Supporting Information

Holophyllane A: A Triterpenoid Possessing an Unprecedented B-nor-3,4-*seco*-17,14-*friedo*-lanostane Architecture from *Abies holophylla*

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Contents

Figure S1. Dose response curves of compounds 1 and 2, and positive controls (etoposide and doxorubicin)

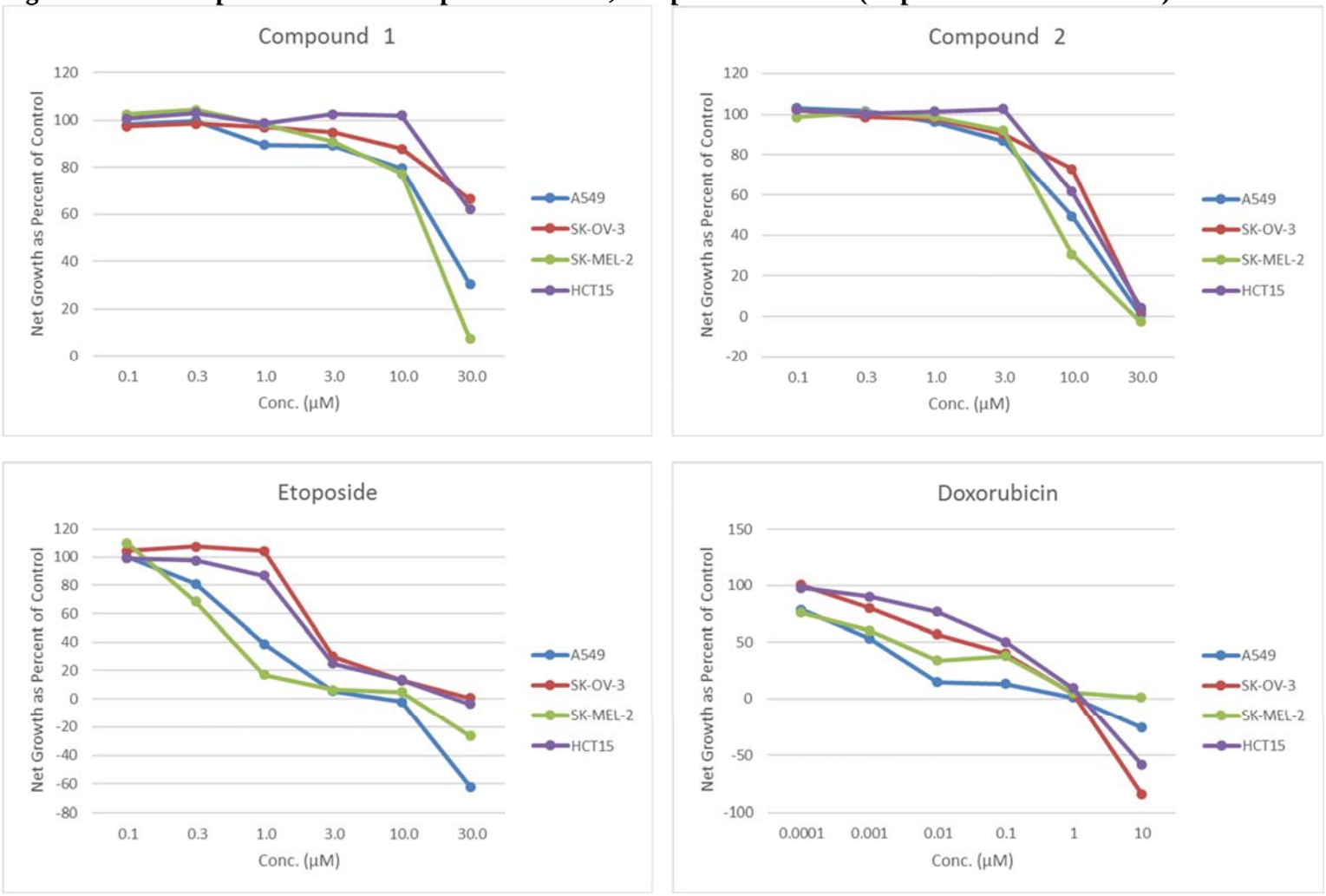


Figure S2. COSY (blue bolds), HMBC (red arrows), and NOESY (yellow dashed) correlations of 2

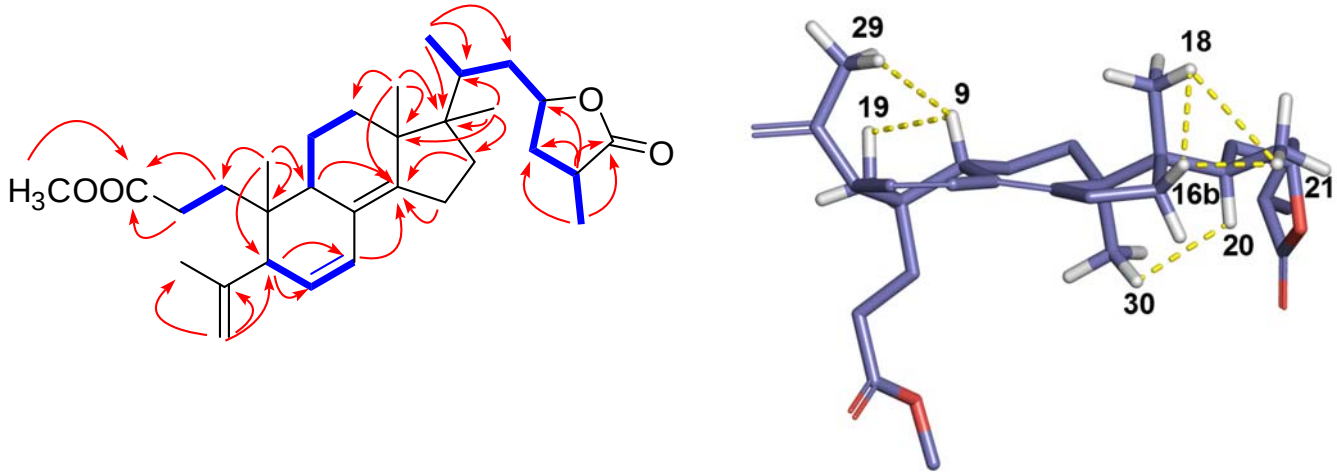
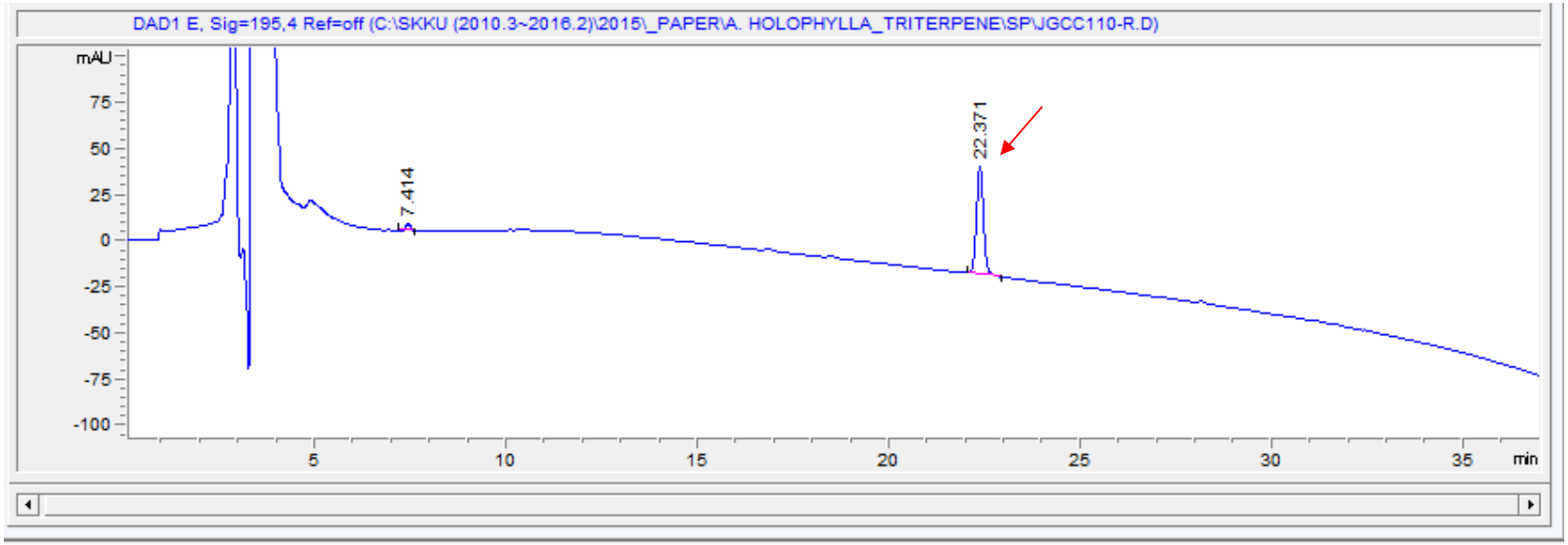


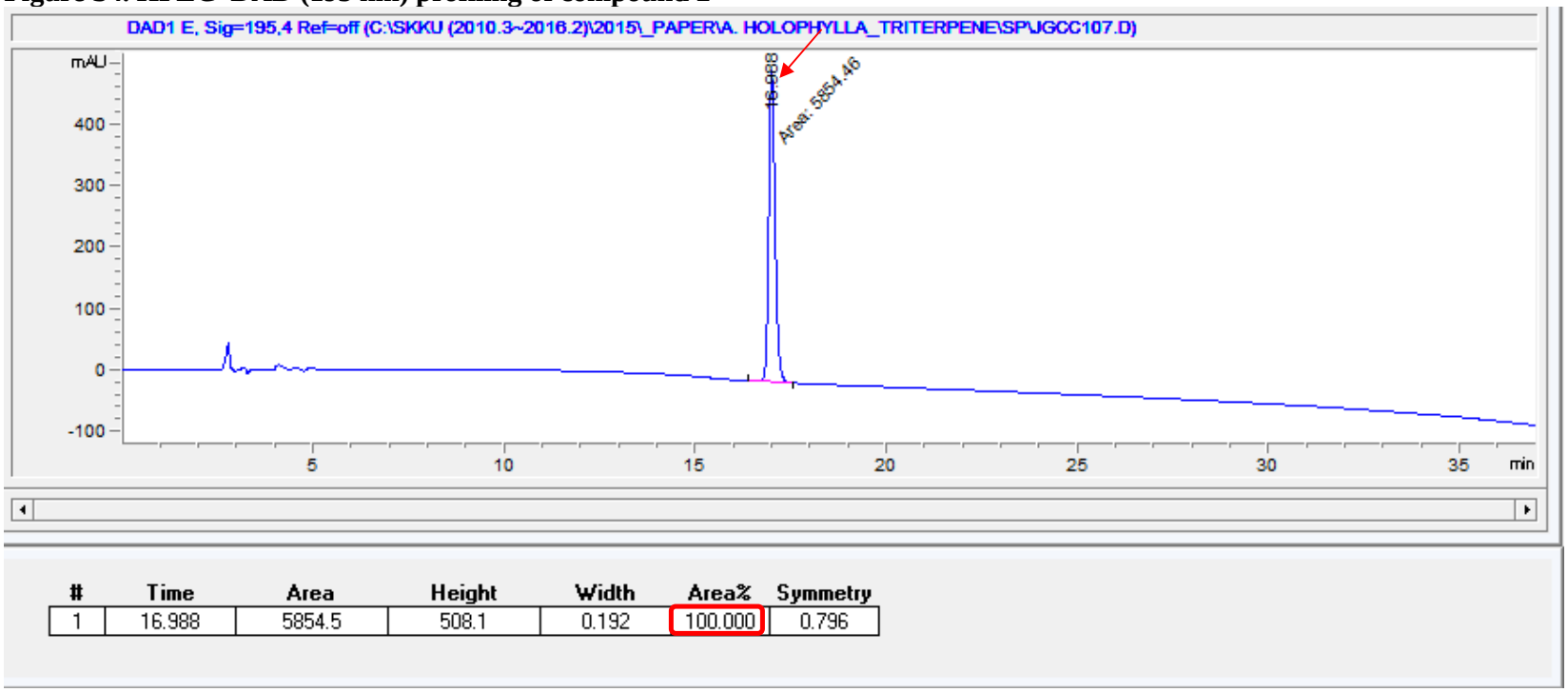
Figure S3. HPLC–DAD (195 nm) profiling of compound 1



