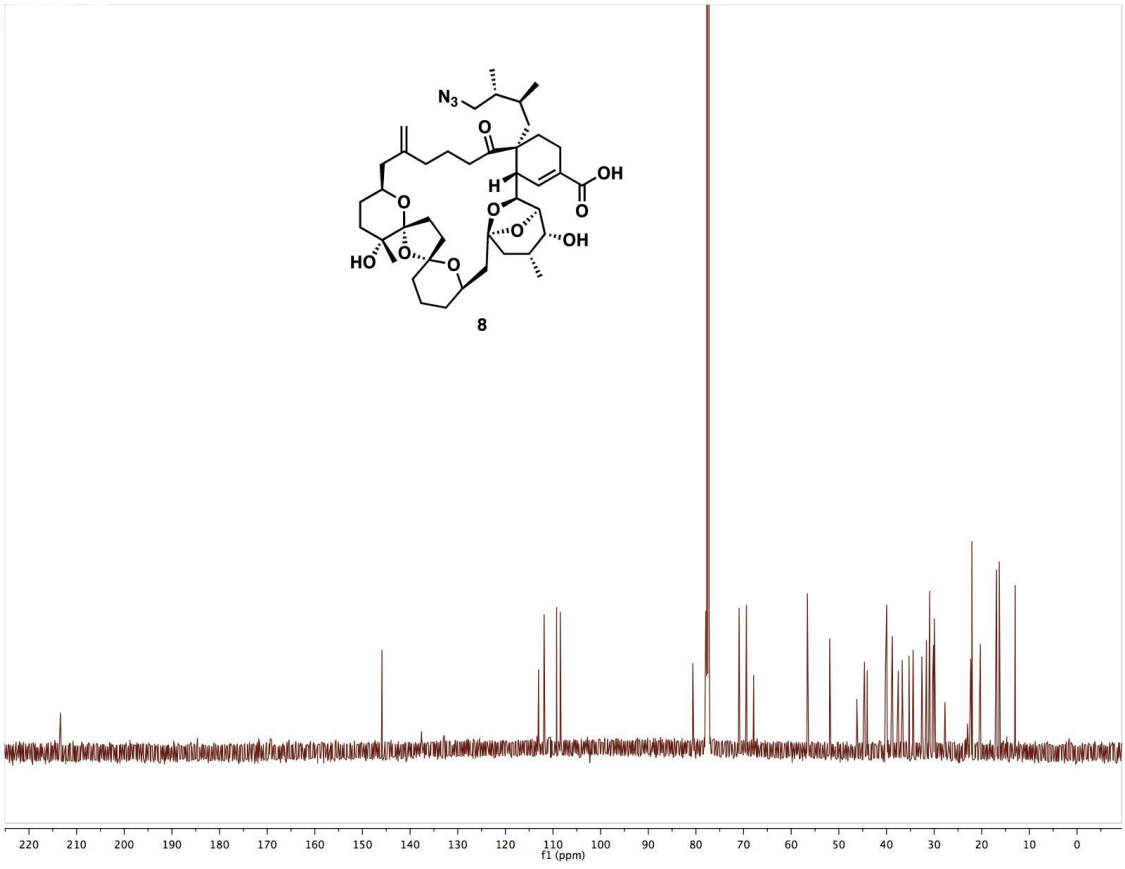
O
OH
H
O
O
O
HO
O
O
OH
8
0.95
2.03
0.98
2.10
1.02
1.19
2.06
0.93
2.88
3.11
4.76
13.64
17.00
10.66
2.79
3.47
2.92
f1 (ppm)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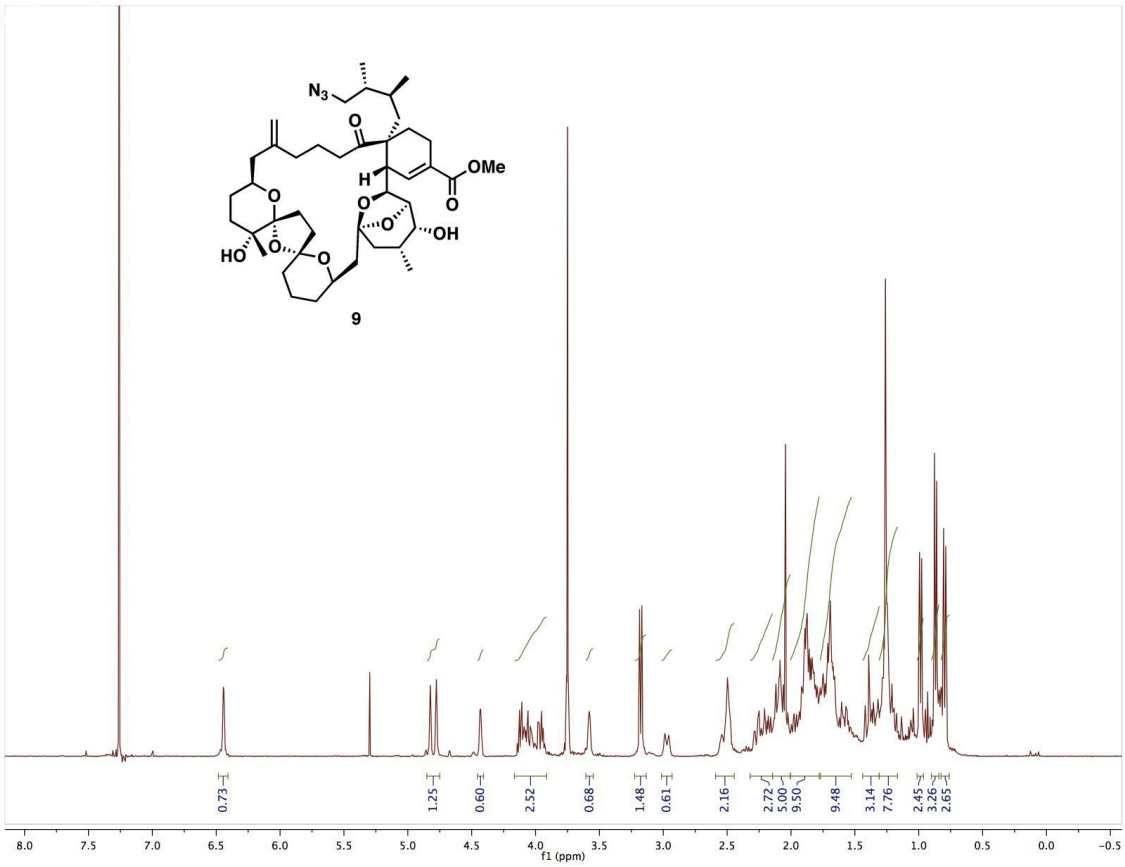
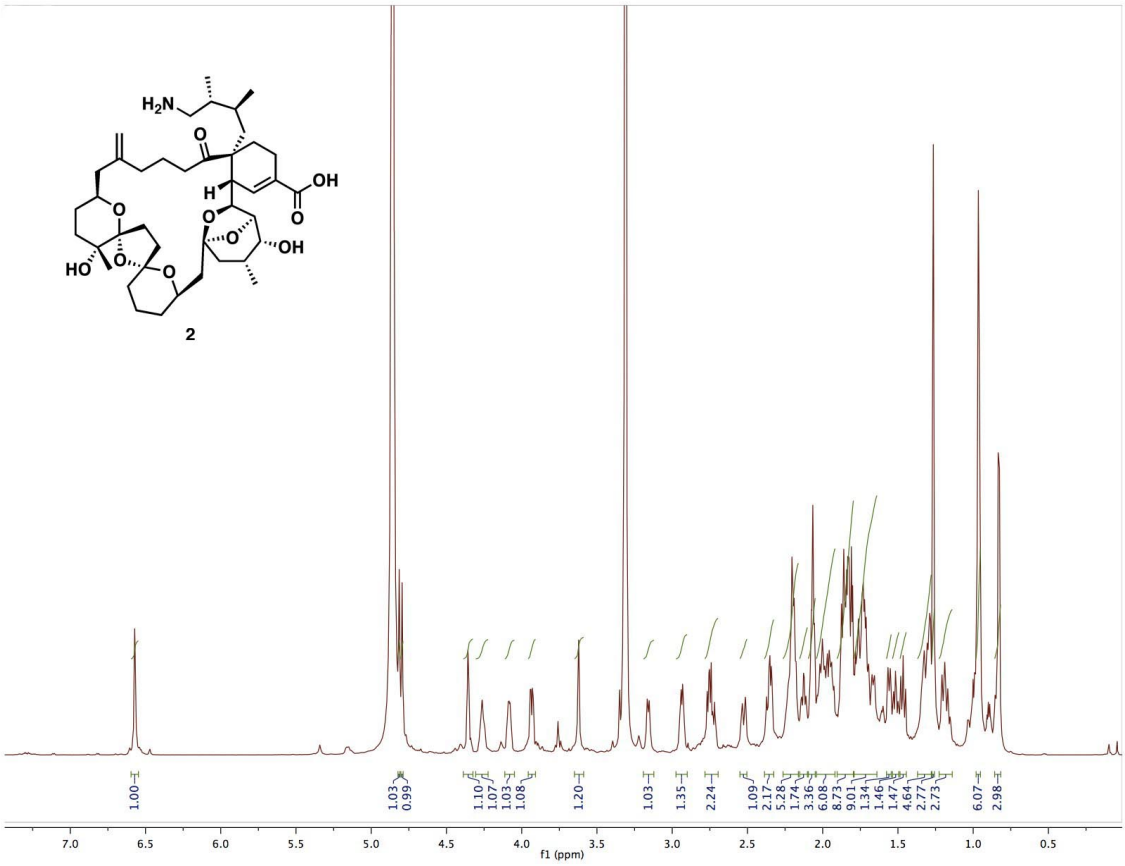
OH
H
O
O
O
HO
O
O
OH
8
f1 (ppm)


N3
O
OMe
H
O
O
O
OH
HO
O
O
9
0.73
1.25
0.60
2.52
0.68
1.48
0.61
2.16
2.72
5.00
9.50
9.48
3.14
7.76
2.45
3.26
2.65
f1 (ppm)


H2N
O
OH
H
O
O
O
OH
HO
O
O
2
1.00
1.03
0.99
1.10
1.07
1.03
1.08
1.20
1.03
1.35
2.24
1.09
2.17
5.28
1.74
3.36
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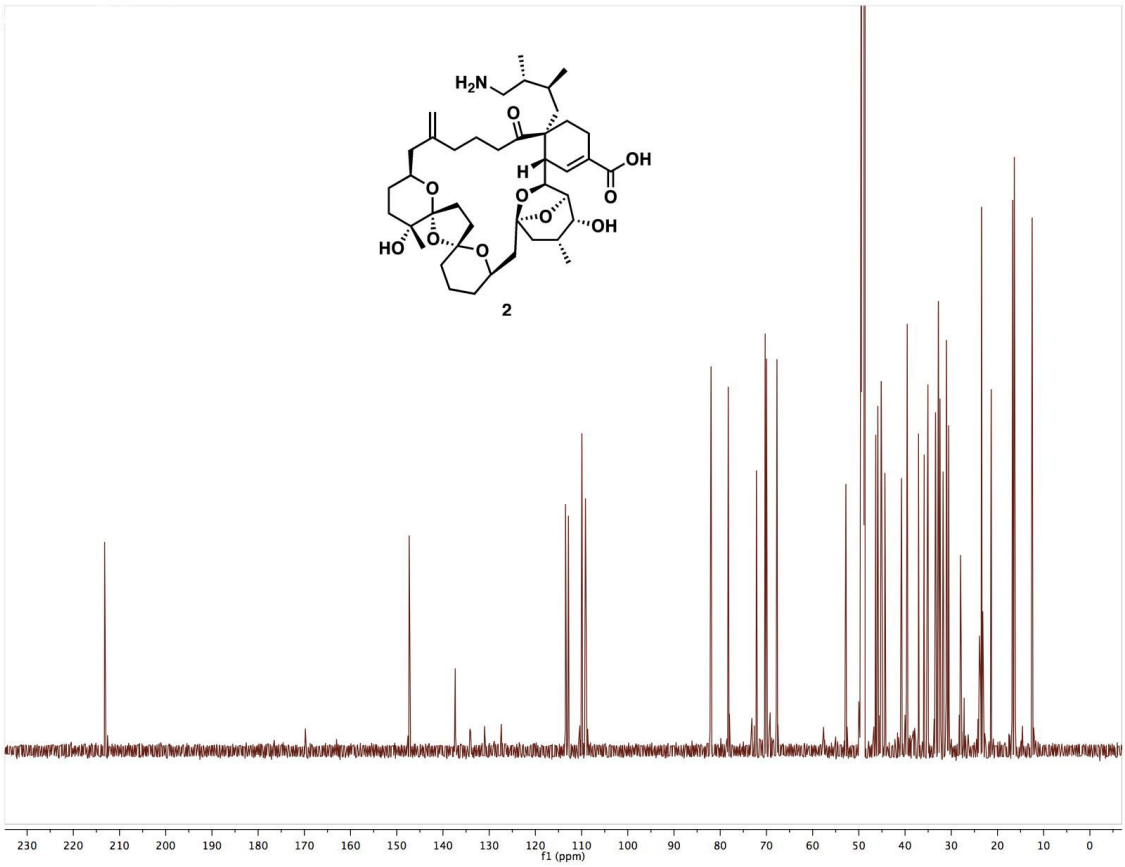
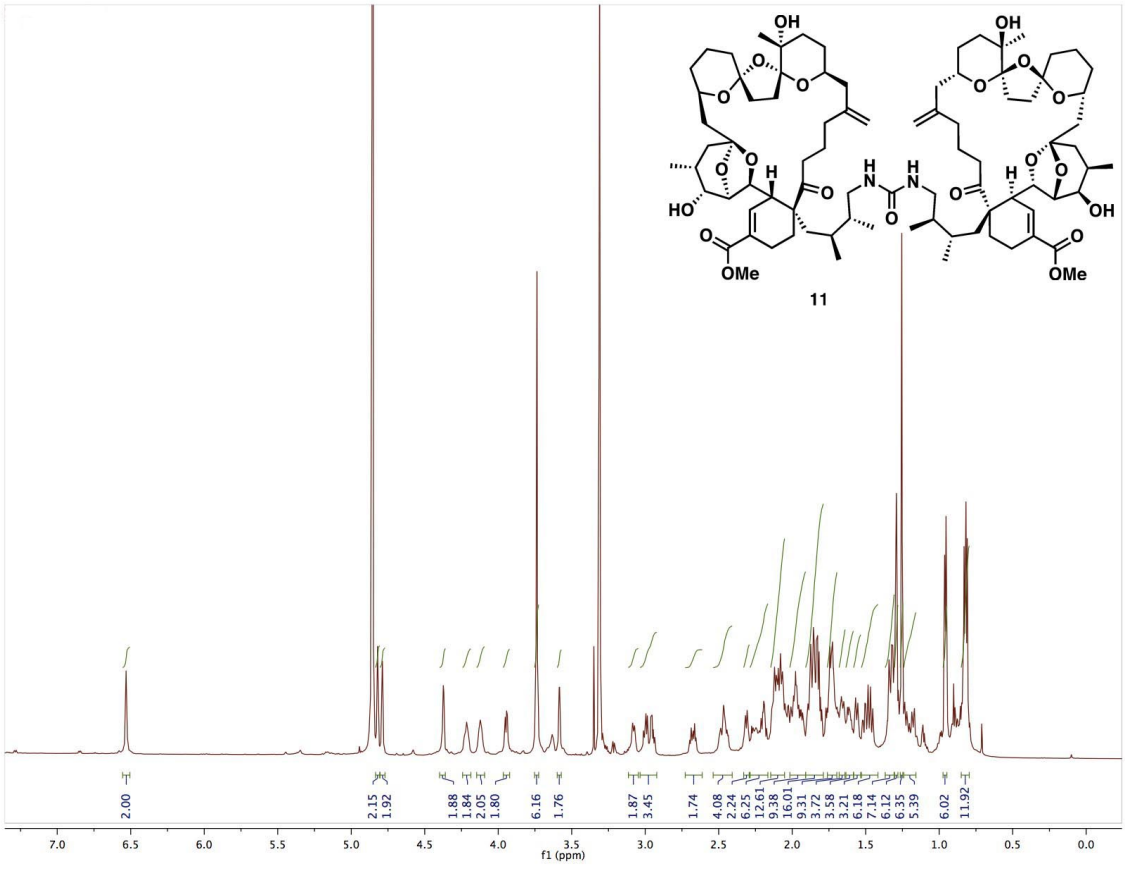
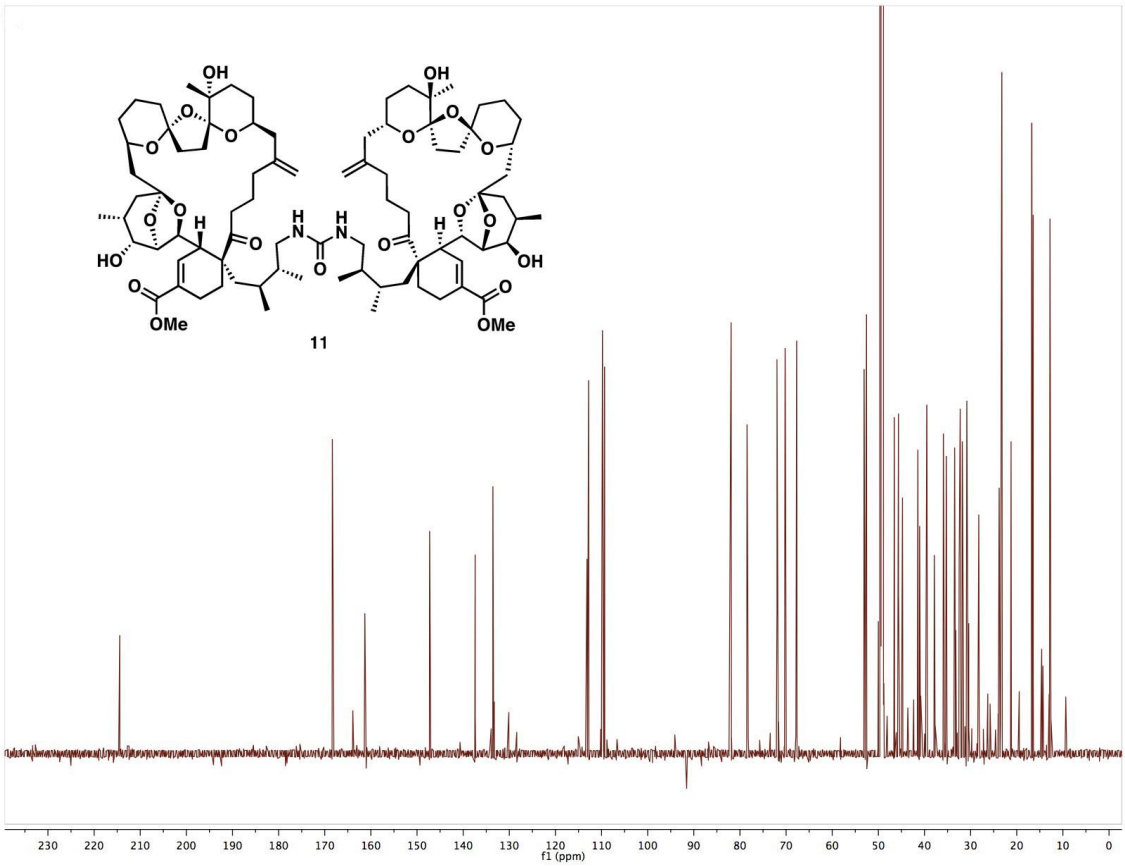
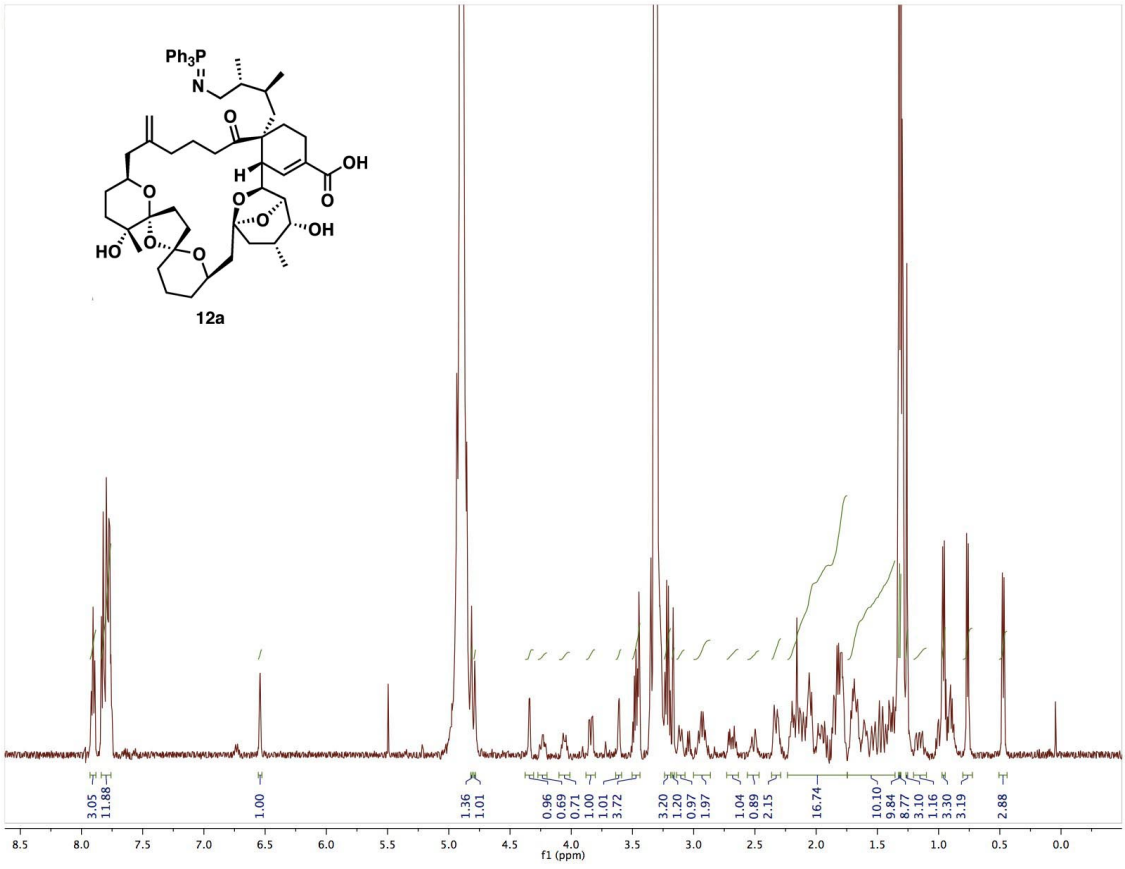
2.77
2.73
6.07
2.98
f1 (ppm)


