ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Is the bioconformation of 5-deoxy-5-fluoro-D-xylulose affected by intramolecular hydrogen bond?

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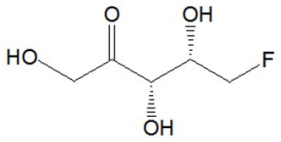
Table S1. Optimized conformations for DFX in the gas phase at the ωB97X-D/6-311++g(d,p) level and respective free energies (kcal mol^{-1}) and key dihedral angles.



Conf	ΔG^0_{rel}	HOC(H_2)C(=O)	OCC=O	O=CCO(H)	C(=O)COH	(H)OCCO(H)	HOCC(F)	OCCF
1g	0.00	-16.8	12.2	9.4	-13.4	57.9	76.2	173.4
2g	0.22	9.6	-4.8	-6.3	2.1	-166.4	-55.3	62.2
3g	0.38	4.0	-1.7	174.7	84.0	52.3	-51.0	56.8
4g	0.47	69.8	159.2	-11.1	6.2	-171.3	-53.5	60.1
5g	0.78	-1.2	0.6	176.7	164.2	-48.8	-56.1	57.7
6g	1.00	-16.6	10.8	101.6	5.1	74.9	-46.9	60.0
7g	1.06	4.1	-1.7	177.6	-172.9	48.6	81.7	-73.5
8g	1.31	-2.9	1.5	172.6	153.8	-42.2	40.7	-54.2
9g	1.32	-18.0	12.1	10.1	-13.5	66.7	64.8	65.2
10g	1.34	0.9	-3.0	-159.3	83.1	51.9	-145.1	178.8
11g	1.51	1.7	-3.6	-151.5	81.9	53.4	-148.7	179.0
12g	1.58	-55.5	156.9	-110.7	48.1	70.9	-51.5	57.8
13g	1.71	5.4	-1.8	177.7	-133.4	50.9	73.6	175.7
14g	1.76	2.7	-2.9	-171.9	83.1	-163.5	76.0	-176.5
15g	1.80	-9.0	6.2	-105.9	82.2	72.6	-166.3	176.9
16g	2.07	-10.2	4.1	2.0	-3.0	-170.9	-159.7	-64.8
17g	2.26	19.1	-13.2	-32.6	31.0	-54.3	169.2	-75.9
18g	2.39	66.9	-142.9	1.9	-4.7	-156.4	76.4	-67.3
19g	2.57	-11.9	8.5	0.8	8.4	70.3	-60.9	172.7
20g	2.66	5.8	-7.5	-34.2	31.0	-53.9	168.4	165.9
21g	2.68	7.5	-1.5	-179.2	-154.8	-175.0	81.5	-68.5
22g	2.70	-56.1	-179.6	-115.9	81.4	50.4	-163.5	178.0
23g	2.83	86.8	-179.6	-26.7	24.4	-47.8	164.1	169.4
24g	2.83	65.0	168.5	-5.1	1.9	-161.6	-159.4	-60.9
25g	2.85	-71.9	-113.2	-0.1	-2.4	-164.9	-61.6	62.4
26g	2.88	-61.7	-157.1	-136.6	158.0	-43.8	42.1	-55.8
27g	2.97	65.8	139.3	157.8	166.3	-50.7	-59.6	59.7
28g	2.97	3.4	-3.9	-152.5	164.9	55.2	-165.4	-72.8
29g	3.13	-82.0	174.7	-3.3	1.0	-154.7	77.9	-63.7
30g	3.15	-64.3	-150.8	-142.3	164.0	-47.7	-56.2	56.3
31g	3.21	-82.7	152.9	-3.9	12.7	75.7	-48.9	60.6
32g	3.63	5.1	-5.0	-156.0	-157.6	74.8	-164.8	-169.3
33g	3.66	67.2	138.1	158.0	160.4	-45.5	40.0	-52.7
34g	3.71	7.2	-3.1	-174.9	63.5	-174.8	84.9	-83.0
35g	3.83	-65.2	139.3	168.9	38.8	-169.7	90.0	-69.5

36g	3.91	-53.7	153.5	152.6	47.0	68.8	-70.2	171.8
37g	4.11	7.4	-2.7	164.5	-77.1	70.0	-54.8	62.1
38g	4.24	0.3	-1.4	-163.4	-163.9	-167.3	68.4	70.9
39g	4.35	-66.3	-131.5	-166.7	-174.1	49.0	82.0	-73.9
40g	4.40	-66.4	-131.4	-166.7	-74.2	49.0	81.8	-73.9
41g	4.45	13.0	-7.9	-17.8	31.2	-161.2	-80.9	179.2
42g	4.48	75.3	157.3	-27.6	25.8	-55.7	171.2	-76.4
43g	4.49	13.3	-8.2	-17.2	29.4	-160.8	-79.5	178.9
44g	4.54	11.3	-7.3	-16.3	30.7	-160.0	-153.2	-178.7
45g	4.70	-1.1	2.5	161.3	-95.8	-52.4	179.6	72.0
46g	4.72	-1.3	2.4	161.4	-94.8	-52.0	177.8	71.8
47g	4.85	17.5	-13.9	-38.7	35.8	-56.5	174.1	64.7
48g	4.85	79.2	-125.0	-177.5	-48.4	-173.9	82.9	-72.1
49g	5.18	67.8	163.0	-17.9	26.3	-166.7	-81.2	174.6
50g	5.37	-52.6	150.1	151.7	50.9	63.3	34.0	-45.0
51g	5.50	84.9	-163.5	-129.4	-72.3	-50.4	166.8	67.2
52g	5.64	65.5	166.3	-14.8	24.6	-159.6	-140.0	179.8
53g	6.21	-74.7	95.2	146.6	98.3	41.3	-167.3	67.1
54g	6.44	-79.3	102.9	-156.8	165.1	42.3	162.2	-72.7
55g	6.64	68.5	96.2	137.9	-161.3	41.4	80.3	-72.4
56g	6.65	-63.8	-141.6	-152.3	65.0	179.2	78.8	-94.1
57g	6.71	84.4	-153.4	-141.8	-65.7	-171.4	60.7	68.7
58g	6.86	-178.2	157.8	144.5	54.8	-50.4	163.6	71.8
59g	6.96	-1.2	1.9	164.5	65.3	-51.8	164.6	69.0
60g	7.26	177.2	-166.0	-12.1	-71.6	-48.8	169.5	70.4
61g	7.47	86.3	-154.9	139.0	-69.6	-47.8	169.7	69.6
62g	7.51	-69.9	-111.8	-10.2	18.5	-158.8	-78.9	174.7
63g	7.71	69.4	-149.1	-52.8	170.1	-52.0	-100.6	179.2
64g	8.45	-62.0	-163.8	-129.8	78.4	-165.2	-157.7	-172.0
65g	11.05	57.2	121.5	-139.3	79.5	-160.5	-84.3	-175.4

Table S2. Optimized conformations for DFX in implicit water at the ωB97X-D/6-311++g(d,p) level and respective free energies (kcal mol^{-1}) and key dihedral angles.