#	Time	Area	Height	Width	Area%	Symmetry
1	7.414	34.9	4	0.1426	4.463	1.056
2	22.371	746.6	58.6	0.1987	95.537	0.935

Purity of compound **1**: **95.5%**

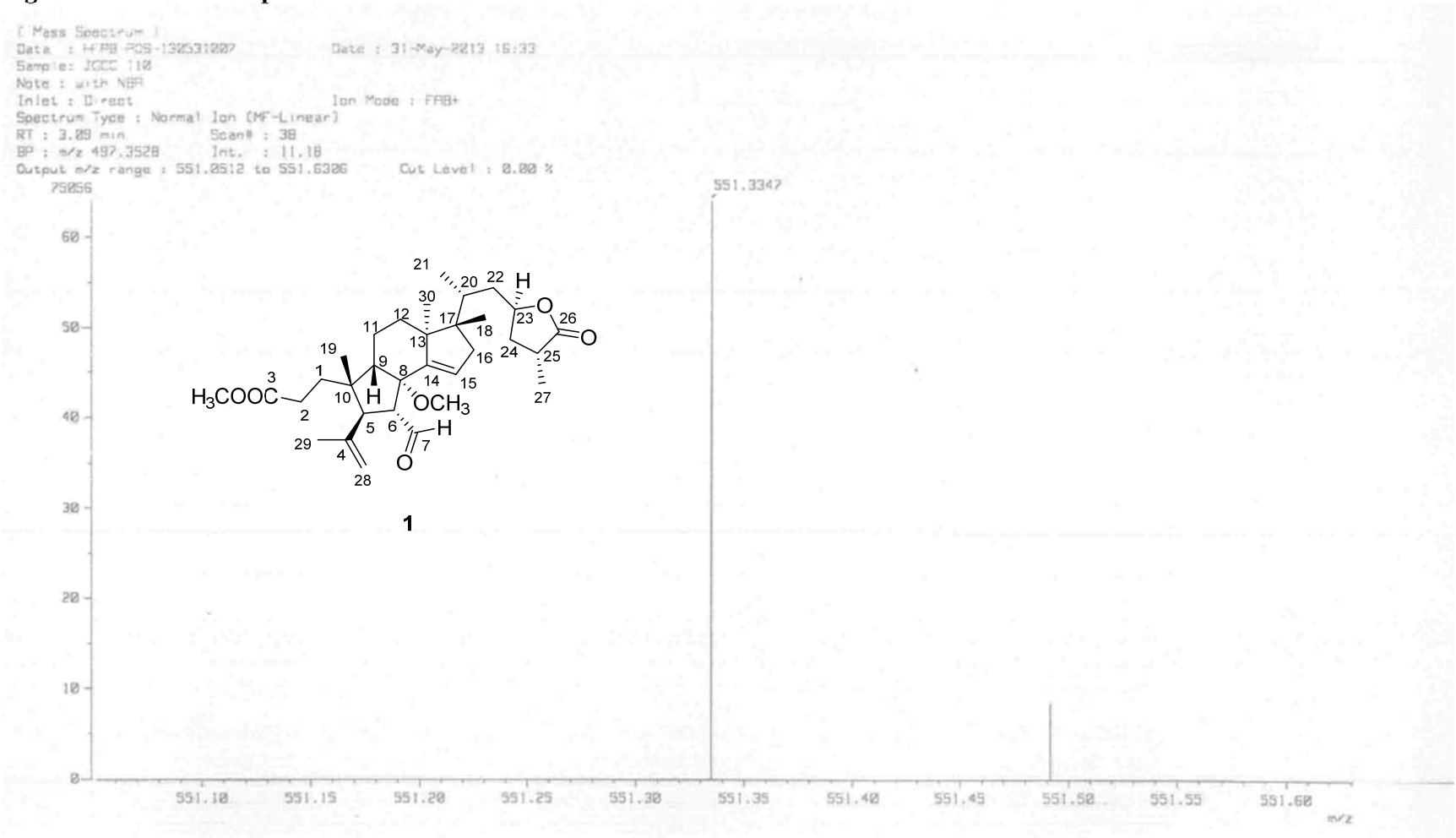
Figure S4. HPLC–DAD (195 nm) profiling of compound 2



#	Time	Area	Height	Width	Area%	Symmetry
1	16.988	5854.5	508.1	0.192	100.000	0.796

Purity of compound **2**: **>98%**

Figure S5. HRFABMS spectra of 1



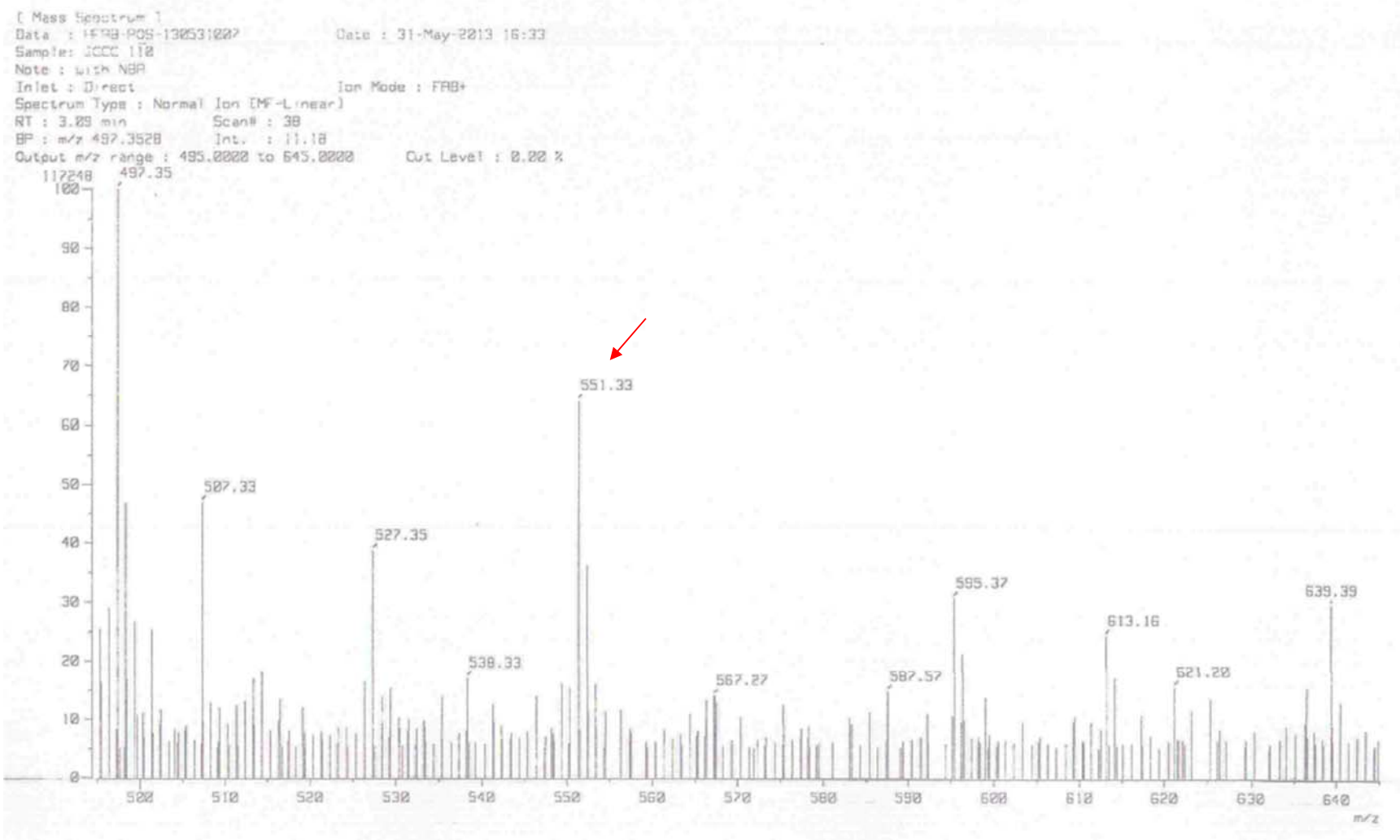

[Mass Spectrum]
Data : FAB-POS-130531027
Date : 31-May-2013 16:33
Sample: JCCC 110
Note : with NBA
Inlet : Direct
Ion Mode : FAB+
Spectrum Type : Normal Ion (MF-Linear)
RT : 3.09 min
Scan# : 38
BP : m/z 497.3528
Int. : 11.18
Output m/z range : 495.0000 to 645.0000
Cut Level : 0.00 %
117248
497.35
551.33
507.33
527.35
538.33
567.27
587.57
595.37
613.16
621.20
639.39
m/z