H2N
O
OH
H
O
O
O
O
O
HO
O
O
OH
2
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OH
O
O
O
O
O
H
HO
O
OMe
H
N
H
N
O
O
H
O
O
OH
O
OMe
11
2.00 2.15 1.92 1.88 1.84 2.05 1.80 6.16 1.76 1.87 3.45 1.74 4.08 2.24 6.25 12.61 9.38 16.01 9.31 3.72 3.58 3.21 6.18 7.14 6.12 6.35 5.39 6.02 11.92
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


OH
O
O
O
O
H
HO
O
O
OMe
H
N
H
N
O
O
OH
O
O
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11


Ph3P
N
O
H
OH
O
O
O
O
HO
O
O
OH
3.05
11.88
1.00
1.36
1.01
0.96
0.69
0.71
1.00
1.01
3.72
3.20
1.20
0.97
1.97
1.04
0.89
2.15
16.74
10.10
9.84
8.77
3.10
1.16
3.30
3.19
2.88
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

12a

Computation data

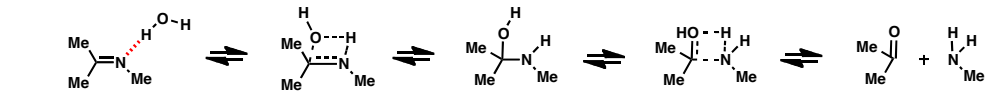
Molecular Modeling:

Three-dimensional coordinates of pinnatoxin A were taken from the docking complexes with nicotinic acetylcholine receptors described previously.[6] This structure was further edited using GaussView5[3] to generate initial coordinates for all other compounds used in this study.

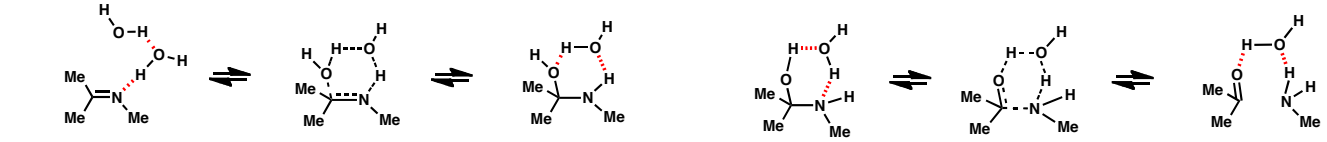
The geometries of the structures **1** and **13** were optimized in gas-phase using Gaussian 09[1,2] with the Becke's three-parameter hybrid exchange functional (B3LYP)[4,5] and the 6-31+G(d,p) basis set. Subsequent vibrational frequency calculations confirmed that these conformations were local minima and maxima, respectively. All the transition states were validated i) by visual inspection, in GaussView5, of the atomic movements corresponding to the imaginary vibrational frequency and ii) by geometry optimization of the structures extracted from the Display Vibrations/Manual Displacement menu of GaussView5 (amplitudes +1 and -1), which led to the corresponding minima.

Images were generated using Chimera.[6]

All calculations were performed using the high-performance computing (HPC) facilities at the Institut de Chimie des Substances Naturelles, Gif sur Yvette, France. These calculations required more than 700 days.cpu on recent computing nodes running with CentOS



for 1:	1a	1b	1c	1d	2e, 2e', 2e"
for 13:	13a	13b	13c	13d	13e



for 1:	1f	1g	1h	1i	1j	2a, 2b, 2c
for 13:	13f	13g	13h	13i	13j	14a, 14b, 14c

structure 1a

ENERGY:

Final Energy in Hartrees: HF = -2406.8866892 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.046652	3.808119	3.416564
2	6	0	-1.007423	2.642198	2.755907
3	6	0	-2.282957	1.875291	2.453360
4	6	0	-2.575240	1.649550	0.960958
5	1	0	-1.790119	1.029450	0.510501
6	6	0	-2.727355	2.947569	0.168780
7	6	0	-3.259401	2.660740	-1.240566
8	6	0	-4.550094	1.818477	-1.219447
9	6	0	-5.745650	2.620439	-0.699897
10	8	0	-4.897657	1.428932	-2.554067
11	8	0	-3.808768	0.892748	0.926335
12	6	0	-4.303446	0.539796	-0.357332
13	6	0	-5.519265	-0.365891	-0.130294
14	6	0	-4.889093	-1.756859	-0.024653
15	6	0	-3.700109	-1.696512	-0.993763
16	6	0	-4.011331	-2.207235	-2.409912
17	6	0	-2.757914	-2.232350	-3.292643
18	6	0	-1.648891	-3.025091	-2.590810
19	6	0	-1.397436	-2.472884	-1.185469
20	1	0	-1.005920	-1.452122	-1.260915
21	8	0	-2.635701	-2.416705	-0.424216
22	8	0	-3.371436	-0.275352	-1.083233
23	6	0	0.274008	1.978546	2.291279
24	6	0	1.598173	2.573099	2.786589
25	6	0	2.865585	1.875104	2.230310
26	6	0	2.970608	1.941568	0.697945
27	7	0	3.070020	3.150553	0.276481
28	1	0	3.425876	4.592482	1.384074
29	6	0	3.171305	3.666090	-1.088781
30	6	0	2.580046	2.924238	-2.315871
31	1	0	3.335159	2.261225	-2.753504
32	6	0	2.255283	3.987727	-3.380391
33	6	0	1.383989	2.048789	-1.892674
34	1	0	0.797646	2.631083	-1.164367
35	6	0	0.439014	1.693611	-3.054388
36	6	0	1.830606	0.722852	-1.233259
37	6	0	3.016863	0.685964	-0.212337
38	6	0	3.016123	-0.731353	0.505744
39	6	0	1.799688	-1.161633	1.367260
40	1	0	1.587819	-0.386720	2.102986
41	6	0	2.003013	-2.511990	2.101495
42	1	0	3.046762	-2.829116	2.158895
43	6	0	1.323345	-2.587561	3.480506
44	1	0	1.835279	-1.935138	4.199366
45	8	0	1.475679	-3.915069	3.991627
46	6	0	-0.162692	-2.160418	3.362253
47	1	0	-0.156108	-1.070241	3.237535
48	6	0	-0.959642	-2.468031	4.634478
49	6	0	-0.827382	-2.756010	2.099801
50	6	0	0.124405	-2.733119	0.890569
51	8	0	0.583448	-1.395992	0.630309
52	6	0	-0.407587	-3.336691	-0.407841
53	8	0	1.308380	-3.447227	1.261935
54	1	0	3.825358	-0.676955	1.255902
55	6	0	3.367561	-1.827926	-0.495242

56	6	0	4.073573	-1.665908	-1.622730
57	6	0	4.302788	-2.845073	-2.602423
58	8	0	5.081571	-2.581778	-3.560468
59	8	0	3.687966	-3.914006	-2.348995
60	6	0	4.630389	-0.321249	-1.996951
61	6	0	4.440962	0.718261	-0.886830
62	1	0	-1.992803	4.240704	3.732059
63	1	0	-0.150304	4.367933	3.662374
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70	1	0	-5.853684	3.534516	-1.292171
71	1	0	-6.668670	2.043322	-0.801321
72	1	0	-5.617651	2.892221	0.350110
73	1	0	-4.200164	0.823553	-2.848528
74	1	0	-6.069552	-0.068699	0.764488
75	1	0	-6.184792	-0.297645	-0.995994
76	1	0	-4.497374	-1.933939	0.980200
77	1	0	-5.577207	-2.567683	-0.278111
78	1	0	-4.403460	-3.227626	-2.310296
79	1	0	-4.805730	-1.593154	-2.848940
80	1	0	-2.992005	-2.674454	-4.268057
81	1	0	-2.413034	-1.207886	-3.483454
82	1	0	-1.937657	-4.082950	-2.515779
83	1	0	-0.713841	-2.983794	-3.159893
84	1	0	0.205739	0.922759	2.579649
85	1	0	0.277201	1.964481	1.192423
86	1	0	1.656171	3.630008	2.513198
87	1	0	1.632615	2.529910	3.882885
88	1	0	3.732574	2.409386	2.635227
89	1	0	2.937108	0.853065	2.600078
90	1	0	2.675973	4.645490	-1.036620
91	1	0	4.232368	3.895727	-1.269846
92	1	0	3.125411	4.633677	-3.551838
93	1	0	1.989799	3.536236	-4.340578
94	1	0	1.424265	4.631749	-3.064625
95	1	0	0.983405	1.196611	-3.866480
96	1	0	-0.337340	1.000709	-2.710961
97	1	0	-0.061203	2.574834	-3.468317
98	1	0	0.954659	0.299157	-0.738474
99	1	0	2.075258	0.014292	-2.029173
100	1	0	1.339489	-4.516348	3.242577
101	1	0	-0.514913	-1.976622	5.508210
102	1	0	-1.992529	-2.113941	4.537061
103	1	0	-0.978938	-3.543495	4.833953
104	1	0	-1.109756	-3.802550	2.275870
105	1	0	-1.744116	-2.213475	1.857326
106	1	0	-0.864059	-4.310248	-0.194229
107	1	0	0.467329	-3.510772	-1.043658
108	1	0	2.993196	-2.829290	-0.306935
109	1	0	5.693519	-0.428471	-2.240728
110	1	0	4.171176	0.010201	-2.939529
111	1	0	4.682795	1.713665	-1.261166
112	1	0	5.168514	0.520894	-0.087058
113	8	0	3.656574	5.388235	1.929037
114	1	0	4.601995	5.522280	1.794452

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	27.4277	34.5531	39.2512
Red. masses --	5.1834	5.9720	5.5536
Frc consts --	0.0023	0.0042	0.0050
IR Inten --	0.0759	3.0913	1.1980

structure 1b

ENERGY:

Final Energy in Hartrees: HF = -2406.8173199 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.037420	3.369737	3.917309
2	6	0	-0.999323	2.308132	3.099109
3	6	0	-2.274857	1.583239	2.706536
4	6	0	-2.586821	1.555539	1.201132
5	1	0	-1.803475	1.008923	0.660973
6	6	0	-2.763844	2.944408	0.587648
7	6	0	-3.309065	2.835058	-0.841606
8	6	0	-4.587597	1.976925	-0.919776
9	6	0	-5.789137	2.690075	-0.295151
10	8	0	-4.939432	1.756302	-2.290871
11	8	0	-3.813292	0.798362	1.085359
12	6	0	-4.316365	0.602888	-0.230251
13	6	0	-5.520014	-0.338630	-0.109104
14	6	0	-4.874565	-1.724280	-0.181896
15	6	0	-3.687393	-1.530791	-1.137717
16	6	0	-3.995138	-1.870600	-2.604976
17	6	0	-2.744090	-1.771661	-3.485908
18	6	0	-1.624416	-2.630821	-2.887357
19	6	0	-1.374143	-2.251141	-1.426591
20	1	0	-0.987692	-1.226827	-1.377319
21	8	0	-2.610961	-2.292638	-0.657574
22	8	0	-3.382755	-0.100113	-1.057950
23	6	0	0.280924	1.717980	2.541230
24	6	0	1.608770	2.265360	3.080614
25	6	0	2.893292	1.641933	2.471379
26	6	0	3.062371	1.851867	0.976533
27	7	0	3.026597	3.131145	0.652564
28	1	0	3.335967	3.706617	1.434281
29	6	0	3.298771	3.825224	-0.615178
30	6	0	2.569321	3.316114	-1.881371
31	1	0	3.257923	2.697758	-2.466145
32	6	0	2.223187	4.542124	-2.744980
33	6	0	1.357448	2.434506	-1.512288
34	1	0	0.811181	2.957028	-0.712100
35	6	0	0.374758	2.241817	-2.681699
36	6	0	1.756607	1.021965	-1.010516
37	6	0	3.025568	0.778617	-0.111045
38	6	0	3.015227	-0.728459	0.391332
39	6	0	1.830799	-1.255531	1.246920
40	1	0	1.646738	-0.579248	2.080664
41	6	0	2.052136	-2.686264	1.800335
42	1	0	3.098587	-3.000109	1.801904
43	6	0	1.393004	-2.945858	3.167113
44	1	0	1.909138	-2.388417	3.959119
45	8	0	1.563615	-4.327285	3.497635
46	6	0	-0.099409	-2.524106	3.125960
47	1	0	-0.104743	-1.426742	3.142502
48	6	0	-0.871761	-3.002755	4.359984
49	6	0	-0.780136	-2.959333	1.806978
50	6	0	0.153417	-2.765742	0.599383
51	8	0	0.593158	-1.397127	0.523260
52	6	0	-0.378720	-3.199585	-0.765093
53	8	0	1.348391	-3.510963	0.860357
54	1	0	3.874966	-0.801304	1.079046
55	6	0	3.227283	-1.667959	-0.791209
56	6	0	3.782255	-1.350400	-1.968222
57	6	0	3.775681	-2.354644	-3.147090
58	8	0	4.478963	-2.009410	-4.135416

59	8	0	3.055934	-3.380481	-3.004498
60	6	0	4.375234	0.011312	-2.190838
61	6	0	4.383769	0.854345	-0.912943
62	1	0	-1.981720	3.750272	4.297976
63	1	0	-0.140773	3.888449	4.240801
64	1	0	-2.216160	0.539367	3.042826
65	1	0	-3.130634	2.036596	3.219836
66	1	0	-3.443668	3.532114	1.218047
67	1	0	-1.802048	3.469858	0.589011
68	1	0	-3.526365	3.824430	-1.260520
69	1	0	-2.549409	2.375158	-1.484306
70	1	0	-5.916040	3.668854	-0.768526
71	1	0	-6.705040	2.116548	-0.460099
72	1	0	-5.655146	2.831624	0.779517
73	1	0	-4.246371	1.186981	-2.659153
74	1	0	-6.066453	-0.161453	0.819289
75	1	0	-6.193359	-0.170528	-0.954778
76	1	0	-4.480294	-2.025375	0.791974
77	1	0	-5.555605	-2.502818	-0.535938
78	1	0	-4.373496	-2.900777	-2.628515
79	1	0	-4.799952	-1.219378	-2.965181
80	1	0	-2.975504	-2.093703	-4.507836
81	1	0	-2.412777	-0.727005	-3.550146
82	1	0	-1.901955	-3.692922	-2.940429
83	1	0	-0.689963	-2.513652	-3.446392
84	1	0	0.232952	0.635769	2.709139
85	1	0	0.263146	1.826601	1.448373
86	1	0	1.638587	3.351195	2.930863
87	1	0	1.655177	2.109253	4.165691
88	1	0	3.787464	2.130516	2.887391
89	1	0	2.975967	0.587745	2.724425
90	1	0	2.975568	4.854689	-0.422481
91	1	0	4.387514	3.848079	-0.741635
92	1	0	3.107486	5.177219	-2.877290
93	1	0	1.877795	4.253564	-3.741252
94	1	0	1.441403	5.153346	-2.275253
95	1	0	0.887559	1.836523	-3.562073
96	1	0	-0.406588	1.526555	-2.403206
97	1	0	-0.117423	3.175629	-2.971290
98	1	0	0.891061	0.611182	-0.486385
99	1	0	1.886840	0.377072	-1.881817
100	1	0	1.417906	-4.826032	2.678259
101	1	0	-0.417748	-2.622681	5.283081
102	1	0	-1.910051	-2.652731	4.324194
103	1	0	-0.875932	-4.095099	4.419268
104	1	0	-1.049560	-4.023016	1.849028
105	1	0	-1.706096	-2.400069	1.651975
106	1	0	-0.831434	-4.194073	-0.674800
107	1	0	0.494171	-3.288442	-1.422713
108	1	0	2.831158	-2.673892	-0.708126
109	1	0	5.398250	-0.104255	-2.567619
110	1	0	3.842765	0.512903	-3.012599
111	1	0	4.674803	1.879831	-1.125102
112	1	0	5.155637	0.495830	-0.226604
113	8	0	5.309452	2.610490	1.621354
114	1	0	6.251326	2.417710	1.726828

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	-1519.6173	24.3908	35.9093
Red. masses --	1.1547	4.9973	4.9883
Frc consts --	1.5710	0.0018	0.0038
IR Inten --	213.4288	0.5175	0.4957

structure 1c

ENERGY:

Final Energy in Hartrees: HF = -2406.8694133 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.617678	3.648437	3.473558
2	6	0	-0.685324	2.407630	2.968568
3	6	0	-2.029963	1.757271	2.688768
4	6	0	-2.434510	1.716954	1.202599
5	1	0	-1.716324	1.115001	0.631414
6	6	0	-2.566932	3.102445	0.568504
7	6	0	-3.215319	3.007988	-0.817610
8	6	0	-4.543198	2.228040	-0.794296
9	6	0	-5.656562	3.015890	-0.100272
10	8	0	-5.001000	2.012195	-2.135145
11	8	0	-3.709009	1.031437	1.176708
12	6	0	-4.300577	0.848728	-0.105406
13	6	0	-5.543803	-0.026404	0.090969
14	6	0	-4.986650	-1.447183	-0.023507
15	6	0	-3.823100	-1.320715	-1.021115
16	6	0	-4.183835	-1.666937	-2.474718
17	6	0	-2.951514	-1.636906	-3.388553
18	6	0	-1.858307	-2.540720	-2.807439
19	6	0	-1.553018	-2.153463	-1.360139
20	1	0	-1.112420	-1.150222	-1.334025
21	8	0	-2.770901	-2.120601	-0.555940
22	8	0	-3.455328	0.096983	-0.978229
23	6	0	0.531048	1.549592	2.667037
24	6	0	1.894273	2.251805	2.718369
25	6	0	3.166201	1.409281	2.442526
26	6	0	3.833995	1.421131	1.020025
27	7	0	3.875854	2.836464	0.670298
28	1	0	4.371358	3.318988	1.412068
29	6	0	4.209665	3.442277	-0.617267
30	6	0	3.145046	3.251685	-1.740485
31	1	0	3.539641	2.560586	-2.493053
32	6	0	2.941107	4.602146	-2.452012
33	6	0	1.837380	2.639895	-1.187122
34	1	0	1.564045	3.234471	-0.306405
35	6	0	0.672560	2.737911	-2.189909
36	6	0	1.946994	1.145801	-0.752083
37	6	0	3.251522	0.534581	-0.166174
38	6	0	3.002795	-0.988763	0.227442
39	6	0	1.831297	-1.361801	1.184774
40	1	0	1.763707	-0.645933	2.000150
41	6	0	1.939436	-2.791126	1.771340
42	1	0	2.954137	-3.196857	1.756791
43	6	0	1.300666	-2.965561	3.161740
44	1	0	1.883550	-2.438312	3.927642
45	8	0	1.369048	-4.351226	3.516792
46	6	0	-0.153546	-2.425598	3.151000
47	1	0	-0.068890	-1.332671	3.135401
48	6	0	-0.924095	-2.809178	4.418989
49	6	0	-0.907262	-2.833443	1.863185
50	6	0	0.002301	-2.731211	0.626670
51	8	0	0.547128	-1.399981	0.531806
52	6	0	-0.593177	-3.145666	-0.716410
53	8	0	1.140354	-3.572772	0.873512
54	1	0	3.903871	-1.277704	0.792794
55	6	0	2.862513	-1.869082	-1.011889
56	6	0	3.158766	-1.542680	-2.276067
57	6	0	2.750301	-2.448012	-3.458326
58	8	0	3.359520	-2.222312	-4.538088

59	8	0	1.834544	-3.289100	-3.228030
60	6	0	3.892528	-0.267104	-2.568783
61	6	0	4.372083	0.386167	-1.268316
62	1	0	-1.520422	4.210933	3.698490
63	1	0	0.325320	4.145802	3.674670
64	1	0	-2.027112	0.722180	3.053109
65	1	0	-2.819905	2.288346	3.232686
66	1	0	-3.164428	3.744181	1.229702
67	1	0	-1.576948	3.564303	0.494017
68	1	0	-3.399825	4.004233	-1.236320
69	1	0	-2.531880	2.494239	-1.503431
70	1	0	-5.760732	3.994629	-0.579549
71	1	0	-6.612651	2.493525	-0.192533
72	1	0	-5.440083	3.161966	0.960279
73	1	0	-4.364342	1.404141	-2.541879
74	1	0	-6.021780	0.177336	1.051403
75	1	0	-6.256278	0.184319	-0.711893
76	1	0	-4.575045	-1.786706	0.930310
77	1	0	-5.728057	-2.177093	-0.359975
78	1	0	-4.606973	-2.680007	-2.473035
79	1	0	-4.969611	-0.986004	-2.823162
80	1	0	-3.224775	-1.959840	-4.400033
81	1	0	-2.574602	-0.609401	-3.474974
82	1	0	-2.192789	-3.587783	-2.833451
83	1	0	-0.928932	-2.487980	-3.384960
84	1	0	0.520004	0.720945	3.391803
85	1	0	0.373616	1.070377	1.696032
86	1	0	1.894927	3.104406	2.032481
87	1	0	2.007337	2.671590	3.726347
88	1	0	3.962082	1.832717	3.067410
89	1	0	3.069463	0.382956	2.799764
90	1	0	4.270181	4.515281	-0.396088
91	1	0	5.207481	3.165409	-1.001355
92	1	0	3.909537	5.034180	-2.734519
93	1	0	2.350814	4.500898	-3.367157
94	1	0	2.434049	5.322872	-1.796496
95	1	0	0.935416	2.276974	-3.150225
96	1	0	-0.201702	2.203064	-1.803915
97	1	0	0.369166	3.772641	-2.379496
98	1	0	1.137391	0.971313	-0.040927
99	1	0	1.680623	0.525401	-1.611470
100	1	0	1.128975	-4.846179	2.717416
101	1	0	-0.411433	-2.447963	5.319014
102	1	0	-1.929829	-2.373043	4.404377
103	1	0	-1.019364	-3.895547	4.507098
104	1	0	-1.257750	-3.871844	1.933361
105	1	0	-1.791283	-2.206356	1.724289
106	1	0	-1.100556	-4.110663	-0.595684
107	1	0	0.243477	-3.287620	-1.413784
108	1	0	2.383257	-2.828720	-0.866048
109	1	0	4.746623	-0.498021	-3.215980
110	1	0	3.267164	0.411213	-3.166132
111	1	0	4.870466	1.328852	-1.490770
112	1	0	5.143261	-0.285579	-0.866092
113	8	0	5.162038	0.924829	1.374336
114	1	0	5.668990	0.802321	0.561639

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	24.8812	33.3830	39.7610
Red. masses --	4.8740	4.9833	5.1658
Frc consts --	0.0018	0.0033	0.0048
IR Inten --	0.4357	1.3669	0.5319

structure 1d

ENERGY:

Final Energy in Hartrees: HF = -2406.8159708 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.520370	3.783176	3.329063
2	6	0	-0.609383	2.514489	2.902701
3	6	0	-1.963785	1.859846	2.690037
4	6	0	-2.414030	1.775287	1.218954
5	1	0	-1.707831	1.163598	0.642920
6	6	0	-2.575529	3.142516	0.552137
7	6	0	-3.260562	3.005699	-0.812107
8	6	0	-4.580740	2.217048	-0.729877
9	6	0	-5.680194	3.014523	-0.024880
10	8	0	-5.074461	1.963057	-2.050794
11	8	0	-3.682524	1.081227	1.249141
12	6	0	-4.306758	0.857519	-0.012711
13	6	0	-5.536044	-0.022680	0.240589
14	6	0	-4.971667	-1.441489	0.138600
15	6	0	-3.843081	-1.328268	-0.899217
16	6	0	-4.253605	-1.688483	-2.335749
17	6	0	-3.053711	-1.657933	-3.291828
18	6	0	-1.939510	-2.556878	-2.744858
19	6	0	-1.586379	-2.170322	-1.307935
20	1	0	-1.131326	-1.173365	-1.296330
21	8	0	-2.775671	-2.121131	-0.461454
22	8	0	-3.475989	0.092511	-0.885484
23	6	0	0.593715	1.628526	2.632200
24	6	0	1.963734	2.319500	2.565971
25	6	0	3.200214	1.401755	2.379397
26	6	0	3.924675	1.190862	1.013359
27	7	0	4.463471	2.673788	0.536536
28	1	0	4.578592	3.152855	1.429328
29	6	0	4.011262	3.704757	-0.448875
30	6	0	3.075206	3.307433	-1.604816
31	1	0	3.597368	2.642628	-2.296950
32	6	0	2.784178	4.611079	-2.376653
33	6	0	1.795609	2.598055	-1.091063
34	1	0	1.488673	3.151456	-0.190548
35	6	0	0.617117	2.695869	-2.080580
36	6	0	1.944620	1.089840	-0.723128
37	6	0	3.267784	0.460111	-0.214819
38	6	0	3.027964	-1.076828	0.115276
39	6	0	1.904743	-1.452737	1.121967
40	1	0	1.886422	-0.744868	1.949873
41	6	0	2.014788	-2.887717	1.687309
42	1	0	3.022325	-3.306416	1.629146
43	6	0	1.426723	-3.064537	3.100146
44	1	0	2.050027	-2.556062	3.846559
45	8	0	1.479520	-4.454726	3.439843
46	6	0	-0.016227	-2.497371	3.151378
47	1	0	0.086278	-1.405048	3.133525
48	6	0	-0.740036	-2.871333	4.449511
49	6	0	-0.827071	-2.892715	1.894586
50	6	0	0.032956	-2.786546	0.623720
51	8	0	0.588387	-1.460755	0.530448
52	6	0	-0.618933	-3.177229	-0.700234
53	8	0	1.169981	-3.645593	0.810699
54	1	0	3.959430	-1.392064	0.610771
55	6	0	2.804712	-1.881000	-1.159142
56	6	0	3.067030	-1.487068	-2.411987
57	6	0	2.558418	-2.296015	-3.625519
58	8	0	3.088122	-1.997995	-4.729210

59	8	0	1.642424	-3.138506	-3.393229
60	6	0	3.832734	-0.216466	-2.658665
61	6	0	4.355704	0.376294	-1.346620
62	1	0	-1.412808	4.367145	3.539042
63	1	0	0.430468	4.283430	3.480839
64	1	0	-1.950290	0.836870	3.086524
65	1	0	-2.734291	2.410197	3.242439
66	1	0	-3.160772	3.796797	1.212041
67	1	0	-1.592407	3.610489	0.436864
68	1	0	-3.464975	3.988645	-1.252454
69	1	0	-2.592082	2.477907	-1.501935
70	1	0	-5.809717	3.977475	-0.529341
71	1	0	-6.633136	2.480575	-0.071754
72	1	0	-5.432721	3.193943	1.023723
73	1	0	-4.445384	1.348769	-2.460066
74	1	0	-5.985609	0.198395	1.210857
75	1	0	-6.274589	0.165609	-0.543998
76	1	0	-4.526433	-1.757672	1.085415
77	1	0	-5.717699	-2.183856	-0.157888
78	1	0	-4.669542	-2.704264	-2.311546
79	1	0	-5.056163	-1.015693	-2.661244
80	1	0	-3.359993	-1.986092	-4.292045
81	1	0	-2.683011	-0.629799	-3.395820
82	1	0	-2.273819	-3.604419	-2.759134
83	1	0	-1.027499	-2.503548	-3.350222
84	1	0	0.619168	0.869809	3.430201
85	1	0	0.403126	1.058858	1.717646
86	1	0	1.942946	3.092765	1.789907
87	1	0	2.108519	2.855941	3.512166
88	1	0	4.011902	1.800259	3.000191
89	1	0	3.012708	0.414770	2.809575
90	1	0	3.503441	4.501926	0.111740
91	1	0	4.925896	4.143446	-0.866177
92	1	0	3.718731	5.122424	-2.637165
93	1	0	2.250618	4.413481	-3.309063
94	1	0	2.178441	5.307155	-1.781800
95	1	0	0.886341	2.273288	-3.055735
96	1	0	-0.231418	2.116698	-1.703014
97	1	0	0.274985	3.724410	-2.232475
98	1	0	1.150860	0.869540	-0.007364
99	1	0	1.662594	0.510845	-1.605388
100	1	0	1.212143	-4.937623	2.641785
101	1	0	-0.186285	-2.517978	5.328141
102	1	0	-1.739707	-2.421896	4.476060
103	1	0	-0.845849	-3.956450	4.540852
104	1	0	-1.182048	-3.928901	1.974200
105	1	0	-1.711356	-2.258119	1.794858
106	1	0	-1.133530	-4.137230	-0.570283
107	1	0	0.188380	-3.320381	-1.430192
108	1	0	2.297681	-2.831107	-1.048941
109	1	0	4.666997	-0.440349	-3.333924
110	1	0	3.210236	0.495837	-3.221596
111	1	0	4.828187	1.343672	-1.530174
112	1	0	5.155343	-0.262111	-0.963266
113	8	0	5.199067	0.755438	1.253056
114	1	0	5.410708	1.905254	0.586931

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	-1340.7609	26.0895	31.6396
Red. masses --	1.1749	5.0466	4.3458
Frc consts --	1.2444	0.0020	0.0026
IR Inten --	380.7681	0.9213	0.8951

structure 2e

ENERGY:

Final Energy in Hartrees: HF = -2406.8896754 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.779615	2.179140	4.541529
2	6	0	-1.547255	1.325360	3.534350
3	6	0	-2.693463	0.609770	2.841928
4	6	0	-2.887819	0.952726	1.355342
5	1	0	-2.001493	0.658731	0.779097
6	6	0	-3.201569	2.427546	1.105335
7	6	0	-3.637611	2.649697	-0.348423
8	6	0	-4.780627	1.707353	-0.772204
9	6	0	-6.106027	2.085941	-0.106892
10	8	0	-5.010584	1.825888	-2.182092
11	8	0	-3.991483	0.122064	0.922482
12	6	0	-4.374897	0.236923	-0.440191
13	6	0	-5.449113	-0.827399	-0.693539
14	6	0	-4.626293	-2.060068	-1.073840
15	6	0	-3.415523	-1.479156	-1.819469
16	6	0	-3.578055	-1.421477	-3.346428
17	6	0	-2.293384	-0.940992	-4.032098
18	6	0	-1.114059	-1.812972	-3.584471
19	6	0	-1.013240	-1.850061	-2.056982
20	1	0	-0.758035	-0.851302	-1.684156
21	8	0	-2.284202	-2.235366	-1.465105
22	8	0	-3.298910	-0.110491	-1.323542
23	6	0	-0.159541	0.972357	3.036102
24	6	0	1.032336	1.487405	3.853486
25	6	0	2.405931	1.038820	3.300255
26	6	0	2.708626	1.681567	1.937041
27	7	0	1.491508	5.464544	0.442170
28	1	0	1.443177	6.455432	0.659769
29	6	0	1.942601	5.250174	-0.941459
30	6	0	2.445001	3.811872	-1.188175
31	1	0	3.343847	3.699111	-0.574709
32	6	0	2.864146	3.675354	-2.662576
33	6	0	1.435276	2.730767	-0.708424
34	1	0	1.042228	3.084714	0.248031
35	6	0	0.228306	2.618615	-1.662653
36	6	0	2.007588	1.302751	-0.506627
37	6	0	3.038270	0.923426	0.627649
38	6	0	3.135233	-0.653316	0.730851
39	6	0	1.885336	-1.472323	1.147737
40	1	0	1.513956	-1.088909	2.098832
41	6	0	2.160933	-2.992847	1.289238
42	1	0	3.222550	-3.245385	1.329783
43	6	0	1.385372	-3.667293	2.434266
44	1	0	1.778767	-3.345487	3.407233
45	8	0	1.615451	-5.077759	2.375249
46	6	0	-0.117635	-3.303424	2.338273
47	1	0	-0.201593	-2.261011	2.671331
48	6	0	-0.983943	-4.151123	3.276014
49	6	0	-0.620155	-3.355125	0.877708
50	6	0	0.418481	-2.794458	-0.112014
51	8	0	0.779784	-1.445281	0.221840
52	6	0	0.039853	-2.853888	-1.590026
53	8	0	1.630529	-3.534308	0.068436
54	1	0	3.814756	-0.841588	1.583516
55	6	0	3.788774	-1.232845	-0.517290
56	6	0	4.651702	-0.584600	-1.311895
57	6	0	5.237830	-1.261856	-2.578475
58	8	0	6.052989	-0.543690	-3.221895

59	8	0	4.839839	-2.429247	-2.827853
60	6	0	5.047146	0.839714	-1.033162
61	6	0	4.511772	1.368672	0.303127
62	1	0	-2.792663	2.393522	4.871902
63	1	0	-0.980053	2.692240	5.065820
64	1	0	-2.537429	-0.475467	2.905325
65	1	0	-3.633300	0.829017	3.361703
66	1	0	-3.990333	2.748398	1.798331
67	1	0	-2.317654	3.034189	1.330525
68	1	0	-3.957643	3.685271	-0.510563
69	1	0	-2.783387	2.473084	-1.011573
70	1	0	-6.331055	3.135248	-0.322040
71	1	0	-6.924502	1.479241	-0.503449
72	1	0	-6.062298	1.948720	0.975741
73	1	0	-4.209173	1.494530	-2.615015
74	1	0	-6.070966	-0.975596	0.191386
75	1	0	-6.084359	-0.505714	-1.523949
76	1	0	-4.259837	-2.578578	-0.184208
77	1	0	-5.175730	-2.776361	-1.690628
78	1	0	-3.814347	-2.436721	-3.690500
79	1	0	-4.434228	-0.784023	-3.594573
80	1	0	-2.409708	-0.978084	-5.121514
81	1	0	-2.097237	0.106005	-3.768103
82	1	0	-1.245640	-2.837364	-3.960506
83	1	0	-0.169560	-1.436411	-3.992432
84	1	0	-0.112032	-0.122378	2.970709
85	1	0	-0.061663	1.316887	1.996781
86	1	0	1.025039	2.581957	3.878256
87	1	0	0.942992	1.138367	4.889795
88	1	0	3.183085	1.419261	3.974823
89	1	0	2.494416	-0.047204	3.297891
90	1	0	1.100068	5.472682	-1.611791
91	1	0	2.760043	5.932021	-1.235159
92	1	0	3.701264	4.345681	-2.889232
93	1	0	3.188152	2.660475	-2.906980
94	1	0	2.042452	3.935129	-3.340557
95	1	0	0.513895	2.197489	-2.633689
96	1	0	-0.537131	1.960750	-1.237710
97	1	0	-0.235988	3.594859	-1.840769
98	1	0	1.140595	0.658326	-0.349067
99	1	0	2.444381	0.949442	-1.445075
100	1	0	1.603027	-5.319658	1.435852
101	1	0	-0.655667	-4.049401	4.317485
102	1	0	-2.033095	-3.838309	3.219781
103	1	0	-0.923188	-5.211077	3.012437
104	1	0	-0.822539	-4.393623	0.583155
105	1	0	-1.559624	-2.807859	0.776394
106	1	0	-0.296070	-3.868496	-1.833714
107	1	0	0.964008	-2.666681	-2.146977
108	1	0	3.543850	-2.250950	-0.805713
109	1	0	6.140250	0.918013	-1.055355
110	1	0	4.719994	1.467996	-1.870102
111	1	0	4.583461	2.457357	0.346322
112	1	0	5.148053	0.988617	1.116403
113	8	0	2.737443	2.908156	1.932474
114	1	0	2.129370	5.024985	1.102740

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	27.8590	35.3493	43.8415
Red. masses --	5.2367	5.2065	5.2020
Frc consts --	0.0024	0.0038	0.0059
IR Inten --	0.4412	0.3584	0.8688

structure 2e'

ENERGY:

Final Energy in Hartrees: HF = -2406.8905871 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.987107	-0.115259	5.098168
2	6	0	1.692017	0.262056	3.846045
3	6	0	2.790590	0.625329	2.861192
4	6	0	2.909021	-0.295352	1.634543
5	1	0	1.992372	-0.246518	1.033253
6	6	0	3.215579	-1.748717	1.994226
7	6	0	3.568837	-2.552850	0.737799
8	6	0	4.690658	-1.891898	-0.086989
9	6	0	6.047528	-1.991664	0.613944
10	8	0	4.848469	-2.582168	-1.332616
11	8	0	3.985326	0.264346	0.844572
12	6	0	4.300673	-0.406268	-0.367806
13	6	0	5.359656	0.440203	-1.084165
14	6	0	4.516842	1.423128	-1.899984
15	6	0	3.275006	0.607329	-2.288466
16	6	0	3.369512	-0.076625	-3.661583
17	6	0	2.057645	-0.777905	-4.034393
18	6	0	0.893412	0.214856	-3.927444
19	6	0	0.865609	0.871524	-2.544814
20	1	0	0.648691	0.113537	-1.783111
21	8	0	2.158391	1.458086	-2.229576
22	8	0	3.183671	-0.433412	-1.266740
23	6	0	0.276317	0.397856	3.321675
24	6	0	-0.874939	0.210769	4.318828
25	6	0	-2.276371	0.375264	3.682376
26	6	0	-2.592244	-0.765907	2.698131
27	7	0	-3.104848	-5.643646	0.068436
28	1	0	-2.956458	-5.411180	1.046480
29	6	0	-1.983248	-5.197159	-0.768594
30	6	0	-1.903076	-3.663651	-0.896717
31	1	0	-2.847801	-3.341417	-1.351025
32	6	0	-0.766815	-3.304260	-1.869737
33	6	0	-1.804868	-2.935316	0.478291
34	1	0	-2.654010	-3.280689	1.072526
35	6	0	-0.526963	-3.311325	1.251957
36	6	0	-1.936837	-1.390804	0.312271
37	6	0	-2.964053	-0.599885	1.202168
38	6	0	-3.106418	0.882360	0.676363
39	6	0	-1.861393	1.805404	0.684199
40	1	0	-1.443002	1.829978	1.691339
41	6	0	-2.159840	3.256857	0.225572
42	1	0	-3.223390	3.504774	0.217975
43	6	0	-1.344694	4.331661	0.965628
44	1	0	-1.682911	4.423673	2.005911
45	8	0	-1.607383	5.602036	0.363265
46	6	0	0.159556	3.959681	0.942326
47	1	0	0.279484	3.136109	1.657398
48	6	0	1.051909	5.110777	1.418507
49	6	0	0.590474	3.422897	-0.441413
50	6	0	-0.483871	2.515155	-1.069892
51	8	0	-0.800294	1.410222	-0.208506
52	6	0	-0.179976	1.981713	-2.467571
53	8	0	-1.699311	3.268804	-1.134668
54	1	0	-3.767969	1.383205	1.407946
55	6	0	-3.801745	0.912883	-0.678329
56	6	0	-4.629975	-0.029461	-1.149953
57	6	0	-5.252876	0.096633	-2.565694
58	8	0	-6.103675	-0.793042	-2.842768

59	8	0	-4.844556	1.053209	-3.275411
60	6	0	-4.956782	-1.254904	-0.342459
61	6	0	-4.407533	-1.204099	1.089772
62	1	0	3.018183	-0.187265	5.434500
63	1	0	1.220949	-0.363082	5.825598
64	1	0	2.623744	1.644343	2.487442
65	1	0	3.759635	0.627036	3.373384
66	1	0	4.043466	-1.773452	2.714794
67	1	0	2.348207	-2.191767	2.495078
68	1	0	3.875698	-3.573558	0.993298
69	1	0	2.679608	-2.636066	0.101560
70	1	0	6.259285	-3.040105	0.846256
71	1	0	6.844881	-1.625045	-0.038000
72	1	0	6.061757	-1.414038	1.540758
73	1	0	4.032412	-2.426419	-1.832181
74	1	0	6.024774	0.926972	-0.368315
75	1	0	5.952453	-0.206530	-1.737526
76	1	0	4.190791	2.266647	-1.286164
77	1	0	5.035124	1.814396	-2.779549
78	1	0	3.587516	0.703761	-4.402110
79	1	0	4.216311	-0.772404	-3.660865
80	1	0	2.123670	-1.188830	-5.048526
81	1	0	1.880446	-1.624282	-3.358901
82	1	0	0.997716	0.996002	-4.693499
83	1	0	-0.065681	-0.284633	-4.102643
84	1	0	0.200877	1.392159	2.862732
85	1	0	0.146755	-0.302857	2.485615
86	1	0	-0.828682	-0.787974	4.765571
87	1	0	-0.773581	0.935867	5.135978
88	1	0	-3.023915	0.279207	4.479557
89	1	0	-2.399558	1.369307	3.252622
90	1	0	-1.005968	-5.586726	-0.430067
91	1	0	-2.147781	-5.609024	-1.771951
92	1	0	-0.955800	-3.737738	-2.858870
93	1	0	-0.676011	-2.222096	-2.000242
94	1	0	0.201905	-3.684190	-1.522016
95	1	0	0.372242	-2.964616	0.729422
96	1	0	-0.537884	-2.861640	2.247416
97	1	0	-0.429852	-4.395195	1.388013
98	1	0	-0.952118	-0.928674	0.436739
99	1	0	-2.227268	-1.159137	-0.715016
100	1	0	-1.646930	5.450096	-0.594132
101	1	0	0.777016	5.431669	2.430583
102	1	0	2.103766	4.802410	1.434999
103	1	0	0.954796	5.978349	0.759253
104	1	0	0.759387	4.256513	-1.135876
105	1	0	1.534530	2.879364	-0.362447
106	1	0	0.127179	2.813868	-3.111632
107	1	0	-1.126986	1.591991	-2.855723
108	1	0	-3.607356	1.752078	-1.339674
109	1	0	-6.044140	-1.388727	-0.323640
110	1	0	-4.590950	-2.142722	-0.873021
111	1	0	-4.416278	-2.199526	1.541028
112	1	0	-5.070353	-0.580288	1.707621
113	8	0	-2.575976	-1.892297	3.181763
114	1	0	-3.216963	-6.651824	0.012627

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	28.6240	35.6940	40.5620
Red. masses --	4.5205	4.4983	5.2323
Frc consts --	0.0022	0.0034	0.0051
IR Inten --	0.4496	0.7572	0.7551

structure 2e"

ENERGY:

Final Energy in Hartrees: HF = -2406.8982746 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.062175	3.543516	3.522679
2	6	0	2.543857	2.973700	2.425529
3	6	0	3.436859	2.388613	1.347555
4	6	0	3.370530	0.854216	1.224427
5	1	0	2.367859	0.539818	0.910604
6	6	0	3.750036	0.121388	2.510451
7	6	0	3.911226	-1.380438	2.246585
8	6	0	4.880550	-1.671308	1.084307
9	6	0	6.331252	-1.358703	1.457234
10	8	0	4.857690	-3.069488	0.768714
11	8	0	4.293684	0.522323	0.158776
12	6	0	4.423153	-0.854704	-0.165309
13	6	0	5.334940	-0.936844	-1.395914
14	6	0	4.348415	-0.804188	-2.559115
15	6	0	3.083314	-1.508145	-2.047651
16	6	0	2.985988	-2.992835	-2.434336
17	6	0	1.656581	-3.608115	-1.980468
18	6	0	0.490117	-2.762572	-2.504781
19	6	0	0.658798	-1.296457	-2.101307
20	1	0	0.593896	-1.207929	-1.011070
21	8	0	1.963630	-0.796362	-2.510771
22	8	0	3.178131	-1.422079	-0.593767
23	6	0	1.051757	2.884636	2.159383
24	6	0	0.125893	2.847045	3.388389
25	6	0	-1.296922	2.369463	3.047120
26	6	0	-1.314337	0.918227	2.528909
27	7	0	-3.340731	-2.611617	-1.461784
28	1	0	-4.095419	-1.917776	-1.575366
29	6	0	-3.641940	-3.488949	-0.313781
30	6	0	-2.583347	-3.520218	0.829040
31	1	0	-1.589161	-3.516603	0.355184
32	6	0	-2.741633	-4.861680	1.573774
33	6	0	-2.660146	-2.290649	1.794143
34	1	0	-3.726549	-2.154385	2.016023
35	6	0	-1.937193	-2.545587	3.132000
36	6	0	-2.120462	-1.021135	1.082403
37	6	0	-2.472230	0.401575	1.649347
38	6	0	-2.810581	1.406452	0.463874
39	6	0	-1.618133	1.944720	-0.356428
40	1	0	-1.078113	2.661860	0.272651
41	6	0	-2.001478	2.619577	-1.694194
42	1	0	-3.055614	2.895397	-1.760985
43	6	0	-1.097632	3.799451	-2.091182
44	1	0	-1.282537	4.660102	-1.435521
45	8	0	-1.462667	4.232057	-3.405463
46	6	0	0.389755	3.380669	-1.994141
47	1	0	0.621937	3.321567	-0.923327
48	6	0	1.330430	4.420409	-2.612513
49	6	0	0.609770	1.971085	-2.584700
50	6	0	-0.521943	1.002505	-2.194177
51	8	0	-0.673004	0.940955	-0.767841
52	6	0	-0.411459	-0.416319	-2.743276
53	8	0	-1.758891	1.572402	-2.649988
54	1	0	-3.193091	2.320530	0.947697
55	6	0	-3.946526	0.805449	-0.337104
56	6	0	-4.995200	0.224220	0.261978
57	6	0	-6.130478	-0.421399	-0.549234
58	8	0	-7.262248	-0.394125	-0.003352

59	8	0	-5.800448	-0.921976	-1.665613
60	6	0	-5.089876	0.143889	1.766526
61	6	0	-3.767989	0.441549	2.531979
62	1	0	4.137166	3.604786	3.672017
63	1	0	2.437954	3.963040	4.306235
64	1	0	3.162408	2.806906	0.369669
65	1	0	4.480600	2.666355	1.534939
66	1	0	4.680475	0.546712	2.910136
67	1	0	2.972300	0.289128	3.262363
68	1	0	4.269095	-1.903513	3.140986
69	1	0	2.932223	-1.805695	1.995140
70	1	0	6.598247	-1.908381	2.365400
71	1	0	7.010260	-1.675715	0.660941
72	1	0	6.475992	-0.290812	1.634513
73	1	0	3.966374	-3.255659	0.436302
74	1	0	6.092371	-0.150925	-1.375927
75	1	0	5.833161	-1.910657	-1.410065
76	1	0	4.101930	0.243948	-2.747468
77	1	0	4.711139	-1.248086	-3.490217
78	1	0	3.058345	-3.052057	-3.528205
79	1	0	3.845765	-3.531190	-2.019558
80	1	0	1.577913	-4.642093	-2.337068
81	1	0	1.617058	-3.646591	-0.884298
82	1	0	0.447414	-2.829360	-3.601758
83	1	0	-0.469942	-3.117601	-2.115283
84	1	0	0.773044	3.731825	1.513002
85	1	0	0.870294	1.989431	1.559189
86	1	0	0.551429	2.164917	4.130039
87	1	0	0.064813	3.837839	3.855243
88	1	0	-1.912480	2.385667	3.957590
89	1	0	-1.792491	3.049190	2.346887
90	1	0	-4.614880	-3.218040	0.120570
91	1	0	-3.752153	-4.522447	-0.670589
92	1	0	-2.698947	-5.697740	0.865367
93	1	0	-1.958759	-5.024745	2.319299
94	1	0	-3.710572	-4.919226	2.088221
95	1	0	-0.888610	-2.822829	2.965886
96	1	0	-1.921936	-1.647851	3.753785
97	1	0	-2.415746	-3.342310	3.710930
98	1	0	-1.030612	-1.104670	1.049265
99	1	0	-2.456921	-1.061254	0.050335
100	1	0	-1.636498	3.428443	-3.920293
101	1	0	1.208391	5.399264	-2.132877
102	1	0	2.376129	4.113680	-2.493325
103	1	0	1.125629	4.547373	-3.679705
104	1	0	0.640025	2.016833	-3.681693
105	1	0	1.568972	1.564825	-2.257323
106	1	0	-0.244570	-0.370954	-3.826084
107	1	0	-1.380049	-0.896306	-2.563804
108	1	0	-3.886961	0.770821	-1.420559
109	1	0	-5.873097	0.831445	2.109723
110	1	0	-5.473196	-0.849096	2.026511
111	1	0	-3.663415	-0.254074	3.371075
112	1	0	-3.835561	1.442770	2.974163
113	8	0	-0.396102	0.187778	2.874923
114	1	0	-3.361161	-3.161106	-2.316088

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	24.0812	38.4166	41.9284
Red. masses --	5.0389	4.8392	4.7674
Frc consts --	0.0017	0.0042	0.0049
IR Inten --	0.1275	0.0473	0.7404

structure 13a

ENERGY:

Final Energy in Hartrees: HF = -905.9109804 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.363119	-2.451251	1.015851
2	6	0	1.301227	-1.199164	0.158234
3	7	0	2.394846	-0.921063	-0.460047
4	1	0	3.958317	-1.870991	-0.355688
5	6	0	2.500661	0.199999	-1.394689
6	6	0	2.555225	1.578329	-0.707214
7	1	0	2.483938	2.321065	-1.517645
8	6	0	3.894844	1.791954	0.016645
9	6	0	1.340411	1.790764	0.234778
10	1	0	1.608003	1.375394	1.214695
11	6	0	1.050690	3.288975	0.430499
12	6	0	0.078283	1.066111	-0.279866
13	6	0	-0.054615	-0.465558	0.023409
14	6	0	-0.952688	-0.666877	1.298432
15	6	0	-0.472147	0.095701	2.549430
16	1	0	0.569681	-0.129189	2.808124
17	1	0	-0.913029	-1.733324	1.556558
18	6	0	-2.408834	-0.342257	1.018928
19	6	0	-2.986930	-0.294867	-0.190150
20	6	0	-4.489356	0.054859	-0.353596
21	8	0	-4.898288	0.052283	-1.548753
22	8	0	-5.128574	0.301221	0.701785
23	6	0	-2.188674	-0.562845	-1.439858
24	6	0	-0.807398	-1.173149	-1.154318
25	1	0	1.211830	-2.227226	2.076702
26	1	0	2.335550	-2.929819	0.889734
27	1	0	3.423740	0.049287	-1.966811
28	1	0	1.678082	0.180263	-2.117887
29	1	0	4.737842	1.717744	-0.680434
30	1	0	3.942973	2.777143	0.492998
31	1	0	4.037637	1.035833	0.797037
32	1	0	0.694779	3.739429	-0.504871
33	1	0	0.273395	3.444447	1.186531
34	1	0	1.941765	3.841768	0.749613
35	1	0	-0.808435	1.546656	0.143314
36	1	0	-0.002084	1.239828	-1.359790
37	1	0	-3.048820	-0.140852	1.877178
38	1	0	-2.767110	-1.224500	-2.093511
39	1	0	-2.095282	0.369989	-2.013562
40	1	0	-0.185509	-1.144847	-2.058838
41	1	0	-0.931202	-2.233112	-0.895428
42	8	0	4.837029	-2.332074	-0.310356
43	1	0	5.347179	-1.831041	0.336620
44	1	0	-0.564738	1.179212	2.423148
45	1	0	-1.097072	-0.180296	3.406055
46	1	0	0.580409	-3.161215	0.725994

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	31.0524	39.7417	45.6927
Red. masses --	6.3093	11.5724	7.2128
Frc consts --	0.0036	0.0108	0.0089
IR Inten --	6.0627	0.4525	11.9175

structure 13b

ENERGY:

Final Energy in Hartrees: HF = -905.8395094 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.300550	2.360277	1.585906
2	6	0	-1.358549	1.299799	0.519860
3	7	0	-2.580372	0.977198	0.126617
4	1	0	-3.184985	1.797416	0.193606
5	6	0	-2.901976	0.175860	-1.066595
6	6	0	-2.856928	-1.334471	-0.809419
7	1	0	-2.863301	-1.809034	-1.802803
8	6	0	-4.102834	-1.806360	-0.041812
9	6	0	-1.542327	-1.740955	-0.096585
10	1	0	-1.706735	-1.607039	0.978749
11	6	0	-1.218929	-3.225948	-0.336098
12	6	0	-0.346869	-0.865414	-0.538185
13	6	0	-0.103634	0.513169	0.161229
14	6	0	0.802869	0.313757	1.443894
15	6	0	0.247795	-0.664914	2.497772
16	1	0	-0.774561	-0.421107	2.812314
17	1	0	0.867625	1.291544	1.936968
18	6	0	2.217544	-0.085836	1.069295
19	6	0	2.802116	0.104455	-0.122161
20	6	0	4.254455	-0.371088	-0.388342
21	8	0	4.673481	-0.140318	-1.556714
22	8	0	4.848214	-0.930297	0.570412
23	6	0	2.049928	0.759054	-1.251103
24	6	0	0.737582	1.423354	-0.811134
25	1	0	-2.164650	3.018316	1.500057
26	1	0	-0.406045	2.972197	1.475050
27	1	0	-3.907499	0.479930	-1.368970
28	1	0	-2.232811	0.488573	-1.870145
29	1	0	-5.019119	-1.602916	-0.609219
30	1	0	-4.071568	-2.881726	0.161479
31	1	0	-4.181472	-1.287159	0.920981
32	1	0	-0.964430	-3.400745	-1.389181
33	1	0	-0.360304	-3.542879	0.265234
34	1	0	-2.063037	-3.877627	-0.083082
35	1	0	0.575706	-1.431298	-0.384442
36	1	0	-0.409022	-0.716291	-1.622939
37	1	0	2.816995	-0.569242	1.839919
38	1	0	2.699600	1.505979	-1.720729
39	1	0	1.877639	0.018612	-2.044513
40	1	0	0.108462	1.700263	-1.660929
41	1	0	0.960403	2.359257	-0.286879
42	8	0	-2.017977	3.083582	-0.976290
43	1	0	-1.712519	3.883636	-1.427011
44	1	0	0.259538	-1.697704	2.135852
45	1	0	0.886725	-0.632790	3.387378
46	1	0	-1.275921	1.889281	2.578552

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	-223.6630	39.2431	47.0723
Red. masses --	2.3588	11.5582	4.8342
Frc consts --	0.0695	0.0105	0.0063
IR Inten --	25.9508	0.2081	9.9373

structure 13c

ENERGY:

Final Energy in Hartrees: HF = -905.8874997 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.395813	-2.824776	0.924686
2	6	0	1.488505	-1.634541	-0.050431
3	7	0	2.726350	-0.910636	0.312993
4	1	0	2.690299	-0.580060	1.270380
5	6	0	3.249368	0.104600	-0.604464
6	6	0	2.767137	1.557118	-0.429495
7	1	0	3.100851	2.080725	-1.340498
8	6	0	3.462456	2.240504	0.762161
9	6	0	1.222438	1.711356	-0.334368
10	1	0	0.968673	1.804335	0.723557
11	6	0	0.790721	3.031636	-1.003395
12	6	0	0.385479	0.551638	-0.924437
13	6	0	0.154408	-0.782647	-0.145704
14	6	0	-0.543730	-0.614961	1.263374
15	6	0	0.194744	0.067607	2.437652
16	1	0	1.215007	-0.298435	2.597056
17	1	0	-0.700688	-1.647630	1.606224
18	6	0	-1.926721	0.002351	1.124408
19	6	0	-2.723345	-0.119167	0.053082
20	6	0	-4.126140	0.539390	0.011740
21	8	0	-4.760844	0.354534	-1.064938
22	8	0	-4.480967	1.179790	1.036659
23	6	0	-2.257227	-0.878213	-1.162647
24	6	0	-0.900268	-1.589162	-0.981278
25	1	0	2.289735	-3.444321	0.796387
26	1	0	0.514403	-3.434672	0.715666
27	1	0	4.347388	0.097938	-0.523659
28	1	0	3.014034	-0.236069	-1.615142
29	1	0	4.552826	2.247706	0.639407
30	1	0	3.131779	3.279008	0.876630
31	1	0	3.234922	1.725829	1.704754
32	1	0	0.919585	2.973194	-2.092499
33	1	0	-0.263501	3.248307	-0.803071
34	1	0	1.384025	3.881558	-0.643941
35	1	0	-0.608242	0.966684	-1.100827
36	1	0	0.776168	0.293504	-1.918557
37	1	0	-2.319383	0.565913	1.969780
38	1	0	-3.024102	-1.611261	-1.439535
39	1	0	-2.234483	-0.190390	-2.018757
40	1	0	-0.478613	-1.829848	-1.960371
41	1	0	-1.072711	-2.548915	-0.477517
42	8	0	1.723514	-2.166802	-1.365206
43	1	0	2.592378	-2.592461	-1.322011
44	1	0	0.233851	1.154909	2.339696
45	1	0	-0.364372	-0.140147	3.358031
46	1	0	1.360262	-2.507506	1.970440