Conf.	ΔG^0_{rel}	HOC(H_2)C(=O)	OCC=O	O=CCO(H)	C(=O)COH	(H)OCCO(H)	HOCC(F)	OCCF
1w	0.00	-18.9	10.7	7.2	-10.5	64.1	67.6	63.2
2w	0.66	-19.1	11.0	5.8	-8.2	59.7	72.9	174.9
3w	0.66	2.0	-0.7	176.9	84.5	54.4	-53.2	59.8
4w	0.86	6.9	-3.2	-7.0	-165.7	176.9	-59.2	65.7
5w	0.87	-18.3	9.7	0.9	4.5	71.1	-59.2	62.3
6w	1.22	-0.8	0.6	-176.3	-170.5	50.3	78.6	-69.1
7w	1.32	2.1	-1.0	-176.6	-125.7	75.7	-48.9	60.6
8w	1.40	-16.8	9.4	-0.5	7.6	68.1	-74.0	177.4
9w	1.47	1.2	-0.3	179.0	83.5	53.5	-71.0	178.3
10w	1.59	6.4	-3.7	-2.0	2.6	-170.3	-161.0	-62.6
11w	1.71	68.2	159.7	-11.4	10.5	-168.6	-57.7	64.8
12w	1.74	-80.6	159.0	-7.0	13.9	70.1	-60.2	62.3
13w	1.74	0.5	1.0	-177.9	-102.8	-75.8	83.2	-66.1
14w	1.82	2.0	-0.7	176.8	84.5	54.4	-53.2	59.8
15w	1.92	-1.1	1.6	165.8	156.6	-45.2	47.1	-59.3
16w	1.96	68.8	153.4	-5.6	6.9	169.9	-66.6	-59.1
17w	1.98	-1.2	1.8	165.8	157.9	-42.3	-79.8	64.8
18w	2.08	2.3	-0.4	171.8	-90.5	66.2	-62.2	63.6
19w	2.39	-89.7	178.2	-6.1	5.0	-156.0	-43.0	-63.0
20w	2.46	19.4	-11.8	-35.7	39.4	-55.2	172.7	-71.9
21w	2.57	3.4	-2.6	-16.7	-12.5	-170.4	70.9	67.1
22w	2.61	0.6	0.8	173.7	-95.7	62.8	-79.0	178.3
23w	2.61	0.6	0.8	173.7	-95.7	84.1	-79.0	178.3
24w	2.63	-56.4	158.4	148.3	49.8	70.5	-60.6	61.3
25w	2.65	1.2	-0.9	-178.1	96.1	40.7	-147.3	-63.0
26w	2.85	-12.9	7.3	-109.0	79.4	72.4	-166.4	178.2
27w	2.93	-2.2	2.5	166.8	-94.3	-50.6	171.5	67.3
28w	3.26	11.0	-8.8	-34.2	34.0	-48.5	168.4	65.2
29w	3.30	17.9	-11.9	-37.5	39.2	-55.8	171.0	166.3
30w	3.32	-56.4	159.3	147.8	49.2	68.6	-75.5	176.5
31w	3.33	4.1	-2.7	-169.6	82.3	-164.7	74.7	-179.3
32w	3.48	75.7	-143.6	-1.0	-0.5	-156.4	76.7	-67.2
33w	3.66	62.5	146.1	151.8	161.6	-47.7	47.9	-59.1
34w	3.67	-55.2	-174.9	-123.3	77.9	52.0	-161.3	179.5
35w	3.68	12.1	-6.6	-16.6	32.6	-161.9	-157.6	-177.2
36w	3.71	13.5	-7.1	-17.7	32.9	-162.0	-77.9	-178.8
37w	3.72	13.9	-7.2	-17.7	32.7	-162.1	-78.1	-178.8

38w	3.74	-64.0	-136.9	159.5	-170.1	49.2	80.4	-70.7
39w	4.11	-79.6	108.5	141.2	98.1	39.9	-172.0	63.7
40w	4.19	-61.1	-156.3	-137.5	164.3	-46.1	-79.1	64.3
41w	4.31	67.6	161.6	-16.5	26.1	-166.2	-81.3	178.1
42w	4.33	62.5	143.7	154.2	163.5	-50.7	-79.6	64.1
43w	4.43	65.7	163.9	-16.1	28.2	-164.2	-124.6	-178.4
44w	4.52	87.8	-178.6	-29.8	30.7	-49.2	167.0	171.5
45w	4.62	87.6	-16.7	-128.9	-69.4	-49.0	168.9	-75.4
46w	4.70	172.7	161.3	142.4	52.9	-50.7	160.8	66.5
47w	4.80	-72.8	-104.9	-3.7	2.6	-167.8	-69.5	65.7
48w	4.80	-1.9	2.3	167.0	-93.6	-50.0	169.8	67.2
49w	4.83	-174.4	-171.4	-124.3	-69.4	165.7	165.7	68.2
50w	4.85	76.7	159.2	-28.2	32.4	-55.5	174.3	-73.0
51w	4.86	-59.6	-157.4	-136.8	163.7	-43.9	45.1	-58.2
52w	4.91	-56.1	155.6	148.8	50.9	60.6	37.4	-50.7
53w	4.92	79.2	-16.3	-171.5	-47.2	174.6	83.9	-69.7
54w	5.02	-72.0	142.2	168.5	39.5	-168.7	87.3	-67.8
55w	5.11	87.9	-170.5	-27.6	-69.7	-47.5	165.6	67.8
56w	5.15	82.9	-156.7	-144.8	-59.3	-71.1	66.7	66.9
57w	5.15	-0.2	0.5	178.0	67.6	-51.2	168.2	63.3
58w	5.17	-173.4	-156.0	-144.5	-55.9	45.4	82.6	-63.8
59w	5.26	64.4	126.2	-178.5	-16.9	51.8	75.3	-69.1
60w	6.06	-83.7	114.8	143.0	108.0	35.3	-172.6	-66.0
61w	6.48	-71.6	-101.9	-12.1	20.4	-164.3	-78.8	176.2
62w	6.76	76.9	-160.6	-43.9	166.2	-53.8	-91.6	179.5
63w	7.09	-63.7	-133.2	-165.5	72.0	-173.9	80.9	-74.8
64w	8.18	-60.7	-154.5	-142.4	75.8	-162.3	-150.8	-169.5
65w	9.61	69.6	110.7	-148.4	87.2	-161.3	-94.9	-175.9