Figure S6. ^{1}H NMR spectrum of 1

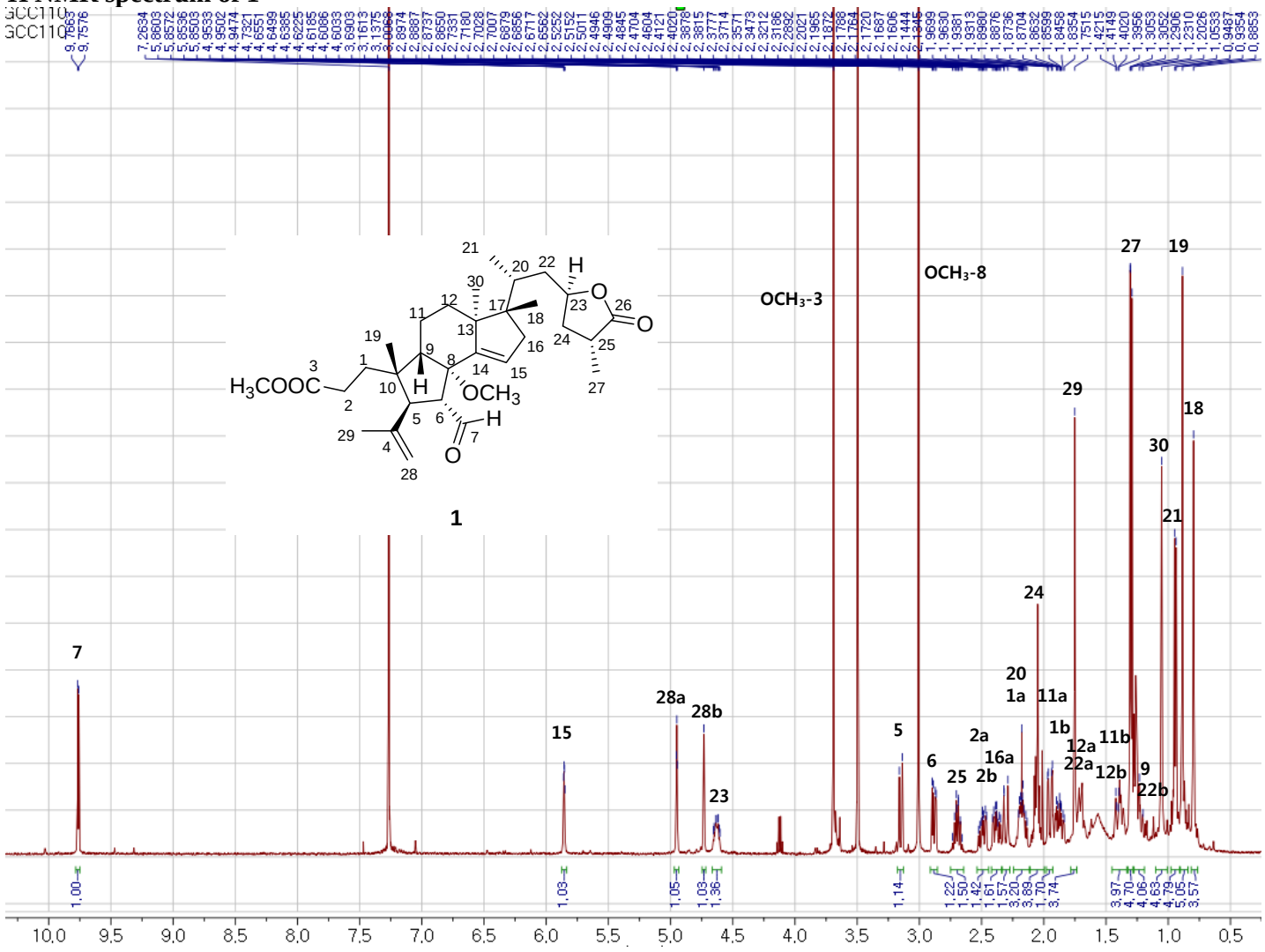


Figure S7. ^{13}C NMR spectrum of 1

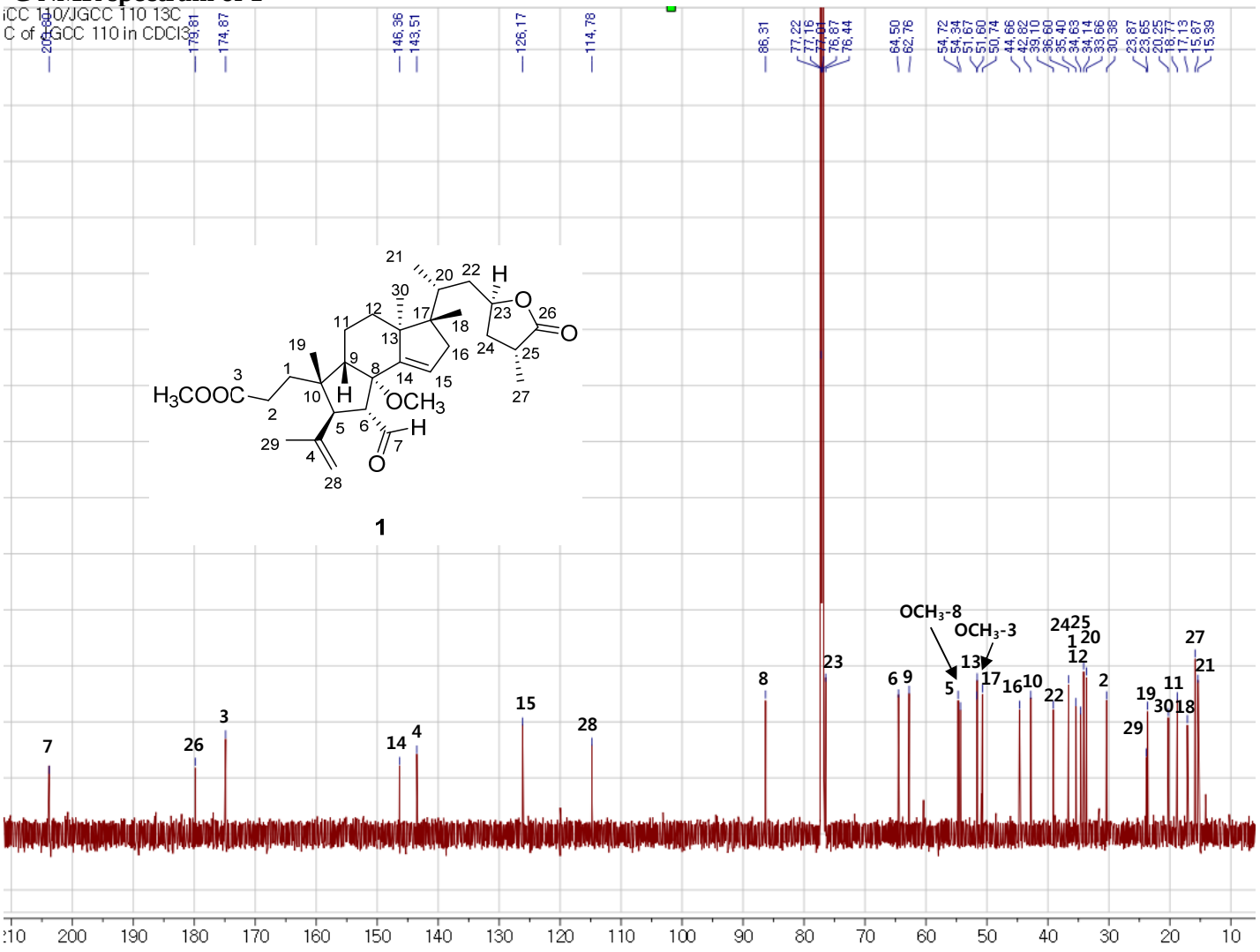


Figure S8. DEPT 90 spectrum of 1

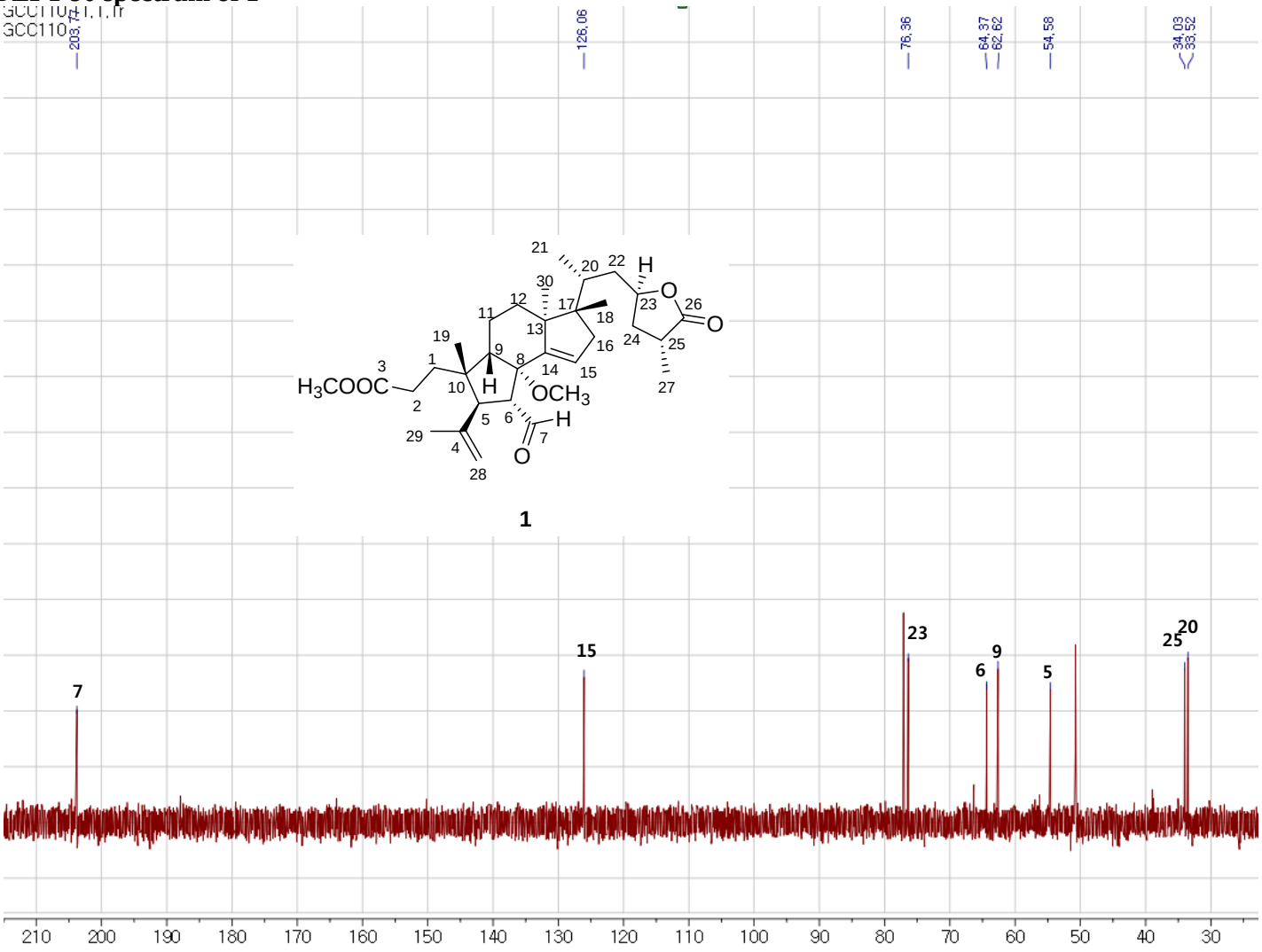


Figure S9. DEPT 135 spectrum of 1