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	22.0696	34.9155	44.3077
Red. masses --	3.3525	12.9538	4.8840
Frc consts --	0.0010	0.0093	0.0056
IR Inten --	1.5735	0.7795	7.4382

structure 13d

ENERGY:

Final Energy in Hartrees: HF = -905.8261583 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.417159	-2.566646	1.310257
2	6	0	1.353180	-1.696814	0.036878
3	7	0	2.855682	-1.021433	0.008703
4	1	0	3.323588	-0.883965	0.906322
5	6	0	3.191490	0.006129	-1.002686
6	6	0	2.866655	1.456571	-0.643184
7	1	0	2.933789	2.013829	-1.591137
8	6	0	3.918134	2.043388	0.316526
9	6	0	1.426820	1.614600	-0.095178
10	1	0	1.484632	1.412819	0.976409
11	6	0	0.941867	3.067142	-0.263112
12	6	0	0.391819	0.646961	-0.731538
13	6	0	0.091689	-0.733871	-0.071395
14	6	0	-0.695123	-0.568364	1.289718
15	6	0	-0.056621	0.254361	2.433892
16	1	0	0.997167	0.017185	2.620624
17	1	0	-0.805687	-1.586828	1.684975
18	6	0	-2.105641	-0.037029	1.072747
19	6	0	-2.808054	-0.089267	-0.067977
20	6	0	-4.231126	0.518396	-0.164677
21	8	0	-4.767303	0.419245	-1.304171
22	8	0	-4.695418	1.043029	0.882442
23	6	0	-2.210156	-0.719784	-1.297685
24	6	0	-0.908346	-1.484557	-1.013884
25	1	0	2.329247	-3.171609	1.266608
26	1	0	0.574928	-3.262978	1.284485
27	1	0	4.264047	-0.093610	-1.218415
28	1	0	2.658717	-0.305142	-1.904073
29	1	0	4.923433	2.001112	-0.120569
30	1	0	3.706774	3.089175	0.559466
31	1	0	3.942007	1.491538	1.265629
32	1	0	0.794748	3.301606	-1.325284
33	1	0	-0.018210	3.217925	0.240524
34	1	0	1.652670	3.795214	0.144741
35	1	0	-0.566555	1.170700	-0.745625
36	1	0	0.645492	0.485945	-1.787951
37	1	0	-2.595752	0.426395	1.928317
38	1	0	-2.948703	-1.394928	-1.744503
39	1	0	-2.060986	0.053734	-2.064736
40	1	0	-0.390147	-1.734317	-1.942440
41	1	0	-1.156450	-2.443763	-0.540097
42	8	0	1.627820	-2.466932	-1.060162
43	1	0	2.856358	-2.043772	-0.620089
44	1	0	-0.139644	1.330226	2.253441
45	1	0	-0.607531	0.051161	3.360069
46	1	0	1.389023	-2.017647	2.255298

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	-1532.4721	15.8273	37.6059
Red. masses --	1.1060	3.4941	11.6085
Frc consts --	1.5303	0.0005	0.0097
IR Inten --	754.2165	2.4569	1.0354

structure 13e

ENERGY:

Final Energy in Hartrees: HF = -905.9031441 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434428	3.580337	0.407040
2	6	0	-0.877742	2.206949	-0.092647
3	7	0	-4.386580	0.135405	-0.074089
4	1	0	-5.228482	0.549930	-0.464704
5	6	0	-3.685146	-0.637133	-1.114492
6	6	0	-2.709567	-1.680909	-0.527832
7	1	0	-2.276898	-2.209375	-1.394197
8	6	0	-3.505009	-2.711214	0.296740
9	6	0	-1.505799	-1.075478	0.263269
10	1	0	-1.924637	-0.431207	1.045925
11	6	0	-0.693713	-2.207568	0.933016
12	6	0	-0.565736	-0.250585	-0.663919
13	6	0	0.136552	1.058635	-0.180353
14	6	0	0.984268	1.011384	1.142449
15	6	0	0.215152	0.754418	2.453766
16	1	0	-0.660793	1.406819	2.557053
17	1	0	1.382203	2.031982	1.251349
18	6	0	2.187044	0.100102	0.989903
19	6	0	2.802806	-0.163112	-0.172351
20	6	0	4.050096	-1.082393	-0.234159
21	8	0	4.533732	-1.228372	-1.391949
22	8	0	4.441751	-1.573580	0.855964
23	6	0	2.297055	0.410221	-1.473746
24	6	0	1.168679	1.446616	-1.303846
25	1	0	-1.145941	4.324426	0.042328
26	1	0	0.579362	3.848951	0.103374
27	1	0	-4.441786	-1.185672	-1.691045
28	1	0	-3.156821	0.016115	-1.822916
29	1	0	-4.363826	-3.076273	-0.280511
30	1	0	-2.898563	-3.578913	0.568983
31	1	0	-3.898040	-2.256510	1.211629
32	1	0	-0.509853	-3.016050	0.213370
33	1	0	0.288715	-1.862389	1.260588
34	1	0	-1.210144	-2.639155	1.796777
35	1	0	0.219380	-0.931062	-1.003183
36	1	0	-1.114520	0.043902	-1.563773
37	1	0	2.608496	-0.350305	1.887728
38	1	0	3.137862	0.867186	-2.007866
39	1	0	1.985741	-0.414924	-2.127188
40	1	0	0.637072	1.586679	-2.255048
41	1	0	1.620158	2.412467	-1.048960
42	8	0	-2.052256	2.073143	-0.420916
43	1	0	-3.791973	0.914368	0.199613
44	1	0	-0.124344	-0.276454	2.554075
45	1	0	0.881204	0.958423	3.300407
46	1	0	-0.460381	3.588072	1.502992

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	37.9255	40.7428	44.5338
Red. masses --	7.7908	6.0373	4.7329
Frc consts --	0.0066	0.0059	0.0055
IR Inten --	6.7261	1.9629	3.4483

structure 1f

ENERGY:

Final Energy in Hartrees: HF = -2483.3348069 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150814	4.472917	2.420083
2	6	0	-0.381894	3.202569	2.058964
3	6	0	-1.796962	2.652298	2.016083
4	6	0	-2.276580	2.158388	0.641300
5	1	0	-1.665214	1.311324	0.305957
6	6	0	-2.280661	3.250448	-0.428559
7	6	0	-3.009443	2.771555	-1.690300
8	6	0	-4.418537	2.225911	-1.383897
9	6	0	-5.389716	3.341691	-0.991374
10	8	0	-4.974343	1.629147	-2.562553
11	8	0	-3.620432	1.670816	0.865344
12	6	0	-4.305630	1.145994	-0.263072
13	6	0	-5.627497	0.565562	0.252703
14	6	0	-5.240959	-0.864071	0.641185
15	6	0	-4.168169	-1.248338	-0.387912
16	6	0	-4.711518	-1.992283	-1.618572
17	6	0	-3.582974	-2.440844	-2.554098
18	6	0	-2.548558	-3.248743	-1.761766
19	6	0	-2.060938	-2.459460	-0.543791
20	1	0	-1.517823	-1.568957	-0.879898
21	8	0	-3.184774	-2.010977	0.264499
22	8	0	-3.613710	0.028083	-0.835731
23	6	0	0.711650	2.208672	1.721431
24	6	0	2.163460	2.664915	1.906539
25	6	0	3.229771	1.636339	1.453228
26	6	0	3.184265	1.334193	-0.051953
27	7	0	3.448031	2.372256	-0.764528
28	1	0	4.185130	3.827894	-0.128629
29	6	0	3.507099	2.523020	-2.221076
30	6	0	2.662368	1.656990	-3.190988
31	1	0	3.235903	0.776108	-3.500932
32	6	0	2.419292	2.493434	-4.459902
33	6	0	1.382925	1.156788	-2.491604
34	1	0	0.994440	1.992478	-1.887967
35	6	0	0.266086	0.748099	-3.468677
36	6	0	1.660605	-0.047614	-1.563067
37	6	0	2.921467	-0.078530	-0.635105
38	6	0	2.749434	-1.274450	0.397273
39	6	0	1.578327	-1.261280	1.415125
40	1	0	1.588845	-0.319787	1.962957
41	6	0	1.624357	-2.436471	2.425270
42	1	0	2.597991	-2.928262	2.482521
43	6	0	1.096130	-2.086719	3.828426
44	1	0	1.788486	-1.408924	4.343828
45	8	0	1.070859	-3.280866	4.615948
46	6	0	-0.297294	-1.416557	3.717906
47	1	0	-0.117419	-0.399153	3.348525
48	6	0	-0.992030	-1.289195	5.078046
49	6	0	-1.188482	-2.126120	2.672764
50	6	0	-0.385519	-2.544910	1.428396
51	8	0	0.265492	-1.406894	0.837036
52	6	0	-1.151057	-3.302578	0.345346
53	8	0	0.691960	-3.377551	1.870864
54	1	0	3.631319	-1.216066	1.059780
55	6	0	2.794824	-2.609784	-0.339771
56	6	0	3.400895	-2.840112	-1.512466
57	6	0	3.309447	-4.223642	-2.205754
58	8	0	3.995228	-4.322641	-3.261003

59	8	0	2.562519	-5.077462	-1.660137
60	6	0	4.147605	-1.745547	-2.221558
61	6	0	4.255921	-0.471188	-1.376986
62	1	0	-0.971111	5.142464	2.666185
63	1	0	0.850775	4.883663	2.494698
64	1	0	-1.878629	1.805062	2.710401
65	1	0	-2.502001	3.417332	2.361308
66	1	0	-2.761495	4.149557	-0.021737
67	1	0	-1.248449	3.529399	-0.668834
68	1	0	-3.098977	3.578462	-2.426774
69	1	0	-2.427775	1.970470	-2.161813
70	1	0	-5.401914	4.103910	-1.776747
71	1	0	-6.404706	2.948481	-0.889013
72	1	0	-5.099982	3.809479	-0.047988
73	1	0	-4.434612	0.845831	-2.749663
74	1	0	-6.015017	1.152928	1.087216
75	1	0	-6.362688	0.570730	-0.557401
76	1	0	-4.785603	-0.891568	1.634362
77	1	0	-6.083170	-1.561013	0.626313
78	1	0	-5.251271	-2.875669	-1.253685
79	1	0	-5.437915	-1.354709	-2.135202
80	1	0	-3.990281	-3.037080	-3.378826
81	1	0	-3.099649	-1.564490	-3.004762
82	1	0	-2.995837	-4.193303	-1.421492
83	1	0	-1.685771	-3.505520	-2.385965
84	1	0	0.523085	1.315684	2.330149
85	1	0	0.563858	1.871632	0.685950
86	1	0	2.334532	3.585607	1.342143
87	1	0	2.347517	2.907569	2.959793
88	1	0	4.210153	2.073632	1.670641
89	1	0	3.166281	0.727600	2.050318
90	1	0	3.209591	3.567821	-2.390620
91	1	0	4.568377	2.482064	-2.506578
92	1	0	3.366902	2.895645	-4.839354
93	1	0	1.973746	1.897451	-5.261234
94	1	0	1.755932	3.344925	-4.259208
95	1	0	0.613738	-0.024833	-4.164817
96	1	0	-0.583930	0.331329	-2.917004
97	1	0	-0.101942	1.595163	-4.056226
98	1	0	0.780532	-0.178373	-0.930662
99	1	0	1.700067	-0.948373	-2.181395
100	1	0	0.754613	-3.989031	4.033056
101	1	0	-0.375707	-0.720433	5.784559
102	1	0	-1.951845	-0.770075	4.973134
103	1	0	-1.176328	-2.273829	5.517728
104	1	0	-1.627906	-3.036610	3.101605
105	1	0	-2.018430	-1.480497	2.375835
106	1	0	-1.739202	-4.101450	0.811711
107	1	0	-0.393607	-3.774549	-0.289814
108	1	0	2.267361	-3.451594	0.097791
109	1	0	5.145749	-2.107936	-2.492628
110	1	0	3.663142	-1.545889	-3.188138
111	1	0	4.632671	0.350124	-1.987053
112	1	0	5.012379	-0.624195	-0.594878
113	8	0	5.358375	4.608100	2.941857
114	1	0	6.305295	4.427161	2.947726
115	8	0	4.637029	4.644019	0.246218
116	1	0	4.087856	5.398610	0.003291
117	1	0	5.103941	4.620503	1.993485

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	24.3855	38.1508	42.2844
Red. masses --	5.1367	5.5853	4.9434
Frc consts --	0.0018	0.0048	0.0052
IR Inten --	0.1053	1.8426	0.8934

structure 1g

ENERGY:

Final Energy in Hartrees: HF = -2483.2882941 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.309001	-3.929119	3.262461
2	6	0	0.506716	-2.738215	2.678612
3	6	0	1.908417	-2.177272	2.512036
4	6	0	2.381764	-1.998168	1.059393
5	1	0	1.739162	-1.278062	0.537218
6	6	0	2.438389	-3.308536	0.273590
7	6	0	3.150553	-3.105167	-1.069304
8	6	0	4.530234	-2.436619	-0.909603
9	6	0	5.552439	-3.385991	-0.280664
10	8	0	5.056361	-2.100193	-2.198894
11	8	0	3.702549	-1.419190	1.161307
12	6	0	4.364074	-1.133143	-0.066001
13	6	0	5.659775	-0.394217	0.286999
14	6	0	5.213859	1.068809	0.342686
15	6	0	4.104827	1.165859	-0.717113
16	6	0	4.582450	1.652771	-2.094335
17	6	0	3.412334	1.847564	-3.067071
18	6	0	2.364947	2.769377	-2.432296
19	6	0	1.936846	2.238616	-1.063650
20	1	0	1.410947	1.285106	-1.188634
21	8	0	3.093712	1.993551	-0.208838
22	8	0	3.622238	-0.210553	-0.868963
23	6	0	-0.614391	-1.846107	2.179520
24	6	0	-2.047637	-2.275236	2.512040
25	6	0	-3.207814	-1.356095	2.031496
26	6	0	-3.433046	-1.308993	0.519793
27	7	0	-3.731395	-2.502464	0.047791
28	1	0	-4.173518	-3.115234	0.744926
29	6	0	-3.943797	-3.017101	-1.312812
30	6	0	-2.905776	-2.625490	-2.395277
31	1	0	-3.320869	-1.821981	-3.011534
32	6	0	-2.719046	-3.845111	-3.316167
33	6	0	-1.594335	-2.095625	-1.771449
34	1	0	-1.320732	-2.785493	-0.958138
35	6	0	-0.424333	-2.085359	-2.771502
36	6	0	-1.718190	-0.659553	-1.194621
37	6	0	-3.017098	-0.186418	-0.444847
38	6	0	-2.762781	1.236046	0.213165
39	6	0	-1.605612	1.428106	1.233891
40	1	0	-1.611235	0.626553	1.969932
41	6	0	-1.648839	2.789337	1.973727
42	1	0	-2.631857	3.266439	1.958573
43	6	0	-1.072993	2.756499	3.401580
44	1	0	-1.728996	2.187866	4.073065
45	8	0	-1.064888	4.091470	3.916618
46	6	0	0.338691	2.113379	3.388939
47	1	0	0.177037	1.037629	3.245837
48	6	0	1.070579	2.291822	4.723266
49	6	0	1.183497	2.603399	2.188895
50	6	0	0.333355	2.715465	0.911619
51	8	0	-0.298955	1.451277	0.629783
52	6	0	1.025688	3.229910	-0.348076
53	8	0	-0.753086	3.604871	1.206879
54	1	0	-3.673948	1.434176	0.801778
55	6	0	-2.597048	2.288261	-0.877048
56	6	0	-2.977825	2.183722	-2.156139
57	6	0	-2.523911	3.226674	-3.203931
58	8	0	-3.149708	3.190049	-4.296722

59	8	0	-1.559367	3.971505	-2.867418
60	6	0	-3.806733	1.015879	-2.606682
61	6	0	-4.206775	0.115208	-1.433988
62	1	0	1.146298	-4.526675	3.613446
63	1	0	-0.680818	-4.346699	3.415132
64	1	0	1.967250	-1.192942	2.994893
65	1	0	2.628684	-2.827791	3.021441
66	1	0	2.958005	-4.065299	0.875810
67	1	0	1.421300	-3.682495	0.110376
68	1	0	3.281129	-4.057009	-1.597119
69	1	0	2.534941	-2.465245	-1.711528
70	1	0	5.609412	-4.302434	-0.876616
71	1	0	6.545864	-2.930027	-0.270681
72	1	0	5.277966	-3.646622	0.743921
73	1	0	4.490635	-1.392226	-2.544036
74	1	0	6.077205	-0.758056	1.227936
75	1	0	6.390534	-0.554304	-0.511131
76	1	0	4.774760	1.309205	1.314220
77	1	0	6.023655	1.776278	0.144834
78	1	0	5.088228	2.615105	-1.941627
79	1	0	5.328286	0.951099	-2.486098
80	1	0	3.774650	2.265900	-4.013369
81	1	0	2.956488	0.877255	-3.303507
82	1	0	2.785089	3.777635	-2.309338
83	1	0	1.474556	2.867778	-3.062522
84	1	0	-0.425498	-0.845149	2.584060
85	1	0	-0.503860	-1.728484	1.095000
86	1	0	-2.228106	-3.282102	2.117725
87	1	0	-2.148566	-2.355735	3.602013
88	1	0	-4.126027	-1.774575	2.445184
89	1	0	-3.124729	-0.351901	2.439473
90	1	0	-3.911809	-4.103638	-1.178947
91	1	0	-4.964829	-2.775588	-1.628247
92	1	0	-3.693209	-4.232108	-3.638938
93	1	0	-2.155122	-3.592279	-4.217920
94	1	0	-2.192691	-4.658763	-2.800187
95	1	0	-0.683555	-1.518072	-3.673408
96	1	0	0.449020	-1.599493	-2.324626
97	1	0	-0.125992	-3.093709	-3.074850
98	1	0	-0.860115	-0.495472	-0.538810
99	1	0	-1.575278	0.048523	-2.013005
100	1	0	-0.762345	4.661848	3.192374
101	1	0	0.489696	1.871726	5.553342
102	1	0	2.042471	1.785226	4.699806
103	1	0	1.237590	3.351054	4.939629
104	1	0	1.604015	3.596624	2.395350
105	1	0	2.025583	1.929202	2.014582
106	1	0	1.599014	4.130299	-0.096311
107	1	0	0.233517	3.520572	-1.051060
108	1	0	-2.023431	3.170207	-0.621464
109	1	0	-4.705980	1.394850	-3.106736
110	1	0	-3.273246	0.464724	-3.395708
111	1	0	-4.679619	-0.792278	-1.800596
112	1	0	-4.982276	0.590367	-0.831453
113	8	0	-5.722413	-0.811699	0.960692
114	1	0	-6.061658	-0.133311	1.559154
115	8	0	-5.911275	-3.209261	1.498941
116	1	0	-6.465857	-3.448862	2.248817
117	1	0	-5.971532	-2.135511	1.329890