Standard coordinates and absolute energies, in hartrees (ωB97X-D/6-311++g**)

1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.882146	1.087791	-0.018167
2	1	0	-1.521562	1.413005	-1.007003
3	1	0	-1.504638	1.807620	0.717396
4	8	0	-3.274323	1.051422	0.029257
5	1	0	-3.539683	0.127914	-0.049126
6	6	0	-1.269641	-0.267201	0.236248
7	8	0	-1.959140	-1.262561	0.231549
8	6	0	0.220091	-0.388747	0.513373
9	1	0	0.401377	0.072154	1.495982
10	6	0	1.071640	0.340593	-0.531037
11	1	0	0.747200	1.381938	-0.609055
12	6	0	2.546733	0.334674	-0.146837
13	1	0	2.907581	-0.683698	0.016191
14	1	0	3.132073	0.821855	-0.928559
15	9	0	2.713018	1.047906	1.036582
16	8	0	0.594600	-1.741059	0.518621
17	1	0	-0.221833	-2.256652	0.557597
18	8	0	0.899287	-0.243029	-1.799347
19	1	0	0.978862	-1.196136	-1.684773

HF=-596.6735887

2g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.779554	-0.955770	-0.416050
2	1	0	-0.989489	-1.713244	-0.416634
3	1	0	-2.103336	-0.849418	-1.462679
4	8	0	-2.837419	-1.337743	0.409240
5	1	0	-3.049859	-0.584772	0.972419
6	6	0	-1.190099	0.367518	-0.004026
7	8	0	-1.693817	1.010811	0.892688
8	6	0	0.018919	0.941211	-0.738291
9	1	0	-0.206992	0.927067	-1.812678
10	6	0	1.296808	0.103043	-0.553649
11	1	0	2.111247	0.700447	-0.980896
12	6	0	1.612911	-0.156843	0.905678
13	1	0	1.724033	0.778998	1.455383
14	1	0	0.857078	-0.791895	1.377470
15	9	0	2.824196	-0.847591	0.966811
16	8	0	0.265181	2.248187	-0.308737
17	1	0	-0.384169	2.445566	0.378940
18	8	0	1.134329	-1.101902	-1.271199
19	1	0	1.923627	-1.634211	-1.150532

HF=-596.6715832

3g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.385444	0.513529	0.293801
2	1	0	-2.589655	1.409777	-0.304154
3	1	0	-1.969314	0.862051	1.251001
4	8	0	-3.544967	-0.233990	0.490717
5	1	0	-3.355469	-1.130388	0.187206
6	6	0	-1.311568	-0.292262	-0.392813
7	8	0	-1.496887	-1.452238	-0.676694
8	6	0	0.022513	0.382526	-0.718474
9	1	0	0.159899	0.271263	-1.798926
10	6	0	1.152448	-0.350003	0.009852
11	1	0	1.008718	-1.429361	-0.112502
12	6	0	2.511518	0.047477	-0.531060
13	1	0	2.650010	-0.316645	-1.551676
14	1	0	2.660460	1.128078	-0.487529
15	9	0	3.486605	-0.545609	0.273405
16	8	0	0.033969	1.757123	-0.431295
17	1	0	0.244251	1.850086	0.504231
18	8	0	1.019706	0.023968	1.370565
19	1	0	1.780284	-0.300878	1.857524

HF=-596.6719263

4g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.929667	-0.780728	-0.690885
2	1	0	2.942499	-0.543079	-1.022017
3	1	0	1.395578	-1.198262	-1.558390
4	8	0	2.015360	-1.686903	0.369588
5	1	0	1.123175	-2.004679	0.555231
6	6	0	1.251536	0.536754	-0.359147
7	8	0	1.432028	1.524793	-1.033764
8	6	0	0.302588	0.633656	0.840021
9	1	0	0.804241	0.191120	1.707658
10	6	0	-1.010502	-0.143749	0.617860
11	1	0	-1.645532	0.072517	1.484494
12	6	0	-1.742991	0.295330	-0.633587
13	1	0	-1.989278	1.356646	-0.592592
14	1	0	-1.173048	0.070123	-1.539647
15	9	0	-2.933160	-0.432392	-0.706134
16	8	0	-0.012619	1.972514	1.089253
17	1	0	0.378740	2.485522	0.368604
18	8	0	-0.720414	-1.532364	0.564360
19	1	0	-1.534561	-2.010277	0.390792

HF=-596.6734943

5g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.461729	0.319469	-0.333227
2	1	0	2.813735	1.140945	0.303965
3	1	0	2.192435	0.775796	-1.294706
4	8	0	3.440930	-0.659909	-0.492700
5	1	0	3.077283	-1.482318	-0.142571
6	6	0	1.207783	-0.245367	0.284547
7	8	0	1.146988	-1.416609	0.586258
8	6	0	0.030550	0.684511	0.524971
9	1	0	-0.201381	0.633197	1.599888
10	6	0	-1.215426	0.236645	-0.257279
11	1	0	-0.952783	0.111062	-1.317164
12	6	0	-1.828178	-1.048733	0.263777
13	1	0	-1.174031	-1.906101	0.115031
14	1	0	-2.097601	-0.952497	1.318418
15	9	0	-3.009952	-1.263490	-0.453074
16	8	0	0.395950	1.988329	0.156864
17	1	0	-0.416263	2.498398	0.077519
18	8	0	-2.127248	1.311823	-0.114700
19	1	0	-2.943539	1.084705	-0.565223