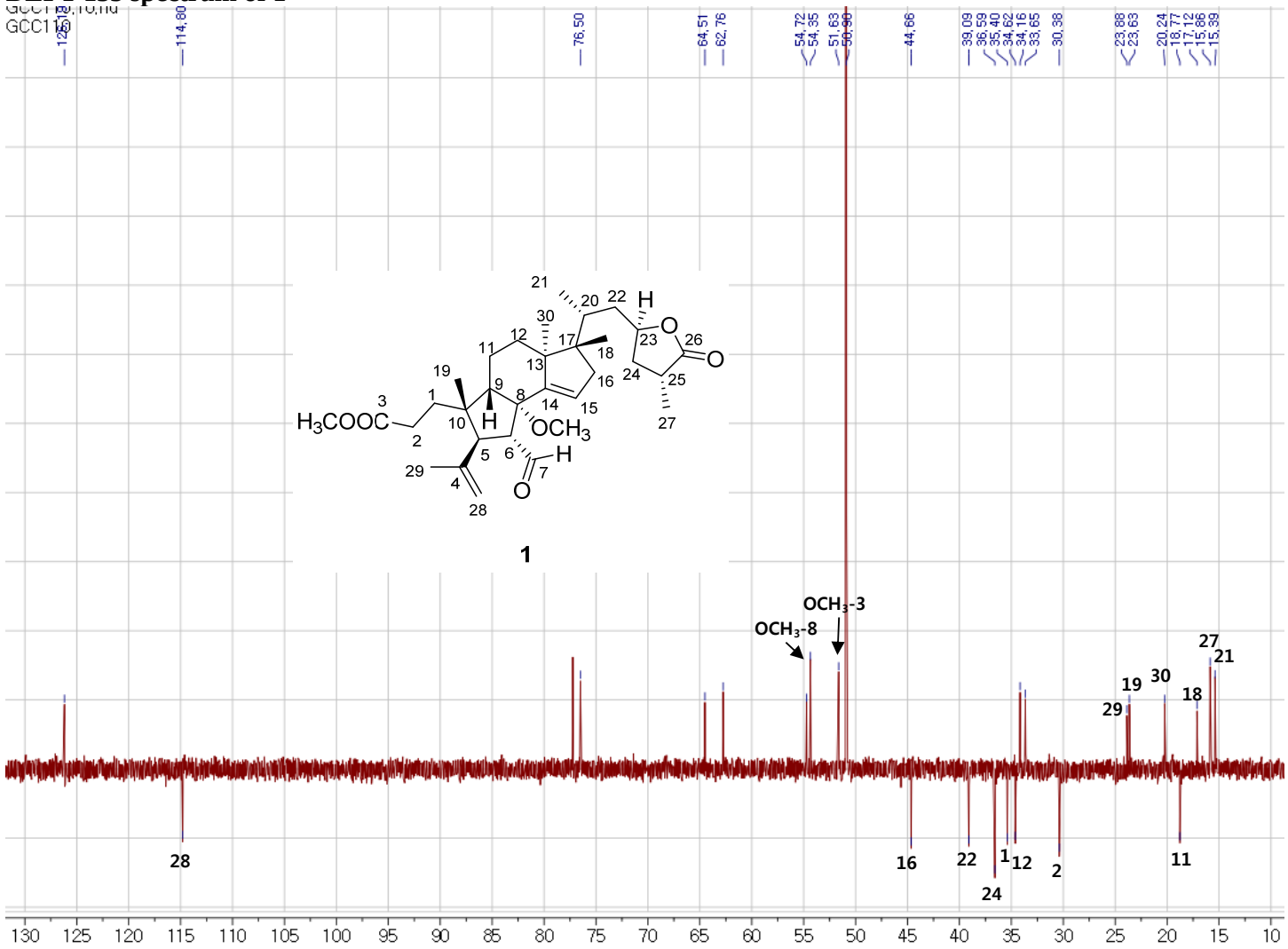


Figure S10. COSY spectrum of 1

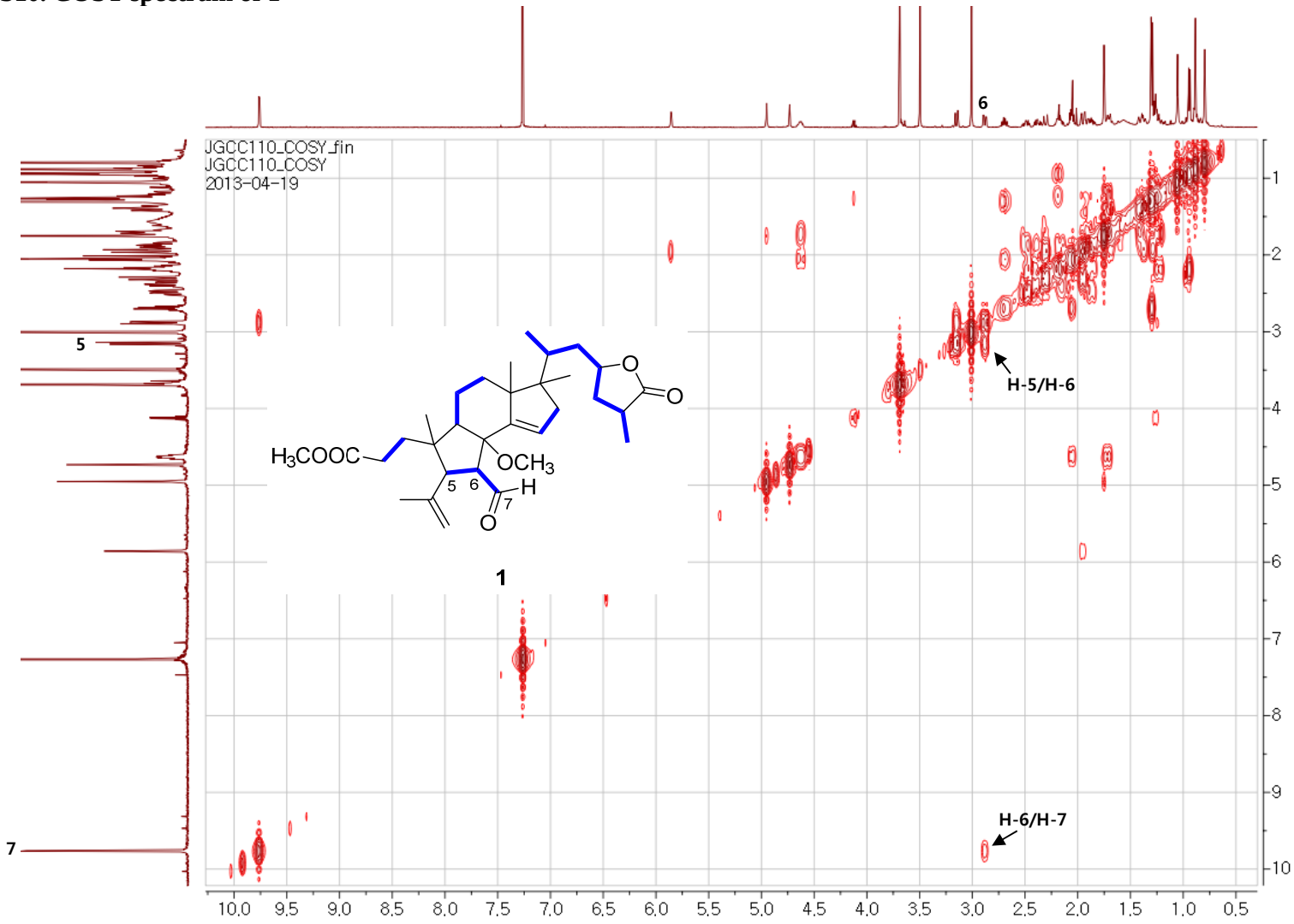


Figure S11. HSQC spectrum of 1

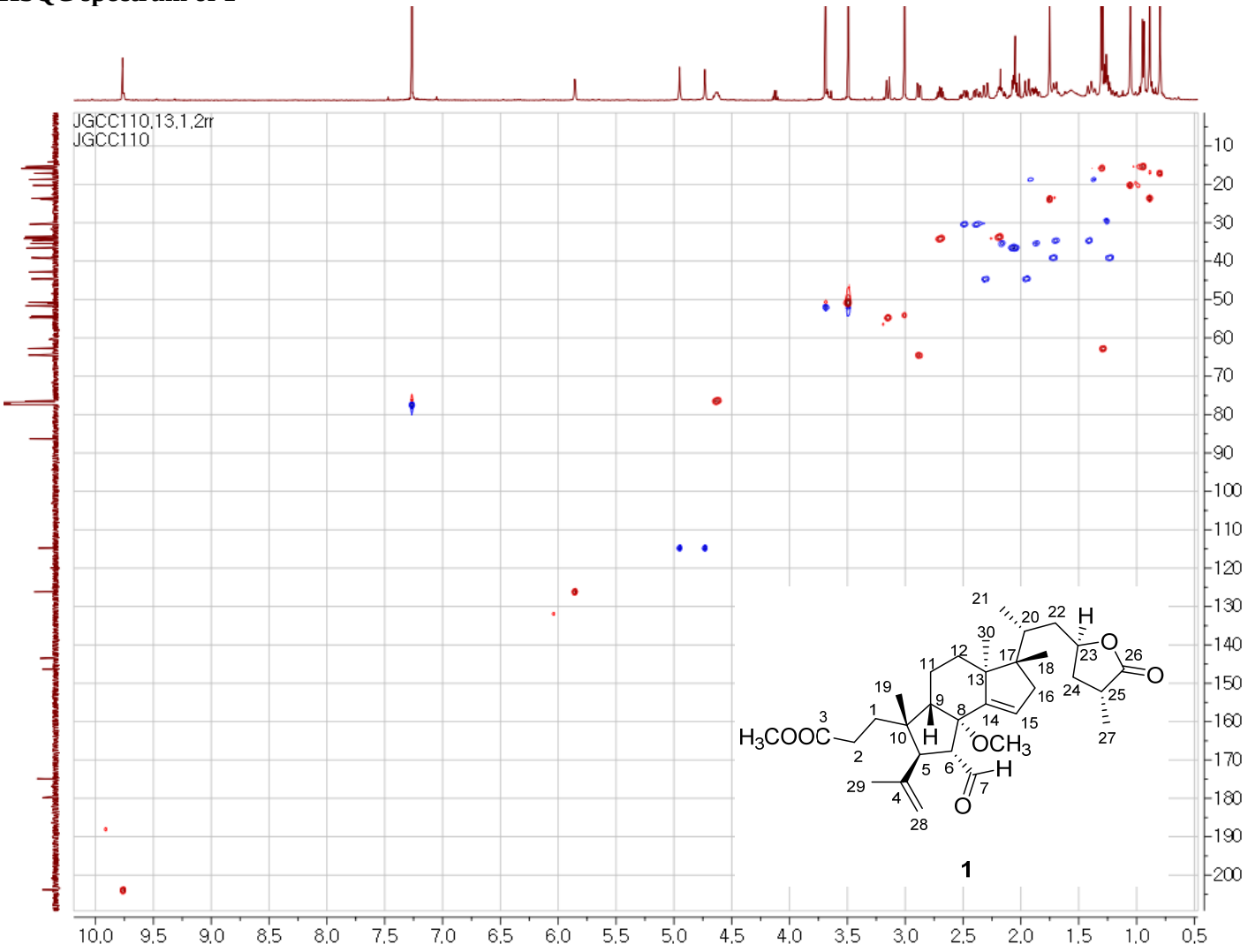


Figure S12. HMBC spectrum of 1

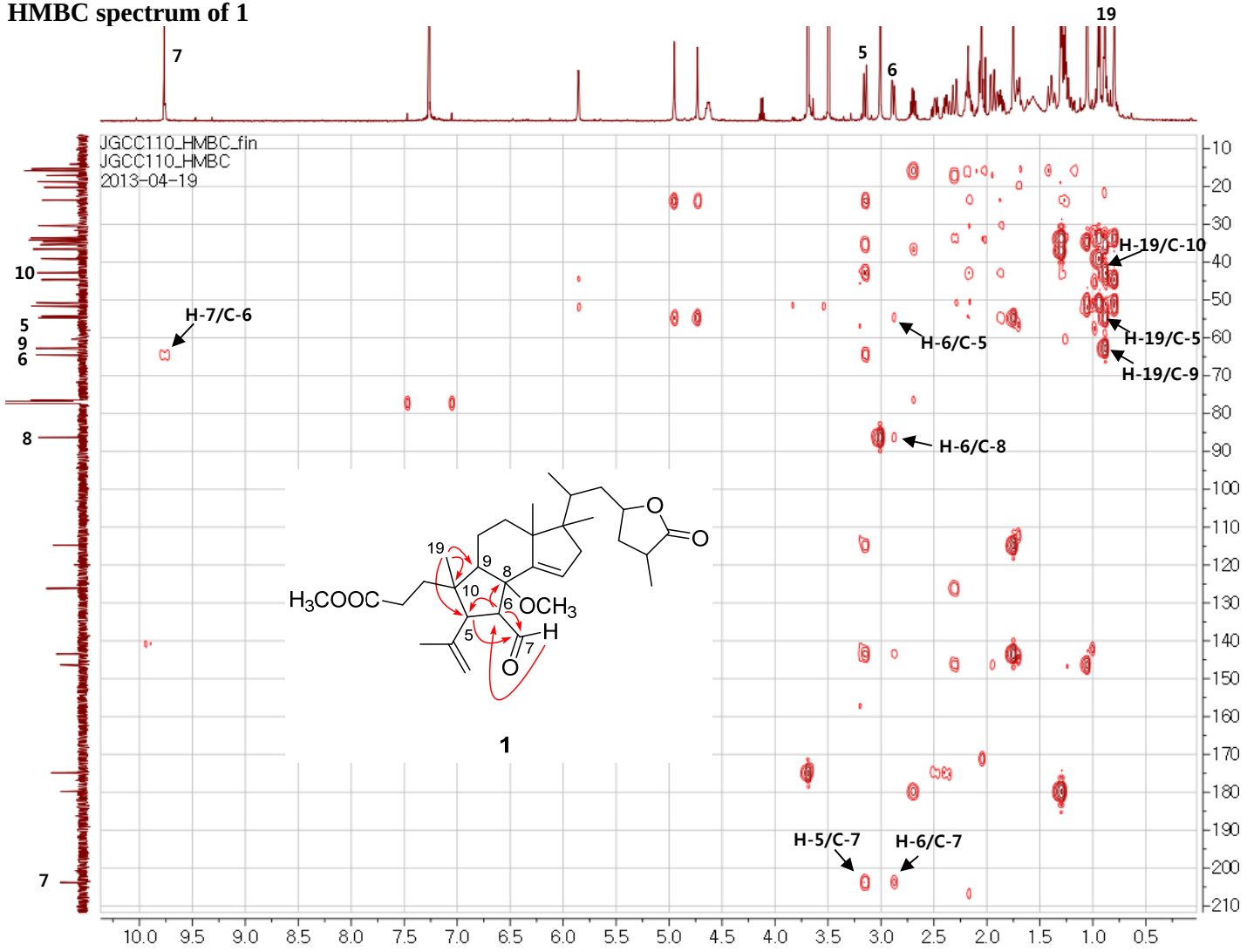
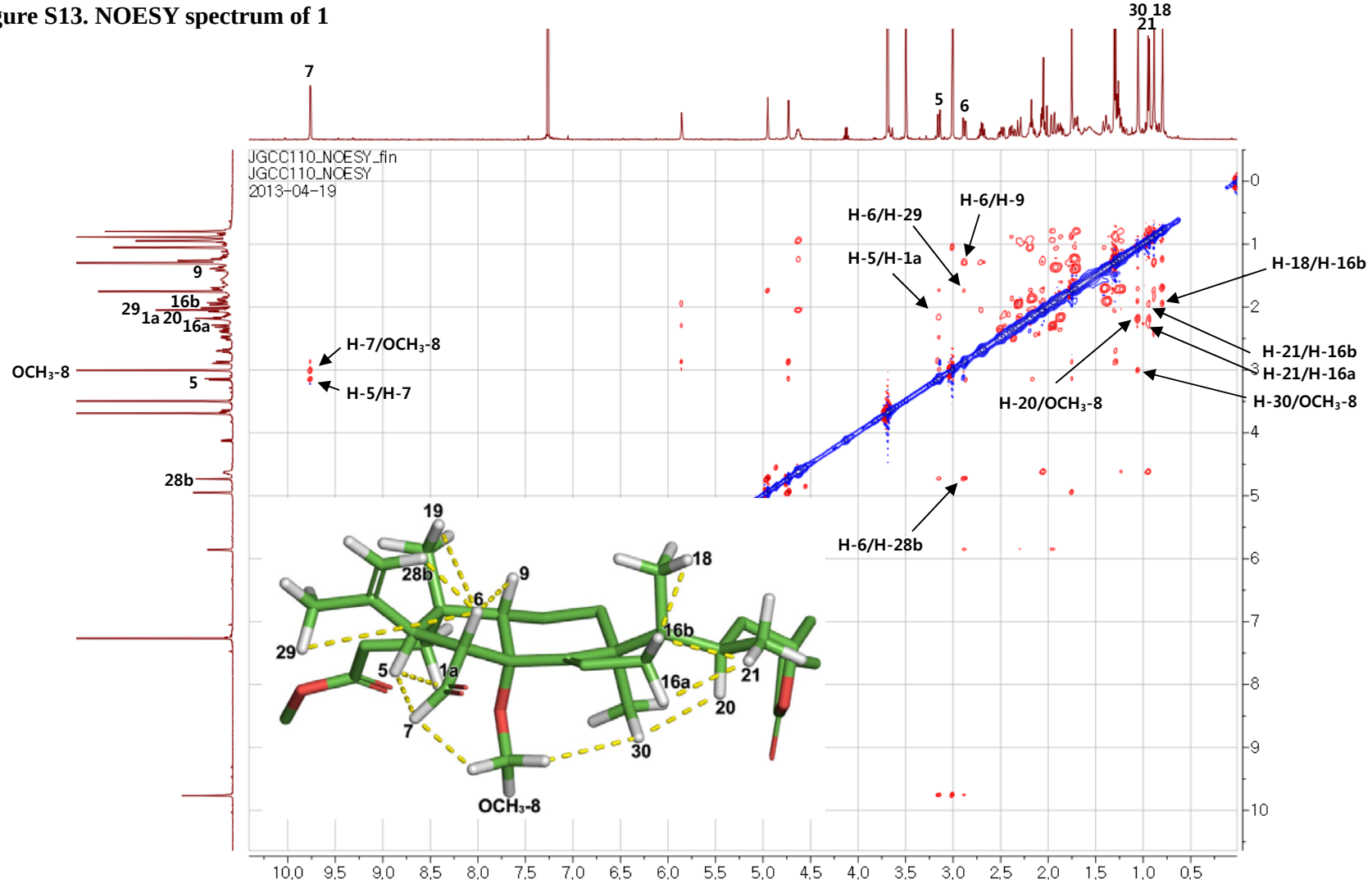