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	-543.3235	27.1937	37.3976
Red. masses --	1.6459	5.2519	4.8766
Frc consts --	0.2863	0.0023	0.0040
IR Inten --	36.5817	0.3841	0.2075

structure 1h

ENERGY:

Final Energy in Hartrees: HF = -2483.3135855 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154331	4.001183	2.988209
2	6	0	-0.387446	2.726463	2.642666
3	6	0	-1.809210	2.203894	2.523980
4	6	0	-2.321573	2.044641	1.079882
5	1	0	-1.713799	1.306006	0.541975
6	6	0	-2.350870	3.357533	0.296214
7	6	0	-3.103823	3.185838	-1.028129
8	6	0	-4.503656	2.573007	-0.832635
9	6	0	-5.470314	3.556279	-0.169030
10	8	0	-5.080172	2.265197	-2.107833
11	8	0	-3.659811	1.510054	1.210707
12	6	0	-4.362043	1.258795	-0.001975
13	6	0	-5.674672	0.562011	0.374264
14	6	0	-5.283540	-0.917658	0.400047
15	6	0	-4.189456	-1.041048	-0.673588
16	6	0	-4.692222	-1.514064	-2.046855
17	6	0	-3.536118	-1.733750	-3.031729
18	6	0	-2.501936	-2.677993	-2.408675
19	6	0	-2.049980	-2.156130	-1.044618
20	1	0	-1.509904	-1.211089	-1.174198
21	8	0	-3.193939	-1.893455	-0.176381
22	8	0	-3.673632	0.320878	-0.831644
23	6	0	0.706611	1.707651	2.373563
24	6	0	2.133674	2.256076	2.248223
25	6	0	3.297346	1.256375	2.002179
26	6	0	3.854139	1.032683	0.545758
27	7	0	4.033979	2.363150	0.035753
28	1	0	4.589901	2.899677	0.692927
29	6	0	4.356559	2.763380	-1.333284
30	6	0	3.202187	2.578777	-2.366147
31	1	0	3.463703	1.765055	-3.050996
32	6	0	3.102984	3.855522	-3.221571
33	6	0	1.873425	2.195456	-1.673653
34	1	0	1.728240	2.916979	-0.859924
35	6	0	0.661835	2.314715	-2.617250
36	6	0	1.840448	0.759720	-1.062254
37	6	0	3.108145	0.072205	-0.477447
38	6	0	2.710511	-1.349824	0.127953
39	6	0	1.572438	-1.460894	1.191056
40	1	0	1.641076	-0.647257	1.908974
41	6	0	1.561086	-2.811680	1.950568
42	1	0	2.522049	-3.332958	1.936946
43	6	0	1.000482	-2.738106	3.383191
44	1	0	1.683485	-2.185867	4.041474
45	8	0	0.952717	-4.066535	3.915273
46	6	0	-0.386284	-2.044482	3.376059
47	1	0	-0.185942	-0.978609	3.217896
48	6	0	-1.111170	-2.183050	4.718976
49	6	0	-1.260114	-2.513781	2.189392
50	6	0	-0.426962	-2.665713	0.905804
51	8	0	0.254310	-1.426037	0.616493
52	6	0	-1.148377	-3.163803	-0.343029
53	8	0	0.626859	-3.597478	1.201249
54	1	0	3.604825	-1.699042	0.681011
55	6	0	2.389701	-2.354711	-0.973050
56	6	0	2.632607	-2.223825	-2.283017
57	6	0	2.035211	-3.215791	-3.305961
58	8	0	2.600612	-3.228699	-4.430686

59	8	0	1.031219	-3.879937	-2.916130
60	6	0	3.483515	-1.092759	-2.778903
61	6	0	4.125314	-0.341075	-1.609310
62	1	0	-0.975790	4.682164	3.195908
63	1	0	0.846810	4.411236	3.069452
64	1	0	-1.889021	1.222372	3.008333
65	1	0	-2.497501	2.877911	3.047011
66	1	0	-2.827549	4.132130	0.911452
67	1	0	-1.325755	3.692899	0.107833
68	1	0	-3.208897	4.143930	-1.550410
69	1	0	-2.530718	2.523202	-1.687124
70	1	0	-5.509563	4.478439	-0.757680
71	1	0	-6.479641	3.137700	-0.132940
72	1	0	-5.156835	3.799072	0.848714
73	1	0	-4.547205	1.543699	-2.476350
74	1	0	-6.056220	0.927360	1.329883
75	1	0	-6.417582	0.760526	-0.403832
76	1	0	-4.843804	-1.191772	1.362284
77	1	0	-6.122254	-1.590037	0.199648
78	1	0	-5.218823	-2.464682	-1.890574
79	1	0	-5.425629	-0.793862	-2.428974
80	1	0	-3.917507	-2.143473	-3.974435
81	1	0	-3.062346	-0.773171	-3.272569
82	1	0	-2.943461	-3.676551	-2.279575
83	1	0	-1.618229	-2.799691	-3.044421
84	1	0	0.666908	0.977748	3.196812
85	1	0	0.424470	1.138490	1.482429
86	1	0	2.167860	3.013008	1.459424
87	1	0	2.367072	2.780477	3.183527
88	1	0	4.168888	1.674757	2.518001
89	1	0	3.123596	0.296634	2.495169
90	1	0	4.562922	3.836952	-1.249715
91	1	0	5.284305	2.310585	-1.715179
92	1	0	4.092399	4.133144	-3.605985
93	1	0	2.443679	3.724042	-4.084442
94	1	0	2.727452	4.701496	-2.630308
95	1	0	0.804363	1.713174	-3.523622
96	1	0	-0.241187	1.942743	-2.121225
97	1	0	0.468893	3.348712	-2.920527
98	1	0	1.063866	0.767005	-0.294952
99	1	0	1.452597	0.078562	-1.823437
100	1	0	0.607104	-4.631590	3.206239
101	1	0	-0.507942	-1.776432	5.539997
102	1	0	-2.064040	-1.641498	4.698913
103	1	0	-1.315101	-3.233217	4.947969
104	1	0	-1.715060	-3.489464	2.406200
105	1	0	-2.078878	-1.810963	2.017251
106	1	0	-1.736543	-4.051333	-0.079176
107	1	0	-0.379140	-3.469207	-1.066011
108	1	0	1.814587	-3.221170	-0.674302
109	1	0	4.259037	-1.506164	-3.434318
110	1	0	2.896989	-0.429803	-3.431147
111	1	0	4.702613	0.504514	-1.970835
112	1	0	4.864748	-1.014674	-1.162373
113	8	0	5.212148	0.468430	0.789421
114	1	0	5.153220	-0.483268	0.953999
115	8	0	6.966732	2.441840	1.739630
116	1	0	7.276033	2.187385	2.616505
117	1	0	6.469234	1.668552	1.401105

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	27.9615	34.8347	39.6334
Red. masses --	5.3012	4.6345	5.2622
Frc consts --	0.0024	0.0033	0.0049
IR Inten --	0.5083	0.8279	1.6042

structure 1i

ENERGY:

Final Energy in Hartrees: HF = -2483.3060189 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.534712	4.218734	2.503745
2	6	0	-0.654287	2.904900	2.261107
3	6	0	-2.026784	2.253154	2.207848
4	6	0	-2.560281	1.975056	0.790986
5	1	0	-1.902410	1.265429	0.273531
6	6	0	-2.732878	3.235036	-0.057849
7	6	0	-3.476292	2.911579	-1.359693
8	6	0	-4.802684	2.166790	-1.111800
9	6	0	-5.865163	3.085745	-0.504279
10	8	0	-5.346119	1.717509	-2.359095
11	8	0	-3.841646	1.333318	0.985195
12	6	0	-4.524294	0.932059	-0.197499
13	6	0	-5.759475	0.136579	0.239253
14	6	0	-5.223992	-1.291730	0.361396
15	6	0	-4.119188	-1.380011	-0.704827
16	6	0	-4.556183	-2.004474	-2.038354
17	6	0	-3.371059	-2.168936	-2.999171
18	6	0	-2.252497	-2.955250	-2.305999
19	6	0	-1.870406	-2.301771	-0.976379
20	1	0	-1.413029	-1.323390	-1.167346
21	8	0	-3.045772	-2.083462	-0.141421
22	8	0	-3.748619	0.012791	-0.969521
23	6	0	0.527960	1.971238	2.068233
24	6	0	1.915930	2.625423	2.033841
25	6	0	3.151013	1.698738	1.941421
26	6	0	3.881829	1.250792	0.616658
27	7	0	4.345931	2.487911	-0.083099
28	1	0	4.228908	3.285468	0.533455
29	6	0	4.037493	2.867529	-1.473913
30	6	0	2.587847	3.195018	-1.868157
31	1	0	2.575440	3.147208	-2.968771
32	6	0	2.208922	4.633823	-1.472313
33	6	0	1.571045	2.152936	-1.345115
34	1	0	1.268256	2.473803	-0.347903
35	6	0	0.304397	2.169867	-2.224068
36	6	0	2.060772	0.684874	-1.277673
37	6	0	3.272135	0.181625	-0.398862
38	6	0	2.884080	-1.191572	0.304930
39	6	0	1.698128	-1.259578	1.309814
40	1	0	1.708100	-0.394256	1.969589
41	6	0	1.700091	-2.552910	2.162870
42	1	0	2.678011	-3.036664	2.219619
43	6	0	1.078831	-2.405596	3.564364
44	1	0	1.718540	-1.791904	4.211228
45	8	0	1.043339	-3.698590	4.178627
46	6	0	-0.325944	-1.759657	3.458204
47	1	0	-0.152629	-0.700166	3.235906
48	6	0	-1.099154	-1.832027	4.779463
49	6	0	-1.137855	-2.337990	2.275495
50	6	0	-0.249571	-2.554478	1.038205
51	8	0	0.397770	-1.314492	0.682294
52	6	0	-0.901391	-3.178954	-0.193708
53	8	0	0.821579	-3.422411	1.435548
54	1	0	3.757698	-1.431439	0.928985
55	6	0	2.665141	-2.276601	-0.743011
56	6	0	3.098223	-2.274077	-2.009711
57	6	0	2.609225	-3.336642	-3.018920
58	8	0	3.275906	-3.403128	-4.086654

59	8	0	1.584249	-3.997277	-2.684171
60	6	0	4.052951	-1.214000	-2.476825
61	6	0	4.471265	-0.303410	-1.315935
62	1	0	-1.412236	4.838651	2.668529
63	1	0	0.425257	4.722396	2.547246
64	1	0	-2.007166	1.295314	2.742184
65	1	0	-2.758077	2.891418	2.717350
66	1	0	-3.282927	3.986058	0.524650
67	1	0	-1.751116	3.665452	-0.278634
68	1	0	-3.687355	3.822550	-1.932077
69	1	0	-2.841642	2.277748	-1.989802
70	1	0	-5.992906	3.964431	-1.144483
71	1	0	-6.828306	2.572304	-0.442567
72	1	0	-5.580668	3.415591	0.497421
73	1	0	-4.747383	1.025115	-2.679447
74	1	0	-6.170923	0.527965	1.171821
75	1	0	-6.521317	0.207298	-0.542581
76	1	0	-4.760016	-1.455452	1.337094
77	1	0	-5.991657	-2.055732	0.210916
78	1	0	-4.980483	-2.991844	-1.814353
79	1	0	-5.357096	-1.396322	-2.475299
80	1	0	-3.694354	-2.681590	-3.912656
81	1	0	-2.997775	-1.182638	-3.304111
82	1	0	-2.590614	-3.983083	-2.112338
83	1	0	-1.355170	-3.027366	-2.929973
84	1	0	0.502758	1.258611	2.905360
85	1	0	0.351872	1.353651	1.180054
86	1	0	1.951998	3.390412	1.251665
87	1	0	2.032590	3.176196	2.976288
88	1	0	3.964615	2.231446	2.447722
89	1	0	3.005707	0.810169	2.558339
90	1	0	4.664092	3.745621	-1.684115
91	1	0	4.397600	2.081789	-2.134277
92	1	0	2.859344	5.360825	-1.973754
93	1	0	1.176007	4.875117	-1.741983
94	1	0	2.306387	4.793704	-0.391660
95	1	0	0.534956	1.811419	-3.234733
96	1	0	-0.468429	1.512661	-1.813797
97	1	0	-0.123306	3.174193	-2.314191
98	1	0	1.187757	0.099515	-0.983763
99	1	0	2.250695	0.380436	-2.310564
100	1	0	0.759911	-4.318895	3.488403
101	1	0	-0.540808	-1.352030	5.592545
102	1	0	-2.067050	-1.325211	4.688187
103	1	0	-1.278636	-2.871110	5.070984
104	1	0	-1.574528	-3.308425	2.546049
105	1	0	-1.968904	-1.674925	2.023790
106	1	0	-1.420552	-4.094143	0.115746
107	1	0	-0.092346	-3.469211	-0.877093
108	1	0	2.023130	-3.100694	-0.463268
109	1	0	4.937247	-1.702613	-2.903923
110	1	0	3.623715	-0.654698	-3.320455
111	1	0	5.066367	0.527776	-1.699842
112	1	0	5.147894	-0.875467	-0.674835
113	8	0	5.040902	0.636673	1.232578
114	1	0	5.823828	0.789520	0.681243
115	8	0	7.187398	2.176537	-0.252549
116	1	0	7.380253	1.913769	-1.160836
117	1	0	6.230342	2.422124	-0.238096

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	25.0802	37.9747	44.5025
Red. masses --	5.1694	5.2480	5.1048
Frc consts --	0.0019	0.0045	0.0060
IR Inten --	0.7462	0.6259	0.8995

structure 1j

ENERGY:

Final Energy in Hartrees: HF = -2483.2903575 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.234103	3.861731	3.159606
2	6	0	-0.444981	2.595992	2.768693
3	6	0	-1.858740	2.066618	2.604002
4	6	0	-2.352305	1.979221	1.147054
5	1	0	-1.738447	1.266147	0.581636
6	6	0	-2.372326	3.328447	0.425624
7	6	0	-3.111445	3.220419	-0.913445
8	6	0	-4.513521	2.599825	-0.762199
9	6	0	-5.487596	3.550429	-0.063310
10	8	0	-5.074882	2.353688	-2.057176
11	8	0	-3.691468	1.443195	1.238175
12	6	0	-4.378485	1.247881	0.005186
13	6	0	-5.692509	0.529526	0.331890
14	6	0	-5.294303	-0.948194	0.293804
15	6	0	-4.182080	-1.017311	-0.766441
16	6	0	-4.658614	-1.430750	-2.167686
17	6	0	-3.484261	-1.591527	-3.142330
18	6	0	-2.452000	-2.555236	-2.547182
19	6	0	-2.028008	-2.098365	-1.150999
20	1	0	-1.487189	-1.147629	-1.224783
21	8	0	-3.187312	-1.879718	-0.289907
22	8	0	-3.675261	0.356055	-0.857936
23	6	0	0.667292	1.595534	2.497854
24	6	0	2.072785	2.182849	2.303729
25	6	0	3.262226	1.193507	2.119321
26	6	0	3.937931	0.829048	0.738104
27	7	0	4.301382	2.380540	0.212486
28	1	0	3.604339	2.992003	0.628977
29	6	0	4.519992	2.842581	-1.188179
30	6	0	3.333520	2.673949	-2.177709
31	1	0	3.572012	1.860294	-2.867953
32	6	0	3.237311	3.959626	-3.021002
33	6	0	2.010183	2.292454	-1.464587
34	1	0	1.889093	2.983219	-0.615372
35	6	0	0.777471	2.514466	-2.362289
36	6	0	1.932717	0.822874	-0.939303
37	6	0	3.167011	0.054318	-0.392978
38	6	0	2.730807	-1.402448	0.093033
39	6	0	1.598381	-1.555542	1.149198
40	1	0	1.683840	-0.786677	1.915059
41	6	0	1.564668	-2.944935	1.830259
42	1	0	2.519156	-3.475341	1.790136
43	6	0	0.996051	-2.947338	3.261880
44	1	0	1.685388	-2.449198	3.955315
45	8	0	0.916366	-4.304241	3.712233
46	6	0	-0.378879	-2.230129	3.289493
47	1	0	-0.161007	-1.160653	3.185641
48	6	0	-1.108833	-2.426299	4.622453
49	6	0	-1.256188	-2.626718	2.078838
50	6	0	-0.419809	-2.713448	0.791332
51	8	0	0.273759	-1.463463	0.583529
52	6	0	-1.138603	-3.139321	-0.486152
53	8	0	0.622529	-3.672468	1.031741
54	1	0	3.628248	-1.788986	0.599398
55	6	0	2.370228	-2.288871	-1.092968
56	6	0	2.645612	-2.061009	-2.382981
57	6	0	1.999567	-2.907722	-3.501085
58	8	0	2.528338	-2.786704	-4.637970

59	8	0	0.989945	-3.596275	-3.170048
60	6	0	3.568980	-0.940263	-2.763798
61	6	0	4.201340	-0.302219	-1.522899
62	1	0	-1.068369	4.525367	3.371372
63	1	0	0.758469	4.282078	3.283815
64	1	0	-1.935021	1.060633	3.035367
65	1	0	-2.560346	2.706165	3.151794
66	1	0	-2.855340	4.073410	1.071701
67	1	0	-1.344993	3.672246	0.265438
68	1	0	-3.210580	4.202550	-1.390380
69	1	0	-2.533136	2.588330	-1.597685
70	1	0	-5.524376	4.498008	-0.610291
71	1	0	-6.496014	3.128360	-0.054345
72	1	0	-5.183129	3.747585	0.966938
73	1	0	-4.543193	1.644263	-2.450502
74	1	0	-6.087256	0.849001	1.298487
75	1	0	-6.426525	0.761256	-0.445473
76	1	0	-4.869484	-1.266230	1.249149
77	1	0	-6.126503	-1.613272	0.047481
78	1	0	-5.176470	-2.393358	-2.064705
79	1	0	-5.394882	-0.701396	-2.526657
80	1	0	-3.845144	-1.958910	-4.110165
81	1	0	-3.016340	-0.615951	-3.328541
82	1	0	-2.887661	-3.562218	-2.474419
83	1	0	-1.554621	-2.640795	-3.170334
84	1	0	0.687120	0.896399	3.347787
85	1	0	0.377789	0.983380	1.638079
86	1	0	2.009806	2.907790	1.481651
87	1	0	2.308820	2.782005	3.190735
88	1	0	4.106885	1.603446	2.682575
89	1	0	3.049484	0.243853	2.613082
90	1	0	4.756905	3.910261	-1.090486
91	1	0	5.424728	2.358104	-1.558790
92	1	0	4.220113	4.221154	-3.431747
93	1	0	2.553971	3.841128	-3.865355
94	1	0	2.891962	4.810990	-2.419077
95	1	0	0.872077	1.959718	-3.303167
96	1	0	-0.121502	2.145631	-1.858443
97	1	0	0.614393	3.570222	-2.599940
98	1	0	1.143711	0.806579	-0.184098
99	1	0	1.532708	0.210801	-1.751088
100	1	0	0.579104	-4.819965	2.962761
101	1	0	-0.501603	-2.070550	5.463885
102	1	0	-2.054578	-1.871716	4.628903
103	1	0	-1.327157	-3.483955	4.797149
104	1	0	-1.719344	-3.608787	2.242662
105	1	0	-2.069397	-1.908892	1.943830
106	1	0	-1.733823	-4.035102	-0.270239
107	1	0	-0.368395	-3.413665	-1.219220
108	1	0	1.750096	-3.148678	-0.878432
109	1	0	4.349141	-1.341696	-3.421497
110	1	0	3.035844	-0.209073	-3.389882
111	1	0	4.810855	0.551662	-1.809482
112	1	0	4.908480	-1.010127	-1.084238
113	8	0	5.118191	0.234087	0.997605
114	1	0	5.848559	1.031010	1.448662
115	8	0	6.383067	2.137100	1.736291
116	1	0	7.310774	2.162107	1.474652
117	1	0	5.223199	2.529944	0.762002