HF=-596.6710102

6g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.935175	-1.011537	-0.450986
2	1	0	-1.352214	-1.762288	0.102933
3	1	0	-1.777727	-1.194448	-1.520423
4	8	0	-3.295000	-1.100592	-0.155655
5	1	0	-3.501794	-0.382530	0.453562
6	6	0	-1.362287	0.335202	-0.080497
7	8	0	-2.003026	1.115619	0.583651
8	6	0	0.037497	0.719400	-0.548664
9	1	0	0.006198	0.752459	-1.648797
10	6	0	1.052782	-0.354983	-0.146297
11	1	0	0.869974	-1.250171	-0.761167
12	6	0	2.467211	0.120159	-0.410071
13	1	0	2.629792	0.322872	-1.471353
14	1	0	2.699230	1.000781	0.188594
15	9	0	3.339756	-0.903688	-0.028826
16	8	0	0.385865	1.978343	-0.059941
17	1	0	-0.327624	2.259607	0.527648
18	8	0	0.855168	-0.652915	1.217430
19	1	0	1.592127	-1.186177	1.523646

HF=-596.6712281

7g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.241987	0.713274	0.205366
2	1	0	-2.240468	1.631595	-0.393732
3	1	0	-1.860248	0.989912	1.198292
4	8	0	-3.522468	0.167562	0.283693
5	1	0	-3.455772	-0.748958	-0.010984
6	6	0	-1.260756	-0.259938	-0.397020
7	8	0	-1.609775	-1.372634	-0.714553
8	6	0	0.187023	0.168204	-0.593945
9	1	0	0.400739	0.043755	-1.663752
10	6	0	1.114596	-0.752361	0.223264
11	1	0	0.790433	-1.785430	0.063415
12	6	0	2.556647	-0.668804	-0.240860
13	1	0	3.211997	-1.187702	0.459717
14	1	0	2.670614	-1.080955	-1.246937
15	9	0	2.981579	0.670650	-0.295515
16	8	0	0.322665	1.515695	-0.193035
17	1	0	1.208889	1.811076	-0.418667
18	8	0	0.976424	-0.483563	1.596640
19	1	0	0.971705	0.472126	1.709507

HF=-596.6711414

8g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.405457	0.462381	-0.112253
2	1	0	2.641130	1.143830	0.715126
3	1	0	2.192542	1.101566	-0.979177
4	8	0	3.460836	-0.410059	-0.375322
5	1	0	3.131685	-1.303870	-0.219742
6	6	0	1.143745	-0.285847	0.241529
7	8	0	1.146950	-1.496264	0.295257
8	6	0	-0.122596	0.509816	0.500153
9	1	0	-0.533021	0.170171	1.461520
10	6	0	-1.172834	0.240551	-0.608908
11	1	0	-0.688367	0.330492	-1.586557
12	6	0	-1.821338	-1.125269	-0.510085
13	1	0	-2.482491	-1.295898	-1.361893
14	1	0	-1.079610	-1.918831	-0.423203
15	9	0	-2.619143	-1.144426	0.640217
16	8	0	0.191672	1.877339	0.540123
17	1	0	-0.607839	2.352688	0.288399
18	8	0	-2.148497	1.265073	-0.562288
19	1	0	-2.804031	1.021170	0.098801

HF=-596.6709873

9g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.894746	-1.098120	-0.306503
2	1	0	-1.356523	-1.717277	0.427965
3	1	0	-1.628977	-1.469289	-1.303285
4	8	0	-3.275324	-1.175569	-0.131878
5	1	0	-3.550622	-0.378410	0.334881
6	6	0	-1.378134	0.307697	-0.132409
7	8	0	-2.085036	1.170225	0.337780
8	6	0	0.043134	0.656061	-0.554600
9	1	0	0.058766	0.618328	-1.656409
10	6	0	1.063812	-0.346120	-0.003472
11	1	0	0.845151	-1.342446	-0.399655
12	6	0	2.466228	0.033728	-0.452437
13	1	0	2.497308	0.174129	-1.537404
14	1	0	2.800651	0.949751	0.040351
15	9	0	3.351083	-0.981029	-0.128969
16	8	0	0.376103	1.939364	-0.100287
17	1	0	-0.447684	2.361633	0.177432
18	8	0	0.949527	-0.448085	1.395079
19	1	0	1.098256	0.425899	1.767821

HF=-596.6710288

10g

1	6	0	-2.401037	0.656597	0.011991
2	1	0	-2.362675	1.555738	-0.617327
3	1	0	-2.305549	1.007153	1.048148
4	8	0	-3.593188	-0.041702	-0.172841
5	1	0	-3.354990	-0.933865	-0.453613
6	6	0	-1.197189	-0.198583	-0.304771
7	8	0	-1.341556	-1.359525	-0.617652
8	6	0	0.184400	0.451152	-0.243845
9	1	0	0.418261	0.769395	-1.266424
10	6	0	1.242176	-0.554450	0.215477
11	1	0	1.126785	-1.477548	-0.357960
12	6	0	2.653882	-0.021170	0.036148
13	1	0	2.787578	0.925882	0.563404
14	1	0	3.379157	-0.754271	0.393096
15	9	0	2.882534	0.201149	-1.316101
16	8	0	0.187495	1.605695	0.559765
17	1	0	0.288234	1.312805	1.472108
18	8	0	1.079969	-0.786877	1.610143
19	1	0	0.525241	-1.557636	1.738153

HF=-596.6697347

11g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.405934	0.681635	0.118894
2	1	0	-2.333362	1.672577	-0.349085
3	1	0	-2.339216	0.850096	1.201394
4	8	0	-3.601160	0.048949	-0.219479
5	1	0	-3.367642	-0.792804	-0.629541
6	6	0	-1.202938	-0.129371	-0.302012
7	8	0	-1.351216	-1.222279	-0.802667
8	6	0	0.180832	0.487863	-0.099339
9	1	0	0.387409	1.090360	-0.991646
10	6	0	1.252952	-0.594805	0.026299
11	1	0	1.143537	-1.300525	-0.801283
12	6	0	2.656876	-0.013796	0.007644
13	1	0	2.788967	0.724705	0.801337
14	1	0	3.394421	-0.811259	0.111450
15	9	0	2.864028	0.620787	-1.211320
16	8	0	0.196656	1.365797	1.001090
17	1	0	0.302899	0.824490	1.790970
18	8	0	1.110374	-1.247415	1.281570
19	1	0	0.518776	-1.994304	1.175253