Figure S13. NOESY spectrum of 1



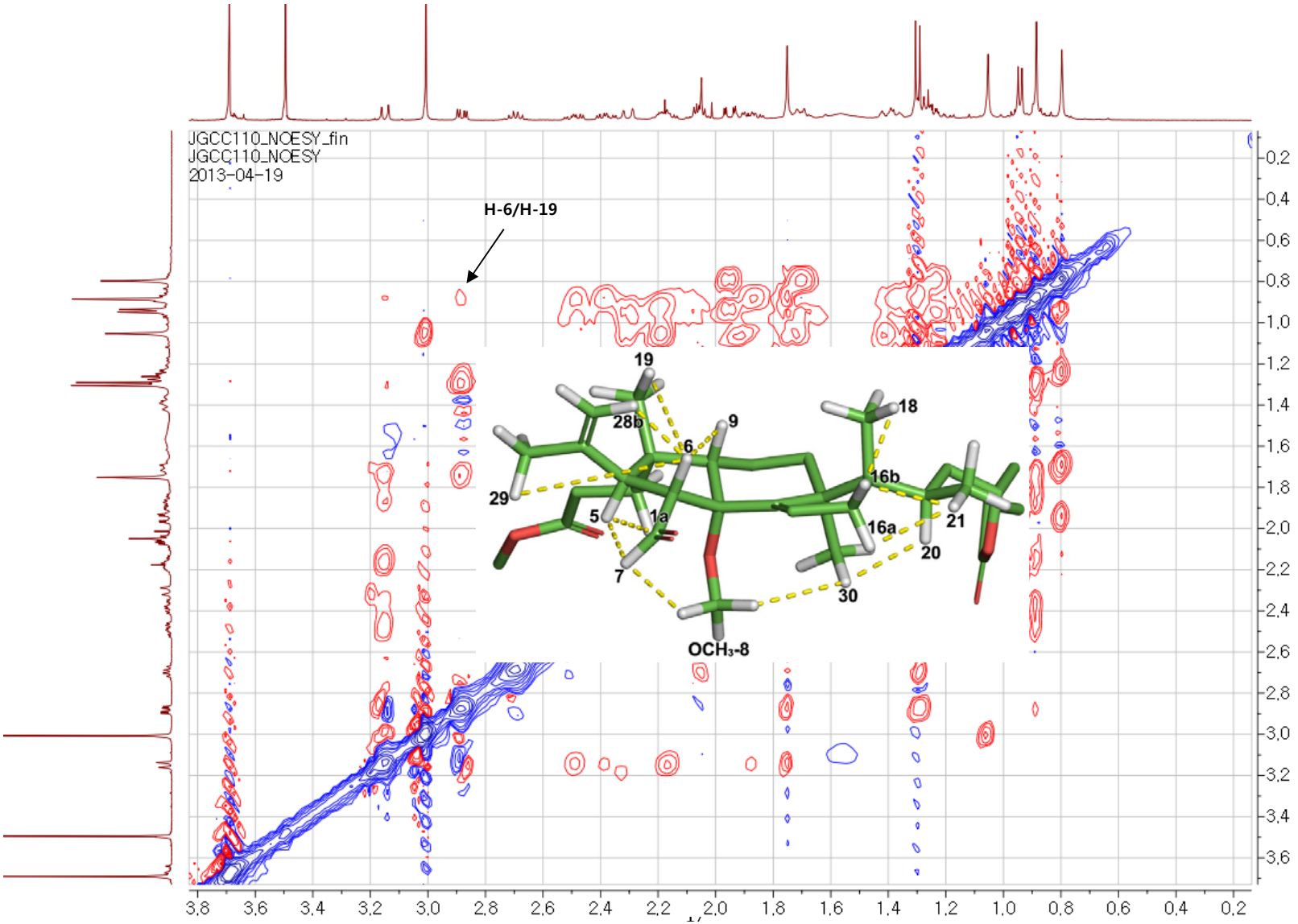
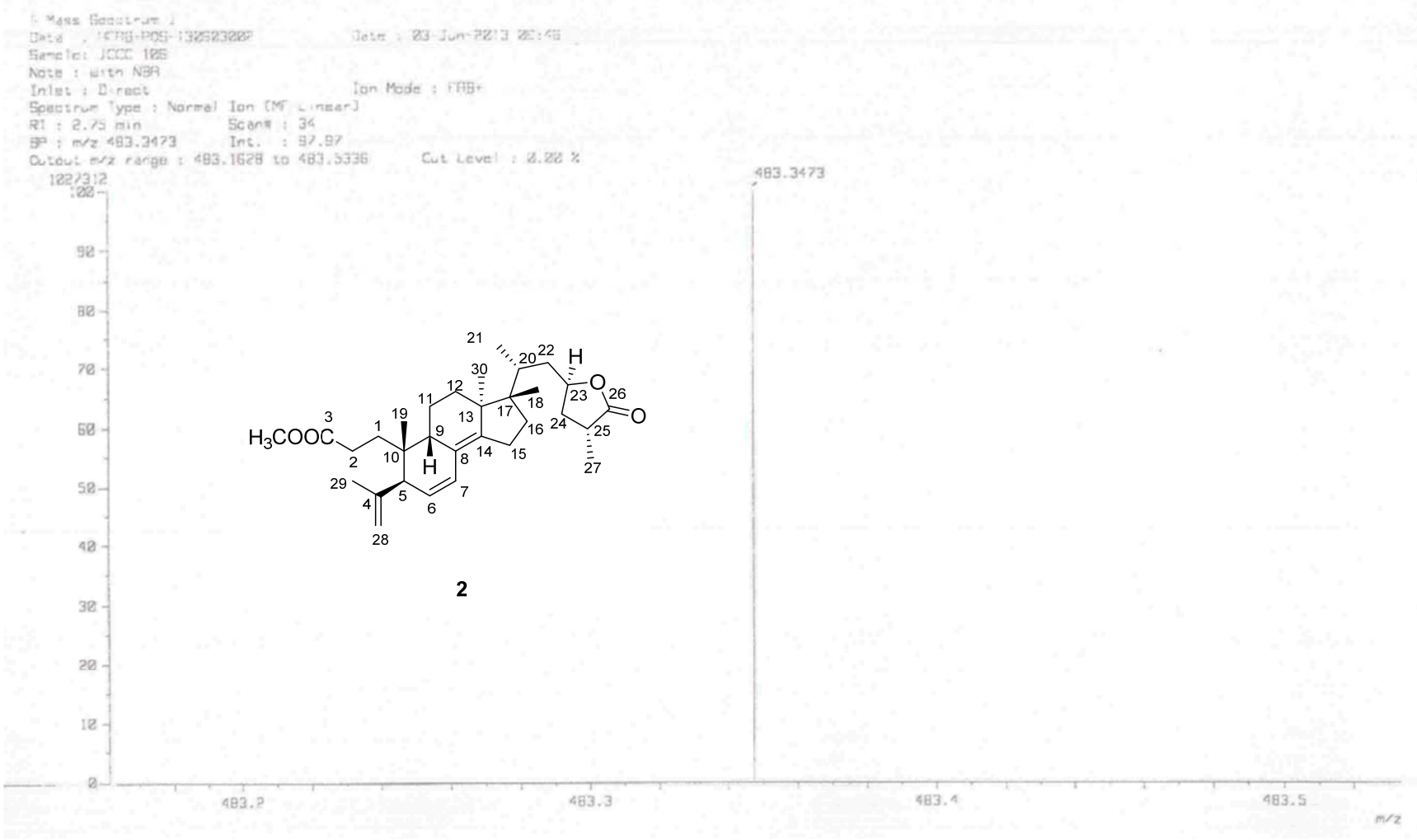

JGCC110_NOESY_fin
JGCC110_NOESY
2013-04-19
H-6/H-19
19
28b
9
18
6
16b
29
5
1a
16a
21
20
7
30
OCH₃-8
3,8
3,6
3,4
3,2
3,0
2,8
2,6
2,4
2,2
2,0
1,8
1,6
1,4
1,2
1,0
0,8
0,6
0,4
0,2

Figure S14. HRFABMS spectra of 2



2

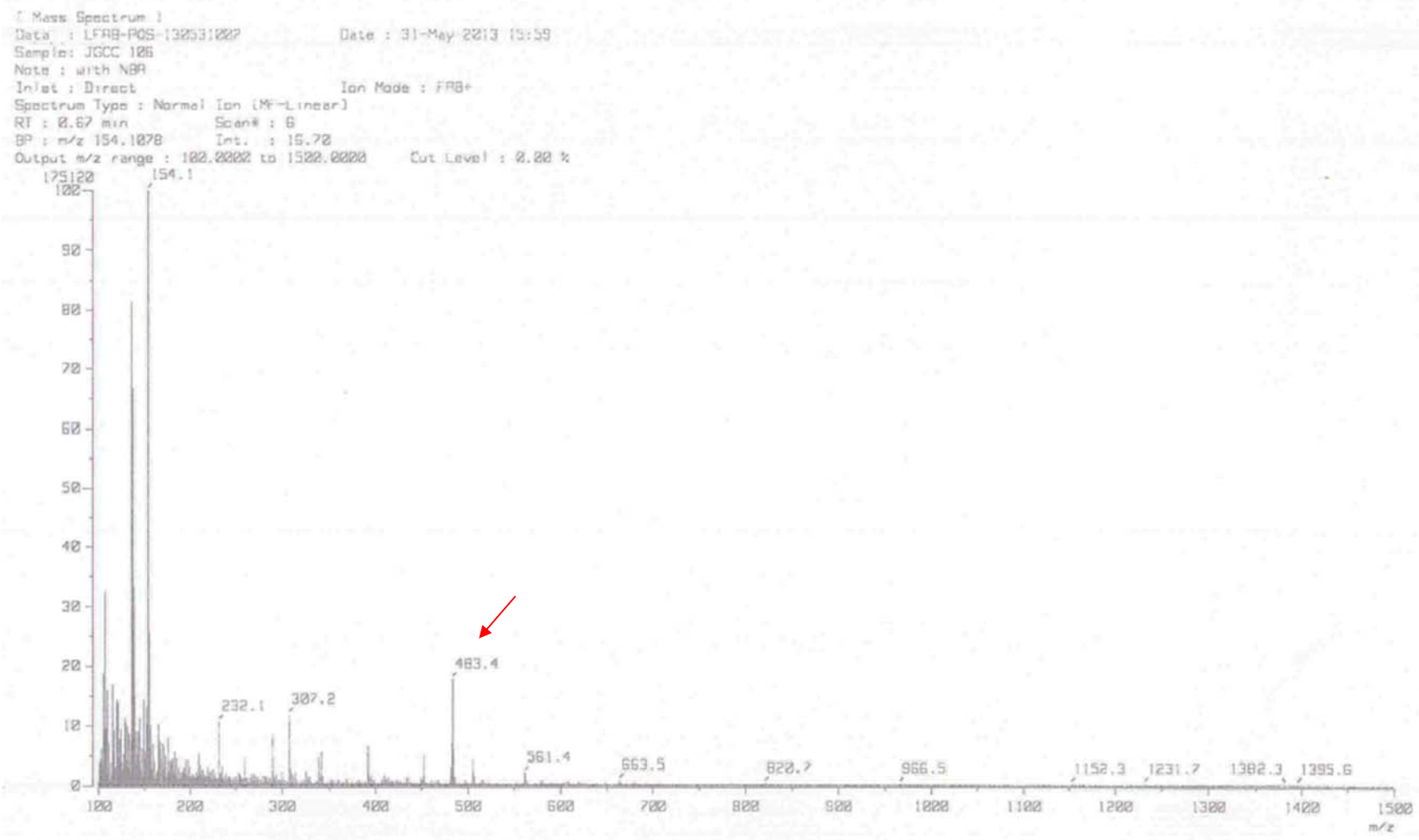

[Mass Spectrum]
Data : LFAB-POS-130531002 Date : 31-May-2013 15:59
Sample: JGCC 106
Note : with NBA
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion (MF-Linear)
RT : 0.67 min Scan# : 6
BP : m/z 154.1078 Int. : 15.72
Output m/z range : 102.2002 to 1502.0000 Cut Level : 0.00 %
175120
154.1
483.4
232.1
307.2
561.4
663.5
820.7
966.5
1152.3
1231.7
1382.3
1395.6
m/z