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	-254.4580	24.2510	35.1397
Red. masses --	3.2762	5.1703	5.2970
Frc consts --	0.1250	0.0018	0.0039
IR Inten --	24.5446	0.7422	0.1629

structure 2a

ENERGY:

Final Energy in Hartrees: HF = -2483.3357173 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.670176	-1.447837	4.917288
2	6	0	1.511821	-0.728773	3.797080
3	6	0	2.711492	-0.272424	2.984927
4	6	0	2.826277	-0.880565	1.575822
5	1	0	1.959298	-0.595068	0.966690
6	6	0	2.974044	-2.401696	1.580164
7	6	0	3.333412	-2.912679	0.179696
8	6	0	4.562933	-2.193552	-0.407754
9	6	0	5.854608	-2.600365	0.305573
10	8	0	4.743175	-2.576798	-1.776385
11	8	0	3.997884	-0.261292	0.994027
12	6	0	4.331101	-0.651110	-0.331962
13	6	0	5.510037	0.224105	-0.773439
14	6	0	4.820284	1.457000	-1.361153
15	6	0	3.537128	0.894513	-1.989763
16	6	0	3.658733	0.549738	-3.482381
17	6	0	2.314671	0.100492	-4.068576
18	6	0	1.245207	1.160472	-3.778008
19	6	0	1.185574	1.474864	-2.280967
20	1	0	0.841215	0.588551	-1.735397
21	8	0	2.503730	1.823295	-1.774307
22	8	0	3.279256	-0.341442	-1.256705
23	6	0	0.162650	-0.282716	3.269759
24	6	0	-1.069902	-0.579327	4.133000
25	6	0	-2.399065	-0.075411	3.517302
26	6	0	-2.824036	-0.901774	2.294212
27	7	0	-2.506296	-5.446575	-1.289082
28	1	0	-2.942667	-6.273127	-1.687952
29	6	0	-2.923026	-4.249969	-2.042708
30	6	0	-2.038593	-3.007528	-1.798816
31	1	0	-2.550625	-2.200273	-2.338530
32	6	0	-0.649479	-3.163130	-2.438478
33	6	0	-2.009713	-2.592730	-0.289262
34	1	0	-2.952696	-2.948905	0.130648
35	6	0	-0.874574	-3.282603	0.493846
36	6	0	-1.955495	-1.048177	-0.097075
37	6	0	-3.013911	-0.368668	0.852868
38	6	0	-2.969933	1.200393	0.677440
39	6	0	-1.640045	1.946443	0.962436
40	1	0	-1.290599	1.686223	1.962334
41	6	0	-1.754451	3.489394	0.853003
42	1	0	-2.783246	3.855846	0.866058
43	6	0	-0.879735	4.257640	1.859474
44	1	0	-1.272974	4.143777	2.878108
45	8	0	-0.968280	5.655155	1.568738
46	6	0	0.575437	3.727209	1.804454
47	1	0	0.563117	2.751045	2.305661
48	6	0	1.551749	4.622349	2.575062
49	6	0	1.035276	3.483003	0.349943
50	6	0	-0.084928	2.878166	-0.516992
51	8	0	-0.570172	1.648796	0.046150
52	6	0	0.251219	2.647427	-1.987930
53	8	0	-1.209059	3.763358	-0.446374
54	1	0	-3.637186	1.600346	1.464231
55	6	0	-3.540588	1.612672	-0.673651
56	6	0	-4.375634	0.886453	-1.429513
57	6	0	-4.854780	1.401198	-2.812500
58	8	0	-5.702511	0.656763	-3.378602

59	8	0	-4.349871	2.481026	-3.215594
60	6	0	-4.854498	-0.464866	-0.979729
61	6	0	-4.479218	-0.776867	0.471794
62	1	0	2.659249	-1.736253	5.263211
63	1	0	0.830585	-1.774801	5.522225
64	1	0	2.678584	0.818696	2.865277
65	1	0	3.634867	-0.507275	3.526848
66	1	0	3.747932	-2.685774	2.305184
67	1	0	2.039212	-2.859309	1.920461
68	1	0	3.527441	-3.991132	0.189322
69	1	0	2.483765	-2.747810	-0.493607
70	1	0	5.957457	-3.689544	0.273498
71	1	0	6.724067	-2.166098	-0.195062
72	1	0	5.854103	-2.275665	1.348392
73	1	0	3.967929	-2.246177	-2.255040
74	1	0	6.167707	0.452603	0.067417
75	1	0	6.082280	-0.308808	-1.538421
76	1	0	4.532230	2.159319	-0.574736
77	1	0	5.431494	1.989108	-2.095068
78	1	0	3.996093	1.455983	-4.001829
79	1	0	4.435007	-0.212408	-3.615276
80	1	0	2.409958	-0.066773	-5.147724
81	1	0	2.013234	-0.856596	-3.624192
82	1	0	1.475430	2.082631	-4.329986
83	1	0	0.257003	0.822608	-4.108762
84	1	0	0.229510	0.799353	3.095350
85	1	0	0.020941	-0.716159	2.270860
86	1	0	-1.167239	-1.657107	4.301345
87	1	0	-0.947255	-0.110496	5.117163
88	1	0	-3.193795	-0.239068	4.255288
89	1	0	-2.360416	0.995980	3.323444
90	1	0	-2.876011	-4.496813	-3.111114
91	1	0	-3.967923	-3.966823	-1.831518
92	1	0	-0.744696	-3.281320	-3.524587
93	1	0	-0.023490	-2.281406	-2.257419
94	1	0	-0.127400	-4.043368	-2.051692
95	1	0	0.102215	-2.902280	0.174526
96	1	0	-0.971305	-3.091505	1.566380
97	1	0	-0.875372	-4.364052	0.339404
98	1	0	-0.956856	-0.754874	0.241128
99	1	0	-2.082609	-0.548122	-1.060120
100	1	0	-0.957620	5.736840	0.601976
101	1	0	1.250337	4.725764	3.624520
102	1	0	2.562385	4.198352	2.553311
103	1	0	1.587064	5.625808	2.140938
104	1	0	1.333936	4.430505	-0.117825
105	1	0	1.910141	2.829767	0.329196
106	1	0	0.679751	3.565034	-2.407352
107	1	0	-0.703010	2.463749	-2.493180
108	1	0	-3.238631	2.571110	-1.085713
109	1	0	-5.941102	-0.517172	-1.110176
110	1	0	-4.464858	-1.231678	-1.661634
111	1	0	-4.627421	-1.837597	0.687592
112	1	0	-5.156075	-0.228283	1.143478
113	8	0	-3.055057	-2.086824	2.532852
114	1	0	-3.520922	-3.921311	2.048884
115	8	0	-3.802776	-4.820283	1.797969
116	1	0	-4.760668	-4.822547	1.909717
117	1	0	-2.830691	-5.387809	-0.323668

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	23.1128	31.0968	37.2714
Red. masses --	5.2263	5.1115	5.6867
Frc consts --	0.0016	0.0029	0.0047
IR Inten --	0.1950	0.3413	4.9136

structure 2b

ENERGY:

Final Energy in Hartrees: HF = -2483.3373149 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.363876	-2.687475	4.368656
2	6	0	1.263994	-1.689985	3.478483
3	6	0	2.506168	-1.027330	2.906991
4	6	0	2.742214	-1.251755	1.403074
5	1	0	1.912188	-0.831918	0.820621
6	6	0	2.940039	-2.721388	1.033547
7	6	0	3.413924	-2.852522	-0.418697
8	6	0	4.659772	-1.992781	-0.708297
9	6	0	5.909561	-2.552759	-0.025348
10	8	0	4.946063	-2.011638	-2.112123
11	8	0	3.932632	-0.490013	1.089469
12	6	0	4.374593	-0.523982	-0.260852
13	6	0	5.554021	0.449887	-0.369543
14	6	0	4.868382	1.783343	-0.675628
15	6	0	3.651143	1.387383	-1.523125
16	6	0	3.884377	1.447383	-3.040765
17	6	0	2.597505	1.153098	-3.821429
18	6	0	1.479045	2.087316	-3.343582
19	6	0	1.307967	1.995766	-1.825023
20	1	0	0.954746	0.993432	-1.555812
21	8	0	2.577428	2.213486	-1.150097
22	8	0	3.384566	-0.002213	-1.158281
23	6	0	-0.057202	-1.118883	3.001733
24	6	0	-1.335154	-1.652074	3.661281
25	6	0	-2.642774	-1.022274	3.114564
26	6	0	-2.979439	-1.504250	1.698393
27	7	0	-3.226789	-4.597990	-2.921569
28	1	0	-3.242143	-4.858978	-1.939538
29	6	0	-1.957454	-3.955601	-3.288919
30	6	0	-1.802995	-2.545862	-2.687065
31	1	0	-2.637177	-1.950346	-3.077941
32	6	0	-0.495791	-1.921922	-3.205696
33	6	0	-1.936952	-2.521341	-1.134052
34	1	0	-2.902142	-2.978741	-0.902416
35	6	0	-0.853002	-3.366037	-0.437451
36	6	0	-1.958617	-1.060162	-0.594538
37	6	0	-3.077400	-0.630525	0.426069
38	6	0	-3.039782	0.932931	0.647857
39	6	0	-1.751996	1.583307	1.216182
40	1	0	-1.467600	1.076519	2.138756
41	6	0	-1.898182	3.102224	1.497245
42	1	0	-2.934689	3.445486	1.522540
43	6	0	-1.119730	3.594702	2.729993
44	1	0	-1.583053	3.224654	3.653755
45	8	0	-1.220501	5.019652	2.794394
46	6	0	0.348091	3.102975	2.653867
47	1	0	0.321423	2.031421	2.887579
48	6	0	1.243920	3.775585	3.699415
49	6	0	0.919658	3.239102	1.223799
50	6	0	-0.119603	2.874371	0.147131
51	8	0	-0.612708	1.537668	0.335596
52	6	0	0.322412	3.039403	-1.304647
53	8	0	-1.266040	3.705164	0.357886
54	1	0	-3.775590	1.127092	1.450785
55	6	0	-3.498492	1.668160	-0.604797
56	6	0	-4.269676	1.158930	-1.575073
57	6	0	-4.622554	1.996866	-2.832116
58	8	0	-5.486409	1.469186	-3.584930

59	8	0	-4.011946	3.090038	-2.966158
60	6	0	-4.790002	-0.248780	-1.496809
61	6	0	-4.509724	-0.921029	-0.147755
62	1	0	2.334999	-3.053959	4.691309
63	1	0	0.495041	-3.171623	4.802483
64	1	0	2.451503	0.057289	3.068834
65	1	0	3.393694	-1.386219	3.440813
66	1	0	3.670735	-3.168921	1.719898
67	1	0	1.999978	-3.264383	1.177154
68	1	0	3.641101	-3.894953	-0.669618
69	1	0	2.610739	-2.528330	-1.091699
70	1	0	6.046690	-3.597723	-0.320835
71	1	0	6.798485	-1.997242	-0.335630
72	1	0	5.827801	-2.500539	1.062517
73	1	0	4.209438	-1.552182	-2.543608
74	1	0	6.139447	0.463573	0.551785
75	1	0	6.199793	0.139573	-1.196201
76	1	0	4.502803	2.255570	0.239703
77	1	0	5.512759	2.494262	-1.199689
78	1	0	4.229098	2.461874	-3.279143
79	1	0	4.690765	0.756059	-3.310717
80	1	0	2.771353	1.276594	-4.896697
81	1	0	2.295813	0.109508	-3.665604
82	1	0	1.718970	3.124836	-3.615451
83	1	0	0.526247	1.839034	-3.823791
84	1	0	-0.004028	-0.031571	3.144709
85	1	0	-0.119338	-1.251158	1.913266
86	1	0	-1.404954	-2.737477	3.538347
87	1	0	-1.293880	-1.462499	4.740454
88	1	0	-3.467494	-1.383437	3.740844
89	1	0	-2.623250	0.063254	3.204951
90	1	0	-1.071684	-4.563217	-3.029587
91	1	0	-1.952495	-3.854880	-4.381107
92	1	0	-0.508268	-1.858423	-4.300090
93	1	0	-0.352983	-0.907733	-2.822167
94	1	0	0.380663	-2.516358	-2.919776
95	1	0	0.147070	-2.951569	-0.608776
96	1	0	-1.023052	-3.402966	0.641058
97	1	0	-0.843726	-4.402088	-0.796042
98	1	0	-0.983311	-0.818484	-0.160510
99	1	0	-2.073176	-0.363734	-1.427921
100	1	0	-1.133289	5.341579	1.883335
101	1	0	0.862561	3.607821	4.713912
102	1	0	2.262676	3.373799	3.650100
103	1	0	1.289136	4.856631	3.538074
104	1	0	1.232707	4.274967	1.036687
105	1	0	1.806605	2.612988	1.106294
106	1	0	0.751426	4.039375	-1.437194
107	1	0	-0.590036	2.985948	-1.908375
108	1	0	-3.153440	2.686616	-0.755234
109	1	0	-5.867112	-0.240452	-1.697108
110	1	0	-4.370661	-0.835369	-2.324231
111	1	0	-4.659429	-2.000805	-0.218329
112	1	0	-5.236066	-0.556982	0.593659
113	8	0	-3.217609	-2.709074	1.594128
114	1	0	-3.579346	-3.872102	2.985968
115	8	0	-3.825907	-4.447494	3.739151
116	1	0	-4.579799	-4.960929	3.426807
117	1	0	-3.369147	-5.447704	-3.459909

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	22.2062	32.9799	35.2448
Red. masses --	3.8003	4.5865	4.5442
Frc consts --	0.0011	0.0029	0.0033
IR Inten --	1.8905	1.5164	0.6961

structure 2c

ENERGY:

Final Energy in Hartrees: HF = -2483.3444967 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.032587	3.248663	3.625499
2	6	0	2.521839	2.756062	2.488930
3	6	0	3.423045	2.303162	1.354825
4	6	0	3.442375	0.780390	1.126169
5	1	0	2.444208	0.429175	0.836355
6	6	0	3.930592	-0.017659	2.333165
7	6	0	4.137544	-1.487682	1.949479
8	6	0	5.045129	-1.653276	0.716252
9	6	0	6.503406	-1.314894	1.033881
10	8	0	5.051492	-3.023821	0.292862
11	8	0	4.324139	0.577934	-0.007449
12	6	0	4.493424	-0.762118	-0.442150
13	6	0	5.347170	-0.718253	-1.715636
14	6	0	4.305229	-0.545864	-2.823205
15	6	0	3.084461	-1.320788	-2.305718
16	6	0	2.993983	-2.773353	-2.800069
17	6	0	1.699228	-3.445963	-2.327066
18	6	0	0.493620	-2.591689	-2.737173
19	6	0	0.651544	-1.150860	-2.245277
20	1	0	0.621377	-1.132971	-1.149512
21	8	0	1.930624	-0.600826	-2.664799
22	8	0	3.248414	-1.345702	-0.857447
23	6	0	1.031811	2.626437	2.229193
24	6	0	0.109413	2.571310	3.458335
25	6	0	-1.329541	2.140519	3.113744
26	6	0	-1.409457	0.726207	2.522533
27	7	0	-3.460302	-2.407219	-1.751230
28	1	0	-4.217321	-1.713075	-1.843500
29	6	0	-3.806462	-3.371013	-0.689438
30	6	0	-2.763991	-3.536540	0.455949
31	1	0	-1.763493	-3.521659	-0.004632
32	6	0	-2.970541	-4.932215	1.079355
33	6	0	-2.817523	-2.392110	1.523479
34	1	0	-3.882161	-2.245052	1.746950
35	6	0	-2.119891	-2.785237	2.840774
36	6	0	-2.234515	-1.082783	0.925785
37	6	0	-2.560389	0.303569	1.594303
38	6	0	-2.884049	1.395039	0.483107
39	6	0	-1.684197	1.973831	-0.298635
40	1	0	-1.147973	2.656220	0.371086
41	6	0	-2.055470	2.719633	-1.602260
42	1	0	-3.109293	2.997209	-1.665575
43	6	0	-1.150471	3.921126	-1.923888
44	1	0	-1.345107	4.743737	-1.223776
45	8	0	-1.502252	4.425292	-3.215802
46	6	0	0.336099	3.499784	-1.832326
47	1	0	0.555258	3.384197	-0.763463
48	6	0	1.282937	4.571737	-2.382389
49	6	0	0.567029	2.123574	-2.492912
50	6	0	-0.567913	1.133048	-2.172834
51	8	0	-0.737890	0.990120	-0.753181
52	6	0	-0.451574	-0.251879	-2.801434
53	8	0	-1.800410	1.725867	-2.610142
54	1	0	-3.259082	2.276612	1.028849
55	6	0	-4.025085	0.859970	-0.355292
56	6	0	-5.085308	0.262508	0.205811
57	6	0	-6.226100	-0.319463	-0.646165
58	8	0	-7.347331	-0.365356	-0.080378

59	8	0	-5.909862	-0.701233	-1.812208
60	6	0	-5.185662	0.099489	1.703085
61	6	0	-3.854613	0.306206	2.484812
62	1	0	4.106596	3.337037	3.766748
63	1	0	2.407111	3.565384	4.454276
64	1	0	3.103027	2.771230	0.414117
65	1	0	4.452313	2.629873	1.542646
66	1	0	4.867611	0.421894	2.701054
67	1	0	3.203828	0.049220	3.148658
68	1	0	4.567248	-2.055824	2.782278
69	1	0	3.162701	-1.937832	1.724503
70	1	0	6.836942	-1.915598	1.885940
71	1	0	7.148708	-1.550966	0.183289
72	1	0	6.621851	-0.257337	1.279644
73	1	0	4.150093	-3.214971	-0.007725
74	1	0	6.073816	0.095322	-1.672499
75	1	0	5.881744	-1.666728	-1.821511
76	1	0	4.018278	0.503019	-2.933025
77	1	0	4.638685	-0.917434	-3.796069
78	1	0	3.011461	-2.749537	-3.897470
79	1	0	3.882274	-3.323609	-2.469697
80	1	0	1.620805	-4.454755	-2.749643
81	1	0	1.715313	-3.558829	-1.235454
82	1	0	0.400086	-2.585890	-3.832821
83	1	0	-0.439871	-2.995738	-2.331076
84	1	0	0.731905	3.466236	1.582845
85	1	0	0.869306	1.728753	1.625113
86	1	0	0.525769	1.872978	4.189791
87	1	0	0.066719	3.551964	3.947820
88	1	0	-1.927202	2.120223	4.036273
89	1	0	-1.821259	2.868120	2.462038
90	1	0	-4.772912	-3.097531	-0.244088
91	1	0	-3.954134	-4.366091	-1.132467
92	1	0	-2.948298	-5.703588	0.300402
93	1	0	-2.198914	-5.185493	1.811559
94	1	0	-3.944942	-5.003800	1.581475
95	1	0	-1.075128	-3.069037	2.659766
96	1	0	-2.100755	-1.949844	3.544133
97	1	0	-2.621620	-3.623174	3.335076
98	1	0	-1.146555	-1.191110	0.897504
99	1	0	-2.556828	-1.032692	-0.110509
100	1	0	-1.663450	3.651811	-3.778482
101	1	0	1.153384	5.523527	-1.852953
102	1	0	2.327302	4.259713	-2.266021
103	1	0	1.091825	4.755192	-3.443869
104	1	0	0.614192	2.226683	-3.585322
105	1	0	1.522760	1.703055	-2.174060
106	1	0	-0.313962	-0.141218	-3.883693
107	1	0	-1.409770	-0.754375	-2.626661
108	1	0	-3.961826	0.885170	-1.438575
109	1	0	-5.941994	0.795771	2.087008
110	1	0	-5.606503	-0.890782	1.906530
111	1	0	-3.763754	-0.453707	3.267852
112	1	0	-3.896619	1.272443	3.001672
113	8	0	-0.550314	-0.082429	2.863048
114	1	0	0.718567	-0.492298	4.150321
115	8	0	1.372544	-0.791287	4.811415
116	1	0	1.191191	-1.731120	4.929590
117	1	0	-3.422908	-2.887777	-2.645346