HF=-596.6698093

12g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.388636	-0.417306	-0.271986
2	1	0	-2.865558	-0.333658	-1.253976
3	1	0	-3.171465	-0.336793	0.487791
4	8	0	-1.757298	-1.665607	-0.086573
5	1	0	-1.008355	-1.712584	-0.695484
6	6	0	-1.467429	0.789646	-0.112390
7	8	0	-1.737740	1.844486	-0.626566
8	6	0	-0.174706	0.636184	0.707095
9	1	0	0.004760	1.612309	1.165443
10	6	0	0.985186	0.369397	-0.261576
11	1	0	1.068315	1.235716	-0.930039
12	6	0	2.289735	0.179792	0.481695
13	1	0	2.572265	1.087208	1.019946
14	1	0	2.235643	-0.667020	1.166262
15	9	0	3.286226	-0.093426	-0.460951
16	8	0	-0.266467	-0.295483	1.752946
17	1	0	-0.660837	-1.105350	1.399766
18	8	0	0.679057	-0.791970	-1.027963
19	1	0	1.443876	-1.016681	-1.562927

HF=-596.6727848

13g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.303238	-0.555628	0.238505
2	1	0	-2.353734	-0.983582	1.246627
3	1	0	-2.029775	-1.379765	-0.436128
4	8	0	-3.522355	0.016321	-0.119849
5	1	0	-3.335371	0.921096	-0.399714
6	6	0	-1.183202	0.454116	0.189508
7	8	0	-1.393952	1.590503	-0.161971
8	6	0	0.226510	0.018907	0.567239
9	1	0	0.568386	0.694434	1.357422
10	6	0	1.152660	0.162516	-0.646918
11	1	0	1.016856	1.161671	-1.065241
12	6	0	2.614793	-0.050044	-0.274597
13	1	0	2.783224	-1.075881	0.068102
14	1	0	3.254900	0.156053	-1.133699
15	9	0	2.975064	0.809553	0.759952
16	8	0	0.221711	-1.335251	0.996823
17	1	0	0.726363	-1.421995	1.804807
18	8	0	0.797558	-0.760443	-1.650976
19	1	0	0.724733	-1.626248	-1.236381

HF=-596.6683796

14g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.103847	-0.571152	0.084990
2	1	0	-2.413188	-0.879626	1.091561
3	1	0	-1.729632	-1.478442	-0.410945
4	8	0	-3.164128	-0.010925	-0.623746
5	1	0	-2.884930	0.867744	-0.907997
6	6	0	-0.946976	0.383309	0.216938
7	8	0	-0.994338	1.476453	-0.314170
8	6	0	0.271240	-0.034392	1.031083
9	1	0	0.222603	0.555444	1.953583
10	6	0	1.590142	0.370423	0.333963
11	1	0	2.397030	-0.033843	0.950372
12	6	0	1.722418	-0.180265	-1.084190
13	1	0	0.995668	0.276914	-1.760233
14	1	0	2.731276	-0.018204	-1.463784
15	9	0	1.477217	-1.564941	-1.085628
16	8	0	0.234661	-1.384461	1.417373
17	1	0	0.560344	-1.922290	0.689901
18	8	0	1.759224	1.764344	0.294081
19	1	0	0.944656	2.145945	-0.056813

HF=-596.6702765

15g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.372308	-0.887381	-0.022334
2	1	0	2.201163	-1.717458	-0.726741
3	1	0	2.324305	-1.311386	0.987314
4	8	0	3.606045	-0.280268	-0.246921
5	1	0	3.429136	0.598548	-0.602415
6	6	0	1.218814	0.067088	-0.189553
7	8	0	1.409392	1.194261	-0.596996
8	6	0	-0.170679	-0.431038	0.216465
9	1	0	-0.315803	-1.448993	-0.157032
10	6	0	-1.270118	0.482660	-0.329594
11	1	0	-1.126114	0.610208	-1.408849
12	6	0	-2.655642	-0.092399	-0.089472
13	1	0	-2.818880	-0.298651	0.970472
14	1	0	-3.415236	0.598880	-0.457718
15	9	0	-2.771804	-1.289763	-0.786755
16	8	0	-0.208646	-0.498487	1.627500
17	1	0	-0.397815	0.393900	1.941188
18	8	0	-1.237165	1.728356	0.341253
19	1	0	-0.459629	2.198354	0.022819

HF=-596.6701092

1w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.905284	-1.102935	-0.324294
2	1	0	-1.352492	-1.749282	0.372738
3	1	0	-1.678564	-1.446804	-1.338186
4	8	0	-3.285580	-1.174641	-0.098977
5	1	0	-3.533483	-0.394049	0.410690
6	6	0	-1.378782	0.296556	-0.133522
7	8	0	-2.076815	1.154950	0.360708
8	6	0	0.037210	0.639163	-0.571468
9	1	0	0.051416	0.563387	-1.668421
10	6	0	1.063252	-0.341568	0.010716
11	1	0	0.822113	-1.355494	-0.319069
12	6	0	2.454616	-0.003235	-0.494967
13	1	0	2.473703	0.028079	-1.586368
14	1	0	2.807625	0.946101	-0.088010
15	9	0	3.347919	-0.995918	-0.084158
16	8	0	0.366123	1.941241	-0.160515
17	1	0	-0.449071	2.355706	0.152264
18	8	0	0.994289	-0.354237	1.420343
19	1	0	1.117264	0.549236	1.730518

HF=-596.6863118

2w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.898019	1.089599	0.038682
2	1	0	-1.520246	1.482340	-0.916764
3	1	0	-1.562810	1.771946	0.825666
4	8	0	-3.296638	1.017890	0.040071
5	1	0	-3.536848	0.100101	-0.134420
6	6	0	-1.267403	-0.265252	0.237609
7	8	0	-1.941019	-1.271356	0.177429
8	6	0	0.221545	-0.372847	0.522622
9	1	0	0.392911	0.097277	1.500680
10	6	0	1.063774	0.360744	-0.528376
11	1	0	0.746565	1.404240	-0.591501
12	6	0	2.546867	0.332725	-0.178317
13	1	0	2.908382	-0.690598	-0.060138
14	1	0	3.119473	0.848839	-0.949501
15	9	0	2.749691	1.001034	1.033567
16	8	0	0.607220	-1.723635	0.547337
17	1	0	-0.203029	-2.249336	0.505460
18	8	0	0.869712	-0.208337	-1.804157
19	1	0	0.993595	-1.160416	-1.720341