Figure S15. ^{1}H NMR spectrum of 2

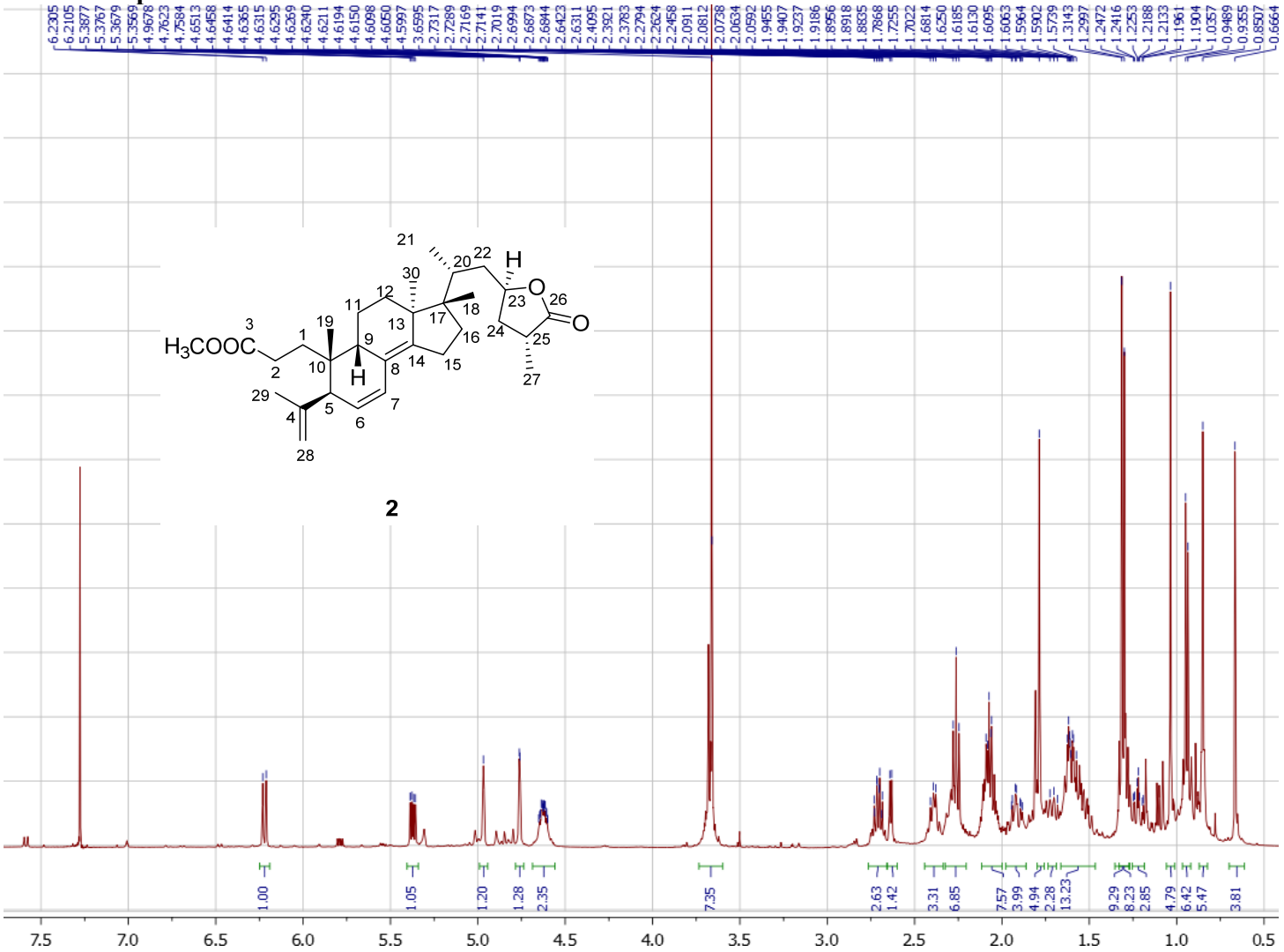


Figure S16. ^{13}C NMR spectrum of 2

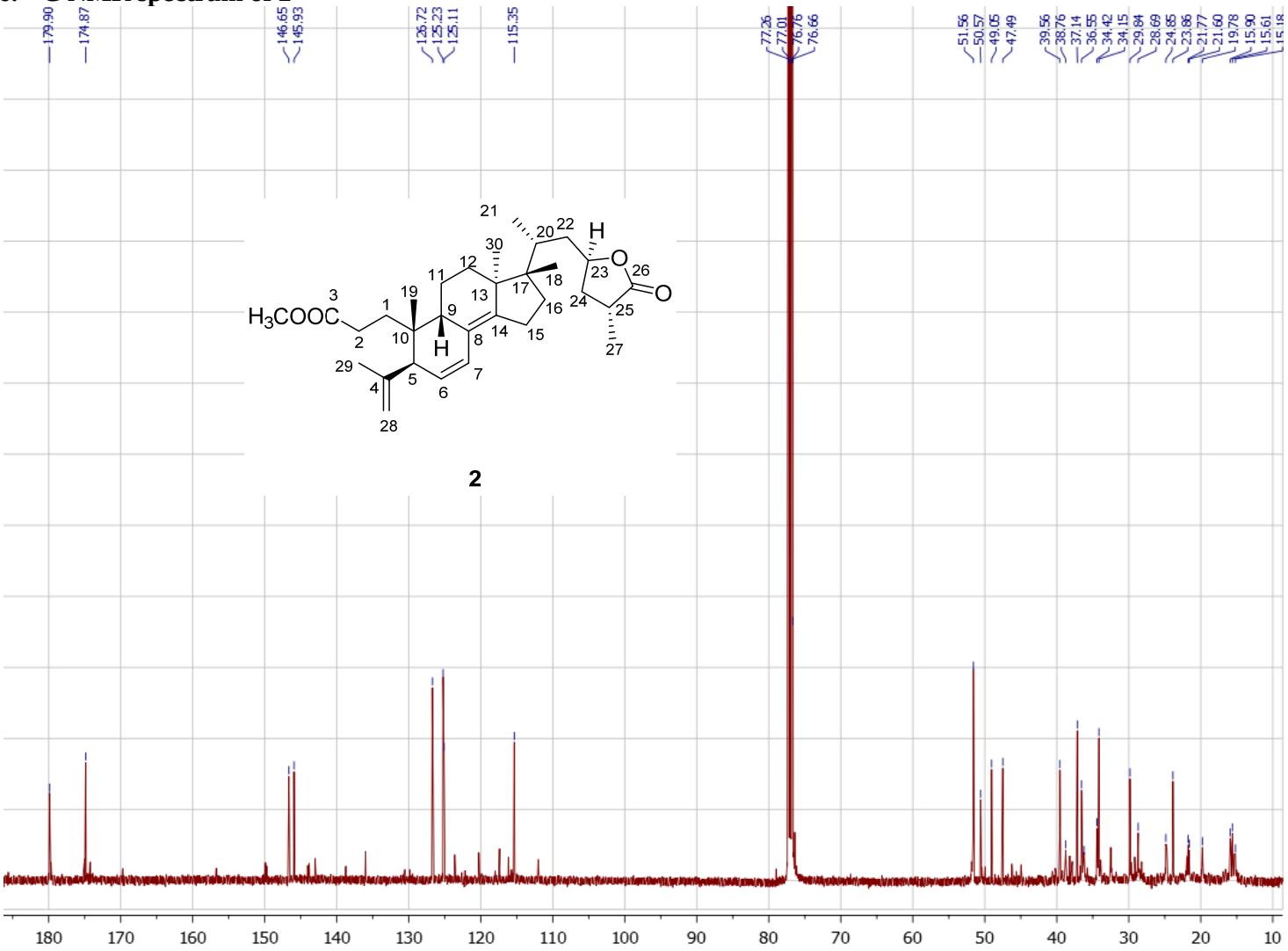


Figure S17. COSY spectrum of 2

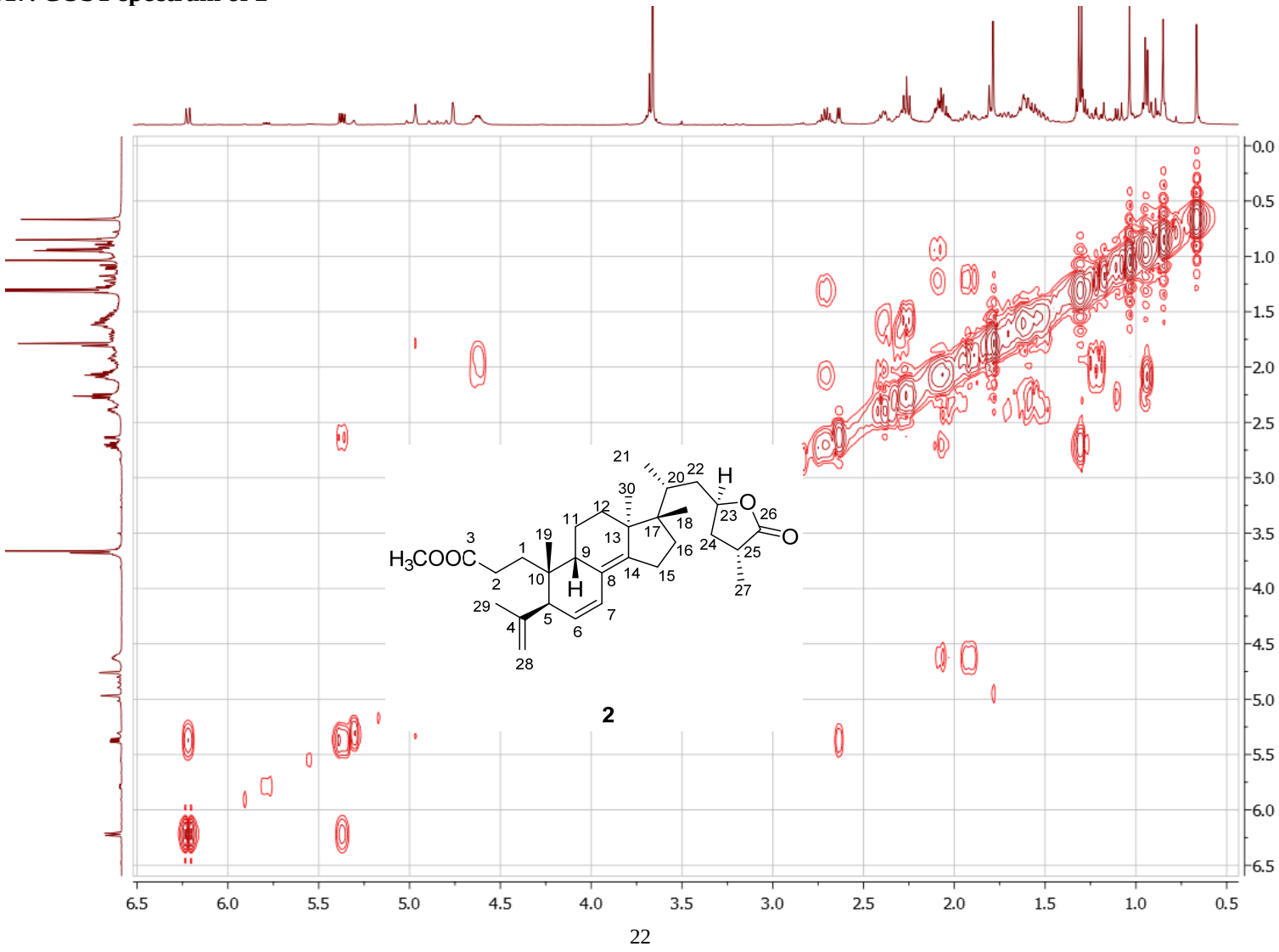


Figure S18. HSQC spectrum of 2

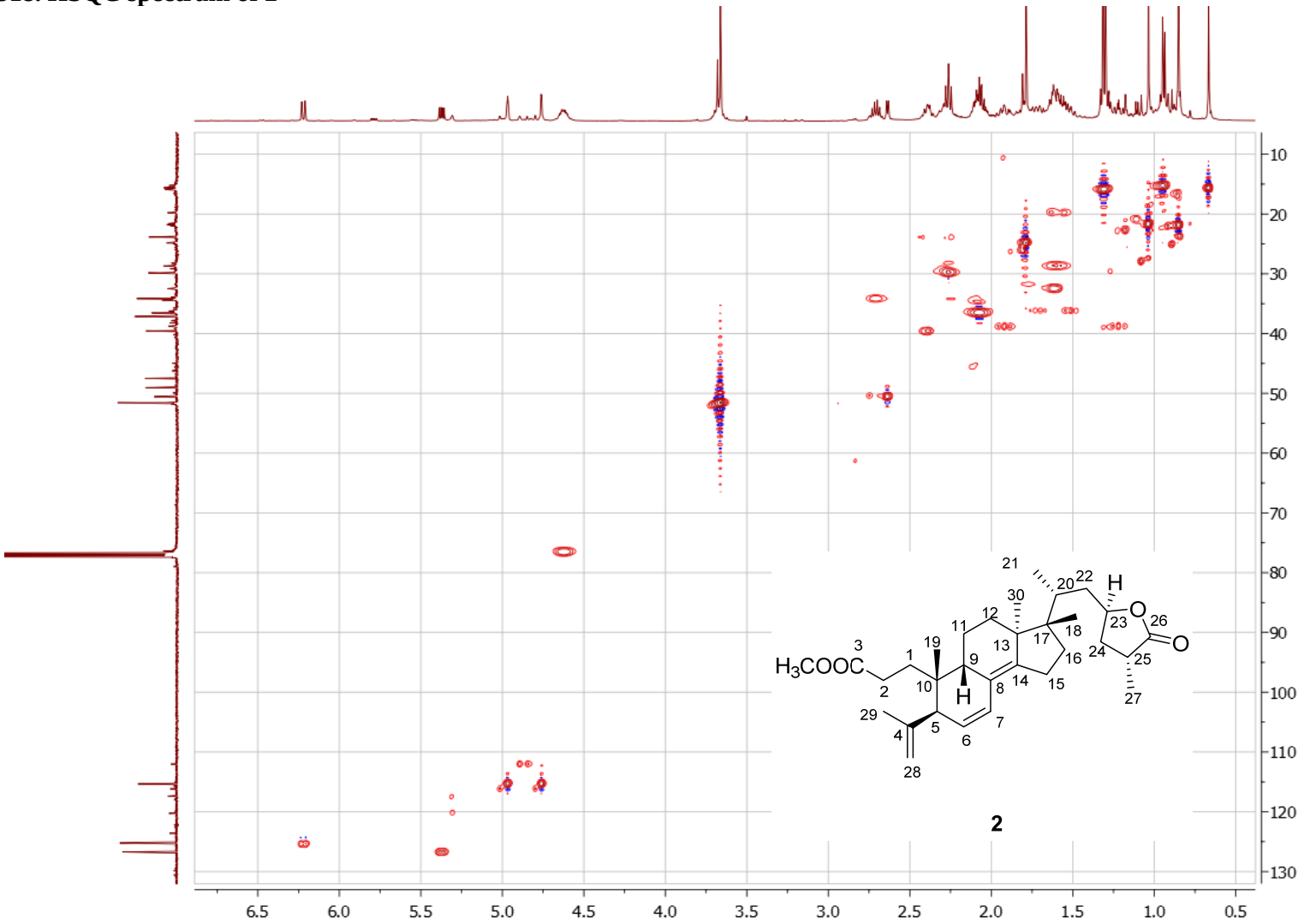


Figure S19. HMBC spectrum of 2

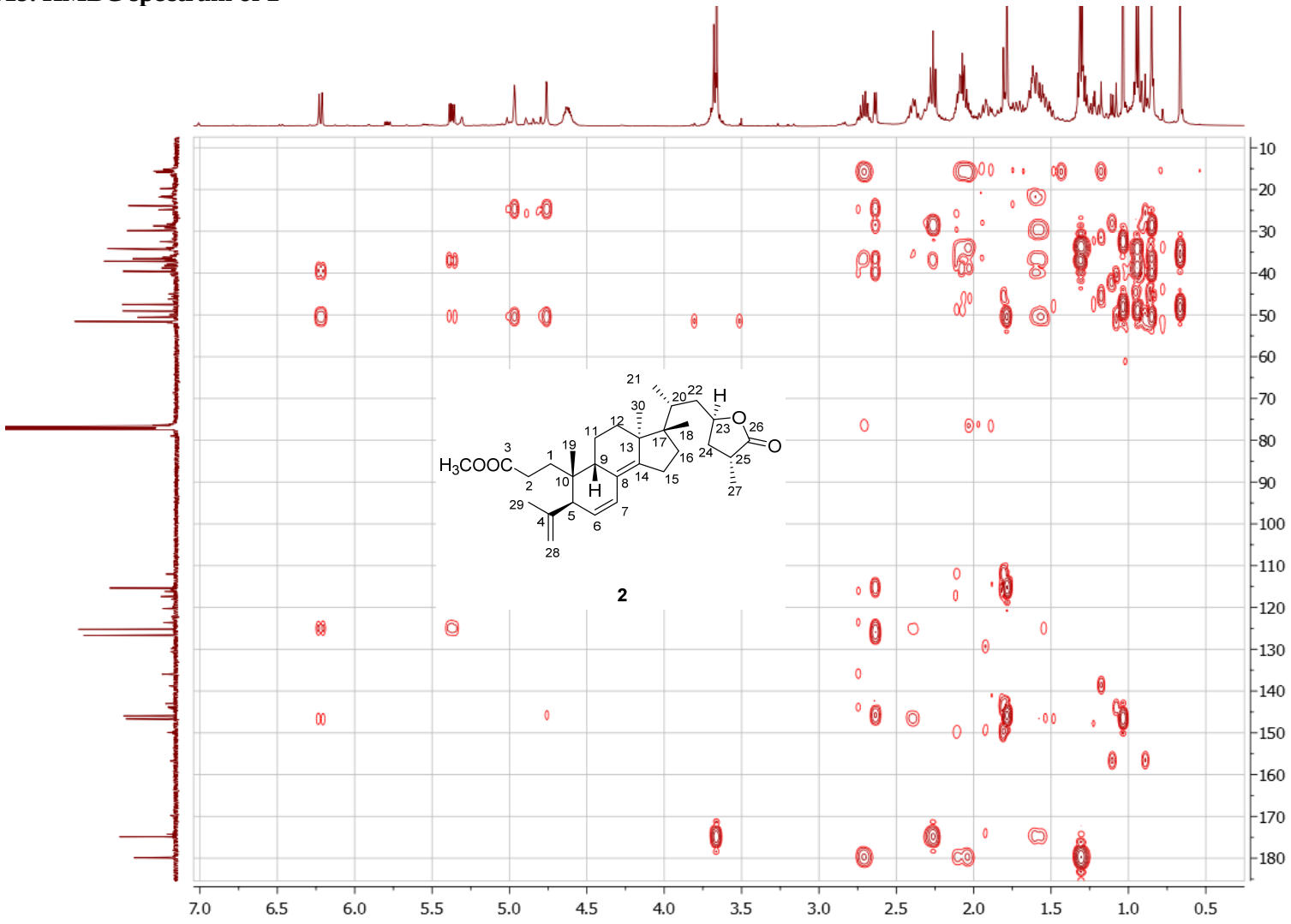


Figure S20. NOESY spectrum of 2

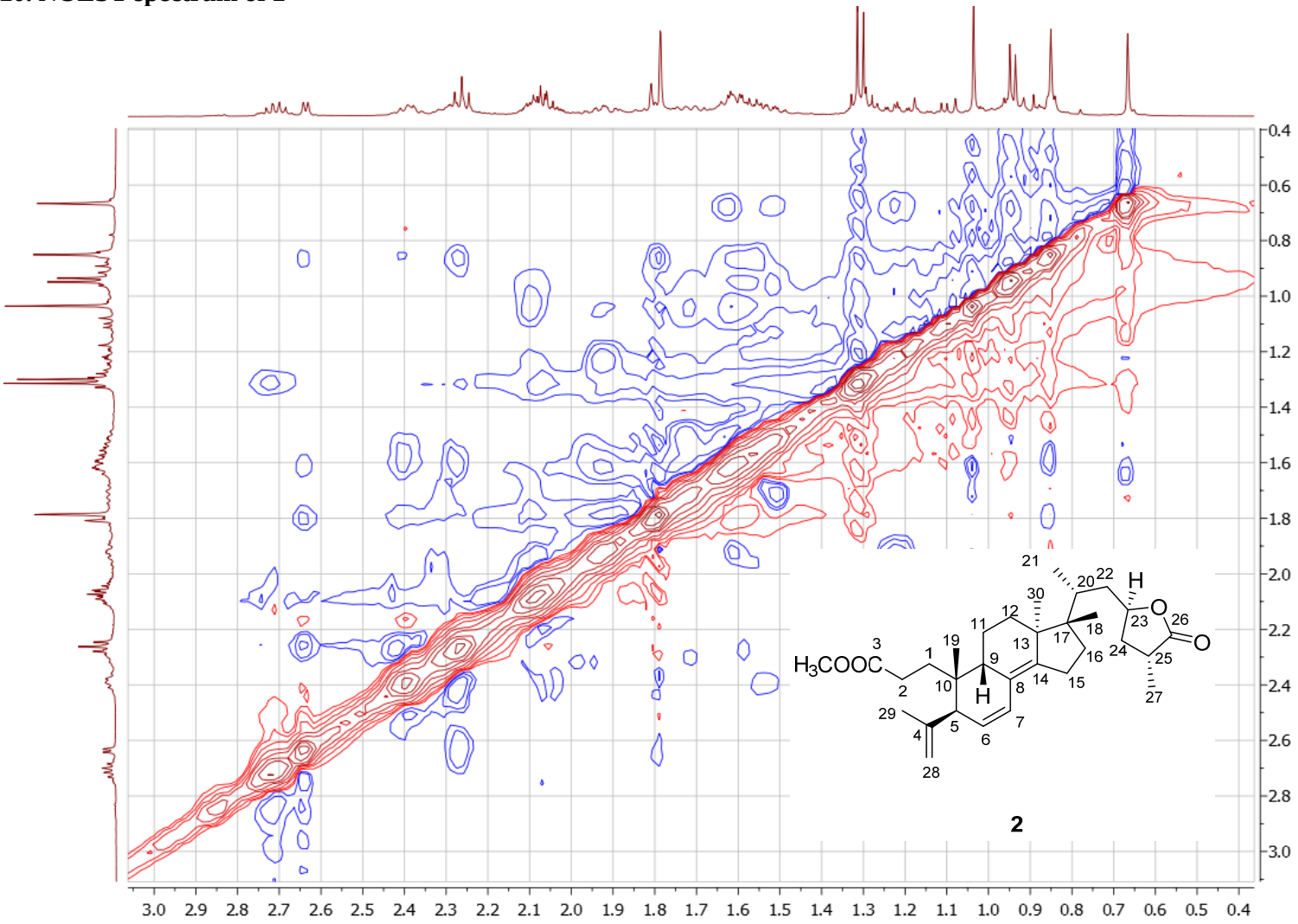


Table S1. Computed thermodynamic data and zero-point vibrational energy of conformers of 1 (PCM, $CHCl_3$) used for chemical shift values and ECD simulation (B3LYP/6-31+(d,p))

Conformer	E_{zpe}	U	H	G
1	-1698.994501	-1698.953878	-1698.952934	-1699.070035
2	-1698.99481	-1698.954304	-1698.95336	-1699.069267
3	-1698.994004	-1698.953515	-1698.95257	-1699.068612
4	-1698.993721	-1698.953367	-1698.952422	-1699.067488
5	-1698.993743	-1698.953287	-1698.952343	-1699.068117
6	-1698.99481	-1698.954304	-1698.95336	-1699.069266
7	-1698.993078	-1698.952547	-1698.951603	-1699.067593
8	-1698.994546	-1698.954063	-1698.953119	-1699.069311
9	-1698.9942	-1698.953798	-1698.952854	-1699.068609
10	-1698.994004	-1698.953515	-1698.952571	-1699.068606
11	-1698.993982	-1698.95355	-1698.952606	-1699.068543
12	-1698.993767	-1698.953294	-1698.95235	-1699.068211
13	-1698.993741	-1698.953287	-1698.952342	-1699.068091
14	-1698.993721	-1698.953367	-1698.952422	-1699.067489
15	-1698.994313	-1698.953751	-1698.952807	-1699.069012
16	-1698.993599	-1698.953133	-1698.952189	-1699.067913
17	-1698.994771	-1698.954274	-1698.95333	-1699.068961
18	-1698.993763	-1698.953401	-1698.952457	-1699.067138
19	-1698.994017	-1698.953514	-1698.95257	-1699.068669
20	-1698.993765	-1698.95326	-1698.952316	-1699.068196
21	-1698.993474	-1698.952937	-1698.951993	-1699.068435
22	-1698.994771	-1698.954274	-1698.95333	-1699.068961
23	-1698.991266	-1698.950749	-1698.949804	-1699.065602
24	-1698.993078	-1698.952547	-1698.951603	-1699.067593
25	-1698.994527	-1698.954042	-1698.953097	-1699.068907
26	-1698.993956	-1698.953532	-1698.952588	-1699.068013
27	-1698.993047	-1698.952516	-1698.951571	-1699.067424
28	-1698.993982	-1698.95355	-1698.952606	-1699.068543
29	-1698.994293	-1698.953812	-1698.952868	-1699.068594
30	-1698.991823	-1698.951509	-1698.950565	-1699.065316
31	-1698.993743	-1698.953287	-1698.952343	-1699.068118
32	-1698.992099	-1698.951788	-1698.950844	-1699.065945
33	-1698.99376	-1698.953264	-1698.95232	-1699.067787
34	-1698.993112	-1698.952613	-1698.951668	-1699.067413
35	-1698.993763	-1698.953401	-1698.952457	-1699.067137
36	-1698.993577	-1698.953079	-1698.952134	-1699.067519
37	-1698.994546	-1698.954063	-1698.953119	-1699.069312
38	-1698.993537	-1698.952932	-1698.951988	-1699.068444
39	-1698.993743	-1698.953287	-1698.952343	-1699.06812