FREQUENCIES:

(B3LYP/3-21G)

	1	2	3
	A	A	A
Frequencies --	31.5242	39.2572	44.0915
Red. masses --	5.2204	4.7938	4.8531
Frc consts --	0.0031	0.0044	0.0056
IR Inten --	0.5364	0.2384	1.0372

structure 13f

ENERGY:

Final Energy in Hartrees: HF = -982.3608130 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.008252	-2.232087	1.309191
2	6	0	0.919680	-1.062946	0.344494
3	7	0	2.019280	-0.785195	-0.264910
4	1	0	3.511768	-1.627150	-0.086532
5	6	0	2.115280	0.274886	-1.271380
6	6	0	2.089922	1.694535	-0.671970
7	1	0	2.024211	2.379124	-1.532427
8	6	0	3.389761	2.005012	0.088334
9	6	0	0.829714	1.917357	0.206596
10	1	0	1.075766	1.583701	1.222898
11	6	0	0.471780	3.411471	0.284641
12	6	0	-0.381287	1.104575	-0.299323
13	6	0	-0.459777	-0.407292	0.104628
14	6	0	-1.404804	-0.566629	1.350586
15	6	0	-1.020627	0.302887	2.564746
16	1	0	0.016382	0.148822	2.887075
17	1	0	-1.326822	-1.610269	1.683325
18	6	0	-2.860470	-0.337526	0.985784
19	6	0	-3.383017	-0.404103	-0.247379
20	6	0	-4.892826	-0.152643	-0.500282
21	8	0	-5.244787	-0.268871	-1.707801
22	8	0	-5.591781	0.134649	0.505356
23	6	0	-2.514865	-0.712560	-1.439827
24	6	0	-1.121989	-1.232148	-1.051853
25	1	0	2.014885	-2.652414	1.285641
26	1	0	0.288692	-3.014562	1.042938
27	1	0	3.065287	0.128492	-1.797741
28	1	0	1.320862	0.171506	-2.018491
29	1	0	4.265839	1.907312	-0.562098
30	1	0	3.382773	3.023250	0.492424
31	1	0	3.521721	1.312288	0.926975
32	1	0	0.130588	3.779105	-0.691549
33	1	0	-0.336718	3.586321	1.002828
34	1	0	1.328798	4.022042	0.590635
35	1	0	-1.302146	1.572388	0.059985
36	1	0	-0.430781	1.201240	-1.390592
37	1	0	-3.549083	-0.113057	1.799397
38	1	0	-3.029743	-1.444367	-2.071370
39	1	0	-2.438301	0.183915	-2.070849
40	1	0	-0.459761	-1.234524	-1.927697
41	1	0	-1.209271	-2.276485	-0.723199
42	8	0	6.696461	-0.576842	-0.547441
43	1	0	6.987609	-0.284842	0.323832
44	1	0	-1.156734	1.369157	2.358060
45	1	0	-1.673562	0.055871	3.409181
46	1	0	0.780974	-1.927467	2.335125
47	8	0	4.405970	-2.090103	-0.030155
48	1	0	5.878120	-1.095066	-0.380458
49	1	0	4.348424	-2.855363	-0.614533

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	13.9793	20.2580	37.7704
Red. masses --	5.9897	5.5352	8.9289

Frc consts	--	0.0007	0.0013	0.0075
IR Inten	--	4.4568	4.8293	1.5012

structure 13g

ENERGY:

Final Energy in Hartrees: HF = -982.3104147 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.399543	-1.997929	1.603772
2	6	0	1.316690	-0.947801	0.523459
3	7	0	2.458571	-0.318175	0.287692
4	1	0	3.278350	-0.856824	0.579146
5	6	0	2.733707	0.488729	-0.916377
6	6	0	2.357334	1.965104	-0.762894
7	1	0	2.351987	2.384033	-1.781160
8	6	0	3.405863	2.725695	0.065410
9	6	0	0.932195	2.111134	-0.174755
10	1	0	1.036303	2.070396	0.913685
11	6	0	0.323443	3.478325	-0.533527
12	6	0	-0.022994	0.982722	-0.634795
13	6	0	-0.055888	-0.388010	0.117489
14	6	0	-0.962370	-0.284917	1.421754
15	6	0	-0.540119	0.764902	2.469498
16	1	0	0.520318	0.703718	2.741778
17	1	0	-0.888053	-1.259571	1.919139
18	6	0	-2.426387	-0.086112	1.073908
19	6	0	-3.009874	-0.391591	-0.093246
20	6	0	-4.521165	-0.134093	-0.328237
21	8	0	-4.938260	-0.478237	-1.469062
22	8	0	-5.158547	0.382708	0.626324
23	6	0	-2.199645	-0.969208	-1.222431
24	6	0	-0.792155	-1.420241	-0.805428
25	1	0	2.380519	-2.472747	1.580194
26	1	0	0.637387	-2.762797	1.460363
27	1	0	3.804142	0.377606	-1.108281
28	1	0	2.215958	0.014189	-1.751322
29	1	0	4.389346	2.698569	-0.418845
30	1	0	3.131815	3.776933	0.201744
31	1	0	3.510072	2.277319	1.061006
32	1	0	0.118596	3.538922	-1.610068
33	1	0	-0.625416	3.636541	-0.010102
34	1	0	0.991409	4.307440	-0.273447
35	1	0	-1.046237	1.360958	-0.568390
36	1	0	0.145190	0.798948	-1.703600
37	1	0	-3.064960	0.336241	1.849051
38	1	0	-2.746024	-1.816996	-1.650525
39	1	0	-2.156762	-0.239519	-2.043112
40	1	0	-0.160136	-1.611444	-1.674820
41	1	0	-0.866590	-2.369360	-0.260721
42	8	0	1.965819	-2.488822	-1.061659
43	1	0	1.492240	-3.294999	-1.302751
44	1	0	-0.749282	1.782532	2.126407
45	1	0	-1.128331	0.611493	3.381371
46	1	0	1.243994	-1.537491	2.587425
47	8	0	4.293068	-2.389681	-0.163478
48	1	0	3.352403	-2.583035	-0.609026
49	1	0	4.696055	-3.231820	0.072408

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	-203.4857	34.9852	38.8500
Red. masses --	3.4358	5.3395	7.2671

Frc consts	--	0.0838	0.0039	0.0065
IR Inten	--	108.2430	2.5339	4.8421

structure 13h

ENERGY:

Final Energy in Hartrees: HF = -982.3381371 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.535364	-2.097975	1.486933
2	6	0	1.475673	-1.076324	0.336839
3	7	0	2.424746	-0.025532	0.653976
4	1	0	3.230453	-0.455031	1.096671
5	6	0	2.887539	0.838973	-0.447142
6	6	0	2.166586	2.191493	-0.519096
7	1	0	2.444354	2.621104	-1.495379
8	6	0	2.667483	3.149212	0.574804
9	6	0	0.617080	2.068843	-0.479897
10	1	0	0.306513	2.242332	0.551132
11	6	0	-0.018732	3.185323	-1.331228
12	6	0	0.038958	0.705007	-0.928757
13	6	0	0.015759	-0.533611	0.022180
14	6	0	-0.807586	-0.321200	1.355658
15	6	0	-0.289122	0.687368	2.406203
16	1	0	0.799822	0.684564	2.494137
17	1	0	-0.762281	-1.298696	1.855045
18	6	0	-2.280434	-0.065355	1.080563
19	6	0	-2.958179	-0.501427	0.010447
20	6	0	-4.469976	-0.215612	-0.175110
21	8	0	-4.965863	-0.700079	-1.231858
22	8	0	-5.033207	0.453554	0.729210
23	6	0	-2.255933	-1.273248	-1.074839
24	6	0	-0.795352	-1.641861	-0.737394
25	1	0	2.544416	-2.523035	1.517547
26	1	0	0.831072	-2.918668	1.330386
27	1	0	3.958731	1.018069	-0.294121
28	1	0	2.799031	0.316270	-1.405312
29	1	0	3.738154	3.361793	0.460022
30	1	0	2.133558	4.106070	0.549074
31	1	0	2.513856	2.705624	1.565174
32	1	0	0.169984	3.015007	-2.399768
33	1	0	-1.103232	3.225618	-1.185552
34	1	0	0.391712	4.169744	-1.075765
35	1	0	-1.005173	0.892714	-1.187293
36	1	0	0.525246	0.403677	-1.868234
37	1	0	-2.842967	0.490196	1.829471
38	1	0	-2.824894	-2.184196	-1.292238
39	1	0	-2.308692	-0.699882	-2.009844
40	1	0	-0.309839	-1.890349	-1.693667
41	1	0	-0.797820	-2.555205	-0.127237
42	8	0	2.016963	-1.778986	-0.847078
43	1	0	1.310685	-2.285877	-1.268651
44	1	0	-0.614387	1.707463	2.183803
45	1	0	-0.723307	0.431243	3.380636
46	1	0	1.322673	-1.637140	2.453519
47	8	0	4.696799	-2.651805	-0.734002
48	1	0	3.767953	-2.352149	-0.825290
49	1	0	4.638858	-3.591652	-0.527256

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	21.4814	26.0010	30.0055
Red. masses --	6.1849	4.0833	6.6919

Frc consts	--	0.0017	0.0016	0.0035
IR Inten	--	7.7038	2.8617	14.2025

structure 13i

ENERGY:

Final Energy in Hartrees: HF = -982.3329737 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.971467	0.201072	2.155319
2	6	0	-1.291169	0.892014	0.955114
3	7	0	-2.308753	1.243890	-0.078222
4	1	0	-3.176733	1.446820	0.410779
5	6	0	-2.582379	0.425697	-1.269182
6	6	0	-2.834522	-1.088634	-1.117013
7	1	0	-2.913282	-1.448291	-2.155994
8	6	0	-4.175233	-1.398339	-0.431751
9	6	0	-1.642060	-1.856465	-0.468747
10	1	0	-1.871076	-2.027390	0.587634
11	6	0	-1.495994	-3.247253	-1.113410
12	6	0	-0.310565	-1.086844	-0.582048
13	6	0	-0.013182	0.161726	0.329818
14	6	0	0.978365	-0.246444	1.488786
15	6	0	0.684345	-1.593790	2.199272
16	1	0	-0.340606	-1.700268	2.559534
17	1	0	0.900509	0.544688	2.248857
18	6	0	2.428051	-0.313562	1.034150
19	6	0	2.926548	0.055300	-0.154201
20	6	0	4.421128	-0.152892	-0.509350
21	8	0	4.744502	0.249745	-1.663025
22	8	0	5.141478	-0.695804	0.368353
23	6	0	2.034507	0.694559	-1.182287
24	6	0	0.734942	1.209761	-0.553346
25	1	0	-2.825260	0.820425	2.453933
26	1	0	-1.291516	0.164133	3.006786
27	1	0	-3.464200	0.878741	-1.740939
28	1	0	-1.760877	0.570282	-1.975812
29	1	0	-5.016789	-0.972374	-0.992357
30	1	0	-4.341392	-2.479102	-0.357991
31	1	0	-4.211705	-0.993022	0.585401
32	1	0	-1.164428	-3.158967	-2.155913
33	1	0	-0.756076	-3.854027	-0.580434
34	1	0	-2.445638	-3.796336	-1.109809
35	1	0	0.508013	-1.793934	-0.424410
36	1	0	-0.203614	-0.791164	-1.632650
37	1	0	3.132935	-0.750220	1.740962
38	1	0	2.579890	1.519217	-1.653538
39	1	0	1.842337	-0.010203	-2.003928
40	1	0	0.060725	1.572138	-1.341876
41	1	0	0.995998	2.070151	0.071254
42	8	0	-0.905901	2.136605	1.559102
43	1	0	-0.800144	2.811297	0.869723
44	1	0	0.905591	-2.443877	1.545707
45	1	0	1.350292	-1.686198	3.064438
46	1	0	-2.327700	-0.804200	1.940699
47	8	0	-1.681207	3.910384	-0.867394
48	1	0	-1.945669	2.967249	-0.727516
49	1	0	-0.997176	3.894340	-1.548013

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	39.2423	40.0386	52.1687
Red. masses --	5.8298	13.2305	5.7661

Frc consts	--	0.0053	0.0125	0.0092
IR Inten	--	7.5236	0.5718	1.9894

structure 13j

ENERGY:

Final Energy in Hartrees: HF = -982.3043186 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.012884	0.518226	2.060023
2	6	0	-1.266607	1.073314	0.829303
3	7	0	-2.416158	1.151294	-0.344988
4	1	0	-3.292714	1.251721	0.166334
5	6	0	-2.589576	0.167977	-1.446544
6	6	0	-2.770355	-1.300760	-1.044935
7	1	0	-2.800832	-1.827947	-2.011172
8	6	0	-4.120368	-1.554778	-0.352022
9	6	0	-1.568953	-1.896459	-0.246609
10	1	0	-1.830106	-1.901160	0.815731
11	6	0	-1.356106	-3.367358	-0.651480
12	6	0	-0.262122	-1.103743	-0.448398
13	6	0	-0.000669	0.259065	0.290348
14	6	0	0.983350	0.022009	1.505095
15	6	0	0.674698	-1.196553	2.413279
16	1	0	-0.339970	-1.218388	2.816159
17	1	0	0.912521	0.923547	2.131900
18	6	0	2.429750	-0.133589	1.061388
19	6	0	2.932221	0.079991	-0.163011
20	6	0	4.417577	-0.217157	-0.492787
21	8	0	4.742873	0.014114	-1.692013
22	8	0	5.129636	-0.658550	0.446849
23	6	0	2.052922	0.614541	-1.259648
24	6	0	0.746883	1.196149	-0.707596
25	1	0	-2.880460	1.163110	2.243156
26	1	0	-1.362094	0.626017	2.927459
27	1	0	-3.465873	0.498779	-2.019083
28	1	0	-1.726296	0.277291	-2.102661
29	1	0	-4.961377	-1.245641	-0.985042
30	1	0	-4.249217	-2.618967	-0.128133
31	1	0	-4.196772	-1.015834	0.599069
32	1	0	-0.988934	-3.437047	-1.683283
33	1	0	-0.616250	-3.848898	-0.003886
34	1	0	-2.285784	-3.946161	-0.586224
35	1	0	0.574211	-1.760165	-0.193933
36	1	0	-0.146697	-0.948641	-1.528420
37	1	0	3.126897	-0.500188	1.814170
38	1	0	2.606470	1.384658	-1.807752
39	1	0	1.873056	-0.171668	-2.007562
40	1	0	0.078064	1.460312	-1.539887
41	1	0	0.971580	2.127885	-0.182470
42	8	0	-0.988177	2.370209	1.108401
43	1	0	-1.242062	3.094215	0.199648
44	1	0	0.853895	-2.140642	1.887761
45	1	0	1.364914	-1.181511	3.264121
46	1	0	-2.341926	-0.519181	1.990564
47	8	0	-1.775743	3.580553	-0.803605
48	1	0	-2.223601	2.145053	-0.776489
49	1	0	-1.104814	3.854514	-1.440643

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	-843.9794	40.1265	42.9404
Red. masses --	1.2585	9.3474	6.9831

Frc consts	--	0.5282	0.0089	0.0076
IR Inten	--	1102.5508	3.4107	6.2303

structure 14

ENERGY:

Final Energy in Hartrees: HF = -982.3479914 (B3LYP/6-31+G(D,P))

COORDINATES:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.448645	-2.206244	1.610934
2	6	0	1.017370	-1.650135	0.268525
3	7	0	3.831894	0.403859	0.314169
4	1	0	4.506449	1.066336	0.686944
5	6	0	3.263162	0.883227	-0.955618
6	6	0	2.249182	2.029807	-0.766544
7	1	0	1.906851	2.301336	-1.778812
8	6	0	2.969782	3.261215	-0.181508
9	6	0	0.985947	1.625467	0.051496
10	1	0	1.351395	1.240871	1.009176
11	6	0	0.102014	2.862461	0.322967
12	6	0	0.132390	0.532079	-0.669340
13	6	0	-0.251156	-0.796027	0.070490
14	6	0	-1.134320	-0.644428	1.355600
15	6	0	-0.589978	0.190820	2.535084
16	1	0	0.437850	-0.056911	2.813673
17	1	0	-1.241569	-1.669792	1.746724
18	6	0	-2.536782	-0.167634	1.010612
19	6	0	-3.145585	-0.307531	-0.175761
20	6	0	-4.583875	0.222214	-0.413151
21	8	0	-5.031064	0.012597	-1.575863
22	8	0	-5.142423	0.794097	0.558790
23	6	0	-2.441377	-0.972011	-1.330371
24	6	0	-1.121402	-1.647534	-0.928926
25	1	0	2.068072	-3.091713	1.451160
26	1	0	0.615526	-2.438810	2.274722
27	1	0	4.037160	1.234163	-1.663024
28	1	0	2.771732	0.030144	-1.427085
29	1	0	3.904154	3.452706	-0.725068
30	1	0	2.362617	4.167848	-0.247857
31	1	0	3.219872	3.109989	0.876218
32	1	0	-0.097649	3.402934	-0.612230
33	1	0	-0.869872	2.575221	0.731566
34	1	0	0.566423	3.564518	1.023334
35	1	0	-0.810823	0.990507	-0.975499
36	1	0	0.631092	0.223735	-1.594076
37	1	0	-3.108527	0.317218	1.800715
38	1	0	-3.115482	-1.710611	-1.778562
39	1	0	-2.283302	-0.235189	-2.129557
40	1	0	-0.516892	-1.875301	-1.812705
41	1	0	-1.345447	-2.607648	-0.441693
42	8	0	1.713896	-1.917676	-0.713576
43	1	0	3.413186	-2.501704	-0.610317
44	1	0	-0.635945	1.261603	2.332002
45	1	0	-1.224256	0.008166	3.410537
46	1	0	2.070218	-1.443093	2.094753
47	8	0	4.384087	-2.646386	-0.545962
48	1	0	4.319037	-0.478705	0.164399
49	1	0	4.664793	-2.900351	-1.432674

FREQUENCIES:

(B3LYP/6-31+G(D,P))

	1	2	3
	A	A	A
Frequencies --	28.4524	38.6377	42.6796
Red. masses --	4.4098	11.2802	5.8591

Frc consts	--	0.0021	0.0099	0.0063
IR Inten	--	10.0393	2.4643	5.3927

[1] Quinoline was removed under high vacuum at elevated temperatures (>120 °C) leading to decomposition of **10**.

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