HF=-596.6863471

3w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.395166	0.512696	0.283030
2	1	0	-2.607226	1.406562	-0.314305
3	1	0	-2.005223	0.860994	1.248670
4	8	0	-3.549299	-0.261689	0.457542
5	1	0	-3.345995	-1.142738	0.116584
6	6	0	-1.303741	-0.273554	-0.398078
7	8	0	-1.486666	-1.430089	-0.707043
8	6	0	0.025510	0.420071	-0.691330
9	1	0	0.158355	0.373972	-1.776364
10	6	0	1.163094	-0.344759	-0.011255
11	1	0	1.049243	-1.411670	-0.231124
12	6	0	2.515517	0.127293	-0.505395
13	1	0	2.647888	-0.099904	-1.564185
14	1	0	2.666818	1.191361	-0.319136
15	9	0	3.504233	-0.565044	0.209223
16	8	0	0.020392	1.777889	-0.322534
17	1	0	0.237985	1.827978	0.615141
18	8	0	1.001165	-0.098040	1.375475
19	1	0	1.744046	-0.476198	1.852372

HF=-596.6853951

4w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.925439	-1.024399	-0.462780
2	1	0	-1.333579	-1.776224	0.077942
3	1	0	-1.784243	-1.202744	-1.532919
4	8	0	-3.286161	-1.122760	-0.143286
5	1	0	-3.482140	-0.424381	0.492661
6	6	0	-1.361615	0.325844	-0.097757
7	8	0	-2.010951	1.106434	0.562971
8	6	0	0.038586	0.710486	-0.557545
9	1	0	0.026765	0.716847	-1.655822
10	6	0	1.052667	-0.343351	-0.104612
11	1	0	0.847036	-1.273131	-0.651987
12	6	0	2.465216	0.094846	-0.433433
13	1	0	2.593579	0.252770	-1.505693
14	1	0	2.741091	0.989339	0.124547
15	9	0	3.340185	-0.931373	-0.045242
16	8	0	0.367274	1.989118	-0.087236
17	1	0	-0.361469	2.277858	0.477822
18	8	0	0.877154	-0.541004	1.284670
19	1	0	1.496275	-1.212834	1.580438

HF=-596.6855755

5w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.785547	-0.957147	-0.398776
2	1	0	-1.003479	-1.721808	-0.361604
3	1	0	-2.095325	-0.873351	-1.449153
4	8	0	-2.866336	-1.304774	0.422963
5	1	0	-3.045169	-0.546368	0.992678
6	6	0	-1.190361	0.367690	-0.003306
7	8	0	-1.689014	1.021181	0.889831
8	6	0	0.019391	0.920760	-0.748906
9	1	0	-0.212397	0.892298	-1.820090
10	6	0	1.295161	0.076405	-0.558110
11	1	0	2.110524	0.664916	-0.994272
12	6	0	1.609951	-0.166868	0.903961
13	1	0	1.672194	0.772657	1.454540
14	1	0	0.884367	-0.837954	1.370537
15	9	0	2.858983	-0.796984	0.986045
16	8	0	0.269120	2.239282	-0.346184
17	1	0	-0.334903	2.434681	0.382550
18	8	0	1.120650	-1.131675	-1.268888
19	1	0	1.926411	-1.649364	-1.200542

HF=-596.683772

6w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.268780	0.736695	0.160330
2	1	0	-2.291209	1.600796	-0.514272
3	1	0	-1.904260	1.101022	1.128189
4	8	0	-3.538953	0.157830	0.283504
5	1	0	-3.459122	-0.755045	-0.022783
6	6	0	-1.265396	-0.253237	-0.374556
7	8	0	-1.606768	-1.383246	-0.644877
8	6	0	0.171719	0.198390	-0.580943
9	1	0	0.353037	0.154762	-1.662366
10	6	0	1.135520	-0.764315	0.136542
11	1	0	0.831242	-1.787192	-0.102106
12	6	0	2.568108	-0.622164	-0.337392
13	1	0	3.231216	-1.243000	0.265436
14	1	0	2.660744	-0.879123	-1.394114
15	9	0	3.003239	0.710789	-0.194666
16	8	0	0.296121	1.516785	-0.089760
17	1	0	1.143580	1.871895	-0.371124
18	8	0	1.014646	-0.611916	1.534980
19	1	0	1.038229	0.330941	1.730469

HF=-596.6852339

7w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.341759	-0.524489	0.261051
2	1	0	-2.394360	-0.910841	1.285406
3	1	0	-2.125138	-1.381526	-0.388932
4	8	0	-3.542703	0.098788	-0.103545
5	1	0	-3.316639	1.001955	-0.362922
6	6	0	-1.180757	0.432654	0.167699
7	8	0	-1.358064	1.571654	-0.205036
8	6	0	0.206248	-0.059683	0.551414
9	1	0	0.528795	0.546941	1.403614
10	6	0	1.184098	0.151375	-0.612839
11	1	0	1.058748	1.164975	-0.997916
12	6	0	2.631369	-0.049843	-0.185643
13	1	0	2.787161	-1.042426	0.244297
14	1	0	3.296620	0.096350	-1.037070
15	9	0	2.963593	0.894369	0.792304
16	8	0	0.163358	-1.436422	0.874532
17	1	0	0.535246	-1.583322	1.745057
18	8	0	0.882026	-0.736656	-1.668540
19	1	0	0.805101	-1.620420	-1.291648

HF=-596.6843881

8w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.919051	-0.990985	-0.401718
2	1	0	-1.510190	-1.689554	0.341903
3	1	0	-1.647746	-1.370878	-1.391644
4	8	0	-3.312978	-0.898889	-0.294359
5	1	0	-3.509595	-0.070111	0.158850
6	6	0	-1.252269	0.342982	-0.174294
7	8	0	-1.893349	1.287536	0.232314
8	6	0	0.235132	0.497694	-0.450626
9	1	0	0.394741	0.282267	-1.514640
10	6	0	1.035295	-0.530631	0.357638
11	1	0	0.774619	-1.532272	-0.005912
12	6	0	2.535559	-0.329612	0.194147
13	1	0	2.820958	0.688850	0.458480
14	1	0	3.086028	-1.048655	0.803606
15	9	0	2.886689	-0.547006	-1.142469
16	8	0	0.644759	1.809563	-0.176920
17	1	0	-0.103085	2.259774	0.236230
18	8	0	0.679057	-0.372192	1.717665
19	1	0	0.966165	-1.141203	2.214863