40	-1698.993868	-1698.953213	-1698.952268	-1699.068652
41	-1698.991223	-1698.950778	-1698.949833	-1699.065069

42	-1698.991397	-1698.951115	-1698.950171	-1699.064753
43	-1698.991881	-1698.951496	-1698.950551	-1699.065722
44	-1698.989261	-1698.948951	-1698.948007	-1699.062882
45	-1698.993956	-1698.953532	-1698.952588	-1699.068014
46	-1698.994526	-1698.954042	-1698.953097	-1699.068905
47	-1698.992463	-1698.951884	-1698.95094	-1699.06701
48	-1698.993868	-1698.953213	-1698.952268	-1699.068652
49	-1698.991774	-1698.951187	-1698.950243	-1699.06654
50	-1698.992998	-1698.952368	-1698.951424	-1699.06767
51	-1698.993764	-1698.95326	-1698.952316	-1699.068194
52	-1698.992794	-1698.952393	-1698.951449	-1699.066465
53	-1698.991763	-1698.951073	-1698.950128	-1699.066546
54	-1698.991543	-1698.951108	-1698.950164	-1699.065693
55	-1698.99219	-1698.95182	-1698.950876	-1699.066227
56	-1698.99161	-1698.951067	-1698.950123	-1699.066114
57	-1698.993223	-1698.952655	-1698.951711	-1699.068107
58	-1698.992297	-1698.951968	-1698.951024	-1699.065288

E_{zpe}, U, H, and G stand for zero-point energy, thermal energy, thermal enthalpy and Gibbs free energy, respectively.

Table S2. Boltzmann populations of conformers shown in Table S1.

Conformer	E_{zpe}	U	H	G
1	3.7%	3.2%	3.2%	10.9%
2	5.1%	5.0%	5.0%	4.9%
3	2.2%	2.2%	2.2%	2.4%
4	1.6%	1.9%	1.8%	0.7%
5	1.6%	1.7%	1.7%	1.4%
6	5.1%	5.0%	5.0%	4.8%
7	0.8%	0.8%	0.8%	0.8%
8	3.9%	3.9%	3.9%	5.1%
9	2.7%	2.9%	2.9%	2.4%
10	2.2%	2.2%	2.2%	2.4%
11	2.1%	2.2%	2.2%	2.3%
12	1.7%	1.7%	1.7%	1.6%
13	1.6%	1.7%	1.7%	1.4%
14	1.6%	1.9%	1.8%	0.7%
15	3.0%	2.8%	2.8%	3.7%
16	1.4%	1.4%	1.4%	1.2%
17	4.9%	4.8%	4.8%	3.5%
18	1.7%	1.9%	1.9%	0.5%
19	2.2%	2.2%	2.2%	2.6%
20	1.7%	1.7%	1.7%	1.6%
21	1.2%	1.2%	1.2%	2.0%
22	4.9%	4.8%	4.8%	3.5%
23	0.1%	0.1%	0.1%	0.1%
24	0.8%	0.8%	0.8%	0.8%
25	3.8%	3.8%	3.8%	3.3%
26	2.1%	2.2%	2.2%	1.3%
27	0.8%	0.8%	0.8%	0.7%
28	2.1%	2.2%	2.2%	2.3%
29	2.9%	3.0%	3.0%	2.4%
30	0.2%	0.3%	0.3%	0.1%
31	1.6%	1.7%	1.7%	1.4%
32	0.3%	0.3%	0.3%	0.1%
33	1.7%	1.7%	1.7%	1.0%
34	0.8%	0.8%	0.8%	0.7%
35	1.7%	1.9%	1.9%	0.5%
36	1.4%	1.4%	1.4%	0.8%
37	3.9%	3.9%	3.9%	5.1%
38	1.3%	1.2%	1.2%	2.0%
39	1.6%	1.7%	1.7%	1.4%
40	1.9%	1.6%	1.6%	2.5%
41	0.1%	0.1%	0.1%	0.1%
42	0.1%	0.2%	0.2%	0.0%
43	0.2%	0.3%	0.3%	0.1%
44	0.0%	0.0%	0.0%	0.0%
45	2.1%	2.2%	2.2%	1.3%
46	3.8%	3.8%	3.8%	3.3%
47	0.4%	0.4%	0.4%	0.4%
48	1.9%	1.6%	1.6%	2.5%
49	0.2%	0.2%	0.2%	0.3%
50	0.7%	0.6%	0.6%	0.9%
51	1.7%	1.7%	1.7%	1.6%
52	0.6%	0.7%	0.7%	0.2%
53	0.2%	0.2%	0.2%	0.3%
54	0.2%	0.2%	0.2%	0.1%
55	0.3%	0.4%	0.4%	0.2%
56	0.2%	0.2%	0.2%	0.2%

57	0.9%	0.9%	0.9%	1.4%
58	0.4%	0.4%	0.4%	0.1%

Table S3. Calculated thermodynamic data and zero-point vibrational energy of conformers of 1 (gas phase) employed for chemical shift values and ECD simulation at the B3LYP/6-311+(2d,p) level