HF=-596.6842887

9w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351755	0.499185	-0.305114
2	1	0	-2.412246	0.798524	-1.357745
3	1	0	-2.142114	1.408430	0.272868
4	8	0	-3.545943	-0.098913	0.118435
5	1	0	-3.313347	-0.982257	0.434740
6	6	0	-1.182846	-0.439767	-0.142438
7	8	0	-1.353820	-1.549686	0.312140
8	6	0	0.202268	0.031516	-0.576306
9	1	0	0.514529	-0.638913	-1.382281
10	6	0	1.185891	-0.106107	0.586450
11	1	0	1.062957	-1.097795	1.031998
12	6	0	2.630513	0.082750	0.145101
13	1	0	2.761658	1.026470	-0.386929
14	1	0	3.301965	0.042514	1.004966
15	9	0	2.983775	-0.955875	-0.721123
16	8	0	0.191084	1.339165	-1.096595
17	1	0	0.234541	1.953705	-0.355791
18	8	0	0.828448	0.921164	1.496783
19	1	0	1.275500	0.792884	2.336007

HF=-596.6841084

10w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.636671	-0.693917	-0.617861
2	1	0	-1.001337	-1.570102	-0.465719
3	1	0	-1.782980	-0.583674	-1.700637
4	8	0	-2.865751	-0.844166	0.042210
5	1	0	-2.989582	-0.057380	0.587650
6	6	0	-0.897278	0.526267	-0.135975
7	8	0	-1.410498	1.272986	0.672748
8	6	0	0.464048	0.883705	-0.718872
9	1	0	0.329256	0.955379	-1.806643
10	6	0	1.568505	-0.173099	-0.468868
11	1	0	2.499750	0.281082	-0.828353
12	6	0	1.787973	-0.472614	0.994247
13	1	0	2.584631	-1.206908	1.115752
14	1	0	2.023951	0.441770	1.539658
15	9	0	0.625583	-1.017620	1.561975
16	8	0	0.890845	2.119400	-0.213550
17	1	0	0.218342	2.412401	0.416449
18	8	0	1.300001	-1.382575	-1.144816
19	1	0	1.451486	-1.261194	-2.084709

HF=-596.6854536

11w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.925759	-0.773292	-0.702632
2	1	0	2.943423	-0.538037	-1.019085
3	1	0	1.395503	-1.170028	-1.580505
4	8	0	1.993278	-1.707526	0.340848
5	1	0	1.089849	-2.001768	0.524133
6	6	0	1.255095	0.541116	-0.349308
7	8	0	1.448306	1.538003	-1.010688
8	6	0	0.297906	0.627856	0.842378
9	1	0	0.791250	0.175206	1.708548
10	6	0	-1.015215	-0.151013	0.609238
11	1	0	-1.665579	0.087190	1.457617
12	6	0	-1.715239	0.265145	-0.667763
13	1	0	-1.897123	1.340107	-0.685527
14	1	0	-1.159013	-0.043336	-1.556434
15	9	0	-2.955697	-0.383680	-0.716225
16	8	0	-0.004210	1.968768	1.110901
17	1	0	0.338580	2.485883	0.368439
18	8	0	-0.713014	-1.536484	0.602932
19	1	0	-1.520331	-2.043054	0.485418

HF=-596.6857057

12w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.140313	0.985445	0.328551
2	1	0	3.227448	0.875800	0.374592
3	1	0	1.797650	1.313697	1.315440
4	8	0	1.727162	1.958857	-0.602397
5	1	0	2.237031	1.860648	-1.409390
6	6	0	1.537384	-0.387961	0.105256
7	8	0	2.056408	-1.383233	0.557101
8	6	0	0.222313	-0.510848	-0.657985
9	1	0	0.345008	-0.032038	-1.635548
10	6	0	-0.872338	0.251239	0.100597
11	1	0	-0.629972	1.319563	0.056881
12	6	0	-2.220464	0.032212	-0.553248
13	1	0	-2.219541	0.377500	-1.588797
14	1	0	-2.523454	-1.013023	-0.494202
15	9	0	-3.175256	0.787837	0.146920
16	8	0	-0.099029	-1.862898	-0.842237
17	1	0	0.475991	-2.367075	-0.250861
18	8	0	-0.865378	-0.204038	1.442082
19	1	0	-1.529397	0.284377	1.934194

HF=-596.6839504

13w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.982718	0.436356	-0.356053
2	1	0	2.357535	1.407239	-0.009660
3	1	0	1.580458	0.591394	-1.363625
4	8	0	3.004245	-0.522381	-0.358682
5	1	0	2.717154	-1.238320	0.223052
6	6	0	0.842959	0.022106	0.536975
7	8	0	0.902482	-1.024053	1.155009
8	6	0	-0.370360	0.933452	0.654698
9	1	0	-0.442565	1.211236	1.711458
10	6	0	-1.680982	0.192550	0.296426
11	1	0	-2.489264	0.910465	0.463278
12	6	0	-1.754277	-0.192607	-1.167601
13	1	0	-2.688514	-0.716845	-1.371051
14	1	0	-1.660370	0.685749	-1.807140
15	9	0	-0.702367	-1.066312	-1.493144
16	8	0	-0.254421	2.064591	-0.177236
17	1	0	-0.012451	2.829453	0.346994
18	8	0	-1.911936	-0.899386	1.155722
19	1	0	-1.083990	-1.384868	1.259819

HF=-596.6843657

14w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.486369	0.521949	0.119741
2	1	0	-2.648349	1.320040	-0.613817
3	1	0	-2.229344	1.011148	1.068215
4	8	0	-3.631604	-0.272942	0.259326
5	1	0	-3.360907	-1.182997	0.079528
6	6	0	-1.299661	-0.299017	-0.319912
7	8	0	-1.408951	-1.496301	-0.468668
8	6	0	0.017553	0.420712	-0.600025
9	1	0	0.133058	0.397065	-1.689215
10	6	0	1.198829	-0.311814	0.057871
11	1	0	1.092624	-1.386063	-0.113602
12	6	0	2.509279	0.160380	-0.533224
13	1	0	2.514566	0.021842	-1.615825
14	1	0	2.700890	1.206500	-0.287792
15	9	0	3.557663	-0.596769	-0.005333
16	8	0	-0.018275	1.771961	-0.210380
17	1	0	0.208618	1.800977	0.727112
18	8	0	1.204639	-0.010350	1.446271
19	1	0	0.765625	-0.709803	1.934291

HF=-596.6844086

15w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.354288	0.468601	-0.200386
2	1	0	2.622392	1.216885	0.553833
3	1	0	2.093788	1.018822	-1.112907
4	8	0	3.414468	-0.418097	-0.432385
5	1	0	3.091920	-1.300597	-0.206454
6	6	0	1.125392	-0.264309	0.278268
7	8	0	1.160174	-1.465568	0.440873
8	6	0	-0.142036	0.528801	0.522019
9	1	0	-0.565629	0.184663	1.474363
10	6	0	-1.180140	0.280603	-0.604484
11	1	0	-0.697811	0.437473	-1.573642
12	6	0	-1.776406	-1.109714	-0.598543
13	1	0	-2.484517	-1.219588	-1.420434
14	1	0	-1.008855	-1.880952	-0.646147
15	9	0	-2.494808	-1.289568	0.594817
16	8	0	0.176569	1.898061	0.577798
17	1	0	-0.630856	2.377926	0.359250
18	8	0	-2.183981	1.275002	-0.506597
19	1	0	-2.791608	1.032398	0.200017

HF=-596.6841611

16w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.346530	0.296784	-0.479175
2	1	0	2.755139	1.195633	-0.003416
3	1	0	1.941770	0.610412	-1.449306
4	8	0	3.333363	-0.685120	-0.637157
5	1	0	3.041152	-1.457508	-0.135664
6	6	0	1.204487	-0.206555	0.367403
7	8	0	1.240335	-1.322785	0.838084
8	6	0	0.013270	0.706331	0.591745
9	1	0	-0.244847	0.651145	1.658254
10	6	0	-1.202251	0.237962	-0.238715
11	1	0	-0.892509	0.086593	-1.280099
12	6	0	-1.812884	-1.040196	0.296649
13	1	0	-1.095977	-1.860594	0.302082
14	1	0	-2.224583	-0.885592	1.295961
15	9	0	-2.874783	-1.401350	-0.543104
16	8	0	0.363984	2.017286	0.228425
17	1	0	-0.463261	2.478558	0.044553
18	8	0	-2.125099	1.312054	-0.163541
19	1	0	-2.739419	1.256059	-0.898360

HF=-596.6834475

17w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.883021	0.302328	0.602080
2	1	0	2.806732	-0.186581	0.914785
3	1	0	1.442079	0.783754	1.485124
4	8	0	2.193907	1.230149	-0.405488
5	1	0	1.394508	1.748908	-0.573907
6	6	0	0.914611	-0.789456	0.187703
7	8	0	0.919990	-1.871193	0.734444
8	6	0	-0.083329	-0.552354	-0.950471
9	1	0	0.496036	-0.228969	-1.823299
10	6	0	-1.130552	0.549543	-0.672923
11	1	0	-1.816250	0.524543	-1.527795
12	6	0	-1.968665	0.294963	0.562322
13	1	0	-2.722099	1.075370	0.685692
14	1	0	-2.452078	-0.681084	0.497989
15	9	0	-1.165264	0.304828	1.709465
16	8	0	-0.757576	-1.745663	-1.238501
17	1	0	-0.489455	-2.383444	-0.561346
18	8	0	-0.453842	1.793673	-0.616788
19	1	0	-1.082441	2.518167	-0.644028

HF=-596.6864921

18w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.277622	0.368083	-0.543736
2	1	0	2.511926	1.424812	-0.374115
3	1	0	1.775034	0.303482	-1.516670
4	8	0	3.442773	-0.411041	-0.515600
5	1	0	3.305077	-1.087175	0.161233
6	6	0	1.291639	-0.088560	0.500731
7	8	0	1.555094	-1.023724	1.223966
8	6	0	-0.049862	0.632179	0.603895
9	1	0	-0.211364	0.859008	1.663295
10	6	0	-1.149792	-0.331009	0.158907
11	1	0	-1.140423	-1.178993	0.854377
12	6	0	-2.508173	0.336703	0.220213
13	1	0	-2.727506	0.698231	1.226460
14	1	0	-2.584565	1.145784	-0.505637
15	9	0	-3.479768	-0.620172	-0.111984
16	8	0	-0.093668	1.799249	-0.187916
17	1	0	0.203101	2.548153	0.331929
18	8	0	-0.840684	-0.766267	-1.152424
19	1	0	-1.490086	-1.421865	-1.417301

HF=-596.6832413

19w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.277406	0.367861	0.543967
2	1	0	-2.511746	1.424663	0.374847
3	1	0	-1.774603	0.302837	1.516778
4	8	0	-3.442518	-0.411286	0.515702
5	1	0	-3.304967	-1.087092	-0.161497
6	6	0	-1.291607	-0.088289	-0.500866
7	8	0	-1.555194	-1.023143	-1.224470
8	6	0	0.049915	0.632425	-0.603860
9	1	0	0.211523	0.859468	-1.663196
10	6	0	1.149731	-0.330982	-0.158962
11	1	0	1.140440	-1.178731	-0.854718
12	6	0	2.508121	0.336720	-0.219803
13	1	0	2.727474	0.698882	-1.225819
14	1	0	2.584543	1.145345	0.506562
15	9	0	3.479716	-0.620386	0.111805
16	8	0	0.093767	1.799312	0.188194
17	1	0	-0.202733	2.548366	-0.331594
18	8	0	0.840316	-0.766601	1.152176
19	1	0	1.489125	-1.422922	1.416720

HF=-596.6832412

20w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.891856	-0.602057	0.316149
2	1	0	-2.938029	-0.326015	0.159645
3	1	0	-1.777847	-0.902369	1.359107
4	8	0	-1.513521	-1.698070	-0.491191
5	1	0	-1.988011	-1.670520	-1.325274
6	6	0	-1.057293	0.649924	0.127261
7	8	0	-1.335396	1.647446	0.756484
8	6	0	0.102230	0.715483	-0.875088
9	1	0	-0.289156	0.391494	-1.847939
10	6	0	1.329461	-0.185746	-0.561443
11	1	0	2.134401	0.236397	-1.170450
12	6	0	1.791380	-0.078054	0.877199
13	1	0	2.704886	-0.653780	1.027735
14	1	0	1.946676	0.963033	1.166902
15	9	0	0.814190	-0.616419	1.733427
16	8	0	0.545922	2.044267	-0.953641
17	1	0	0.046769	2.542084	-0.290085
18	8	0	1.167587	-1.521049	-0.968242
19	1	0	0.272335	-1.810608	-0.732226

HF=-596.6858806