Conformer	E_{zpe}	U	H	G
1	-1699.368641	-1699.327891	-1699.326947	-1699.444577
2	-1699.368936	-1699.328404	-1699.32746	-1699.443481
3	-1699.368073	-1699.327447	-1699.326502	-1699.444741
4	-1699.368221	-1699.327728	-1699.326784	-1699.442408
5	-1699.367829	-1699.327197	-1699.326253	-1699.442967
6	-1699.368936	-1699.328404	-1699.32746	-1699.443481
7	-1699.368221	-1699.327728	-1699.326784	-1699.442409
8	-1699.368902	-1699.328219	-1699.327275	-1699.444321
9	-1699.368344	-1699.327739	-1699.326795	-1699.444072
10	-1699.368073	-1699.327447	-1699.326502	-1699.444746
11	-1699.368164	-1699.327533	-1699.326589	-1699.443503
12	-1699.367689	-1699.32722	-1699.326275	-1699.442275
13	-1699.367828	-1699.327197	-1699.326253	-1699.442965
14	-1699.368221	-1699.327728	-1699.326784	-1699.442406
15	-1699.368379	-1699.327747	-1699.326802	-1699.443647
16	-1699.367881	-1699.327257	-1699.326312	-1699.443019
17	-1699.368962	-1699.328419	-1699.327474	-1699.44353
18	-1699.36814	-1699.327695	-1699.326751	-1699.442089
19	-1699.368	-1699.327442	-1699.326498	-1699.443189
20	-1699.367762	-1699.327182	-1699.326238	-1699.442577
21	-1699.367308	-1699.326743	-1699.325799	-1699.442843
22	-1699.368962	-1699.328418	-1699.327474	-1699.443528
23	-1699.366089	-1699.325628	-1699.324684	-1699.439542
24	-1699.368221	-1699.327728	-1699.326784	-1699.442409
25	-1699.368714	-1699.32811	-1699.327166	-1699.443571
26	-1699.368081	-1699.327542	-1699.326598	-1699.442775
27	-1699.36814	-1699.327695	-1699.326751	-1699.442089
28	-1699.368164	-1699.327533	-1699.326589	-1699.443505
29	-1699.368417	-1699.327799	-1699.326855	-1699.443914
30	-1699.366199	-1699.325874	-1699.32493	-1699.440017
31	-1699.367828	-1699.327197	-1699.326253	-1699.442968
32	-1699.366785	-1699.326423	-1699.325478	-1699.440731
33	-1699.367746	-1699.327209	-1699.326265	-1699.442502
34	-1699.367836	-1699.327229	-1699.326285	-1699.442462
35	-1699.36814	-1699.327695	-1699.326751	-1699.442091
36	-1699.367742	-1699.327179	-1699.326235	-1699.442159
37	-1699.368902	-1699.328219	-1699.327275	-1699.44432
38	-1699.367366	-1699.326788	-1699.325843	-1699.442635
39	-1699.367829	-1699.327197	-1699.326253	-1699.442968
40	-1699.368052	-1699.327345	-1699.326401	-1699.443022
41	-1699.366268	-1699.325715	-1699.324771	-1699.440527
42	-1699.366267	-1699.325902	-1699.324958	-1699.439889
43	-1699.366427	-1699.326043	-1699.325099	-1699.440591
44	-1699.364234	-1699.32393	-1699.322985	-1699.437867
45	-1699.368081	-1699.327542	-1699.326598	-1699.442775
46	-1699.368714	-1699.32811	-1699.327166	-1699.443571
47	-1699.36695	-1699.32631	-1699.325366	-1699.441539
48	-1699.368052	-1699.327345	-1699.326401	-1699.443022
49	-1699.365718	-1699.325088	-1699.324144	-1699.440566
50	-1699.36648	-1699.325721	-1699.324777	-1699.441934
51	-1699.367762	-1699.327182	-1699.326238	-1699.442577
52	-1699.36682	-1699.32627	-1699.325326	-1699.441654
53	-1699.368714	-1699.32811	-1699.327166	-1699.443571
54	-1699.365654	-1699.325166	-1699.324222	-1699.43998

55	-1699.36682	-1699.326398	-1699.325454	-1699.44099
56	-1699.36695	-1699.32631	-1699.325366	-1699.441538
57	-1699.367825	-1699.327185	-1699.326241	-1699.442499
58	-1699.366508	-1699.325919	-1699.324975	-1699.441411

Table S4. Boltzmann populations of conformers described in Table S3

Conformer	E_{zpe}	U	H	G
1	3.2%	2.7%	2.7%	7.6%
2	4.4%	4.7%	4.7%	2.4%
3	1.8%	1.7%	1.7%	9.1%
4	2.1%	2.3%	2.3%	0.8%
5	1.4%	1.3%	1.3%	1.4%
6	4.4%	4.7%	4.7%	2.4%
7	2.1%	2.3%	2.3%	0.8%
8	4.3%	3.8%	3.8%	5.8%
9	2.4%	2.3%	2.3%	4.5%
10	1.8%	1.7%	1.7%	9.1%
11	2.0%	1.8%	1.8%	2.4%
12	1.2%	1.3%	1.3%	0.7%
13	1.4%	1.3%	1.3%	1.4%
14	2.1%	2.3%	2.3%	0.8%
15	2.5%	2.3%	2.3%	2.8%
16	1.4%	1.4%	1.4%	1.5%
17	4.5%	4.7%	4.7%	2.5%
18	1.9%	2.2%	2.2%	0.5%
19	1.6%	1.7%	1.7%	1.8%
20	1.3%	1.3%	1.3%	0.9%
21	0.8%	0.8%	0.8%	1.2%
22	4.5%	4.7%	4.7%	2.5%
23	0.2%	0.2%	0.2%	0.0%
24	2.1%	2.3%	2.3%	0.8%
25	3.5%	3.4%	3.4%	2.6%
26	1.8%	1.9%	1.9%	1.1%
27	1.9%	2.2%	2.2%	0.5%
28	2.0%	1.8%	1.8%	2.4%
29	2.6%	2.5%	2.5%	3.8%
30	0.2%	0.3%	0.3%	0.1%
31	1.4%	1.3%	1.3%	1.4%
32	0.5%	0.6%	0.6%	0.1%
33	1.3%	1.3%	1.3%	0.8%
34	1.4%	1.3%	1.3%	0.8%
35	1.9%	2.2%	2.2%	0.5%
36	1.2%	1.3%	1.3%	0.6%
37	4.3%	3.8%	3.8%	5.8%
38	0.8%	0.8%	0.8%	1.0%
39	1.4%	1.3%	1.3%	1.4%
40	1.7%	1.5%	1.5%	1.5%
41	0.3%	0.3%	0.3%	0.1%
42	0.3%	0.3%	0.3%	0.1%
43	0.3%	0.4%	0.4%	0.1%
44	0.0%	0.0%	0.0%	0.0%
45	1.8%	1.9%	1.9%	1.1%
46	3.5%	3.4%	3.4%	2.6%
47	0.5%	0.5%	0.5%	0.3%
48	1.7%	1.5%	1.5%	1.5%
49	0.1%	0.1%	0.1%	0.1%
50	0.3%	0.3%	0.3%	0.5%
51	1.3%	1.3%	1.3%	0.9%
52	0.5%	0.5%	0.5%	0.3%
53	3.5%	3.4%	3.4%	2.6%

54	0.1%	0.2%	0.2%	0.1%
55	0.5%	0.6%	0.6%	0.2%
56	0.5%	0.5%	0.5%	0.3%
57	1.4%	1.3%	1.3%	0.8%
58	0.3%	0.3%	0.3%	0.3%

Table S5. Experimental and PCM calculation ($CHCl_3$) for ^{13}C chemical shift values of compound 1 at B3LYP/6-31G+(d,p) and B3LYP/6-311G+(2d,p)

	Experimental	B3LYP/6-31G+(d,p)	B3LYP/6-311G+(2d,p)
C-12	34.60	37.18	38.62
C-11	18.80	23.8	24.44
C-5	54.70	55.81	61.33
C-6	64.50	65.6	70.33
C-8	86.30	90.99	95.75
C-9	62.80	64.79	69.57
C-7	203.80	203.86	215.82
C-16	44.70	47.32	50.83
C-17	50.70	54.9	60.1
C-13	51.70	57.83	60.76
C-14	146.40	146.28	156.58
C-15	126.20	127.43	135.97
C-18	17.10	17.28	18.52
C-30	20.30	20.93	22.28
C-20	33.70	37.47	40.33
C-22	39.10	41.07	43.16
C-23	76.40	78.75	81.01
C-24	36.60	37.61	40.38
C-25	34.10	37.98	40.37
C-26	179.80	176.29	188.37
C-27	15.90	16.75	17.65
C-10	42.80	50.57	50.32
C-19	23.70	21.89	22.84
C-1	35.40	38.62	40.54
C-2	30.40	31.57	34.84
C-3	174.90	173.36	184.8
OCH_3-3	51.60	52.26	54.93
C-4	143.50	145.54	158.6
C-28	114.80	109.81	118.93
C-29	23.90	25.8	27.66
OCH_3-8	54.30	53.87	56.89
C-21	15.40	15.68	15.96

Coordinates of conformers found at B3LYP/6-311G+(2d,p) in the gas phase
1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.066123	0.153046	-1.161120
2	6	0	0.329712	0.796008	-1.055589
3	1	0	-1.092159	-0.403250	-2.098701
4	1	0	-1.815173	0.944596	-1.249149
5	1	0	0.378406	1.501882	-0.225808
6	1	0	0.519497	1.367904	-1.969025
7	6	0	3.553060	-1.177539	-0.169238
8	6	0	2.379814	-2.061994	0.328805
9	6	0	1.172933	-1.075947	0.428031
10	6	0	1.375526	-0.301708	-0.889619
11	6	0	2.773689	-2.859840	1.552945
12	1	0	2.087765	-2.793877	-0.423907
13	8	0	1.344594	-0.119354	1.492233
14	6	0	-2.082305	-3.067777	0.658423
15	6	0	-2.537008	-1.909188	-0.283386
16	6	0	-1.425918	-0.781734	0.026605
17	6	0	-0.220930	-1.657925	0.435500
18	6	0	-0.600502	-2.880927	0.792637
19	1	0	-2.564075	-2.999087	1.642602
20	1	0	-2.346214	-4.050466	0.258633
21	6	0	-2.414293	-2.433595	-1.728227
22	6	0	-1.825174	0.098697	1.234626
23	1	0	0.061539	-3.657291	1.154391
24	1	0	-2.704676	-1.696450	-2.477294
25	1	0	-1.390678	-2.743670	-1.946313
26	1	0	-3.052402	-3.308190	-1.866518
27	1	0	-1.002787	0.758854	1.506292
28	1	0	-2.691200	0.723834	1.013119
29	1	0	-2.066500	-0.502719	2.112926
30	6	0	-4.013929	-1.497557	0.024495
31	6	0	-4.546212	-0.380433	-0.898258
32	6	0	-5.854320	0.267032	-0.447903
33	6	0	-6.295454	1.463833	-1.311354
34	6	0	-5.756439	2.681091	-0.553281
35	6	0	-5.657077	2.171520	0.881646
36	8	0	-5.711941	0.814213	0.894838
37	1	0	-6.644448	-0.478940	-0.373239
38	1	0	-7.386393	1.511109	-1.358156
39	1	0	-5.921328	1.389233	-2.332784
40	1	0	-4.723718	2.884943	-0.860289
41	6	0	-6.565527	3.968503	-0.670984
42	1	0	-4.027612	-1.107439	1.043687
43	1	0	-4.722565	-0.781062	-1.902435
44	1	0	-3.799314	0.407879	-1.011766
45	8	0	-5.535055	2.816533	1.884340
46	1	0	-6.152928	4.738989	-0.018901
47	1	0	-6.554419	4.340091	-1.697775
48	1	0	-7.605664	3.803331	-0.380096
49	1	0	1.166653	-1.044074	-1.669765
50	6	0	2.898559	0.013128	-1.017595

51	6	0	3.282884	-0.016002	-2.504943
52	6	0	3.210435	1.408456	-0.417662
53	1	0	4.344887	0.170015	-2.669942
54	1	0	3.052170	-0.980838	-2.958637
55	1	0	2.727584	0.753720	-3.048331
56	6	0	4.672759	1.851922	-0.408442
57	6	0	4.841518	3.271681	0.090126
58	8	0	3.970492	4.099755	0.182476
59	8	0	6.132561	3.518802	0.408588
60	6	0	6.419720	4.857159	0.851322
61	6	0	4.677272	-1.973688	-0.822230
62	1	0	3.985689	-0.712453	0.723688
63	6	0	4.496939	-3.146125	-1.430816
64	6	0	6.065791	-1.391649	-0.723975
65	1	0	5.333763	-3.674930	-1.872166
66	1	0	3.533366	-3.630279	-1.518338
67	1	0	6.150184	-0.441946	-1.257243
68	1	0	6.332358	-1.191172	0.318984
69	1	0	6.808592	-2.073944	-1.138434
70	1	0	5.113291	1.831334	-1.410817
71	1	0	5.300960	1.208525	0.209101
72	1	0	2.829960	1.444839	0.602478
73	1	0	2.643498	2.155473	-0.976974
74	8	0	2.340070	-3.949904	1.836303
75	1	0	3.546769	-2.390124	2.197488
76	6	0	1.166110	-0.565418	2.828816
77	1	0	1.005587	0.327320	3.433542
78	1	0	0.303475	-1.227117	2.931292
79	1	0	2.055154	-1.081997	3.205838
80	6	0	-4.978894	-2.698539	0.005195
81	1	0	-5.965862	-2.408553	0.370136
82	1	0	-5.109011	-3.105563	-1.000926
83	1	0	-4.634019	-3.506991	0.649676
84	1	0	5.855298	5.088754	1.754231
85	1	0	7.487874	4.874026	1.052441
86	1	0	6.163379	5.578471	0.075674

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.857634	0.150912	-1.032275
2	6	0	0.513337	0.811110	-0.788746
3	1	0	-0.838356	-0.255552	-2.044192
4	1	0	-1.629044	0.925684	-1.023371
5	1	0	0.513717	1.390805	0.135893
6	1	0	0.699455	1.509700	-1.608677
7	6	0	3.760618	-1.143050	0.008584
8	6	0	2.620644	-2.157895	0.239632
9	6	0	1.369749	-1.237009	0.425722
10	6	0	1.596674	-0.263734	-0.748157
11	6	0	2.971126	-3.144490	1.333091
12	1	0	2.415234	-2.752327	-0.652601
13	8	0	1.465163	-0.437990	1.622287
14	6	0	-1.815085	-3.340312	0.228778
15	6	0	-2.286300	-2.061520	-0.531115
16	6	0	-1.221864	-0.964635	-0.014907
17	6	0	0.000009	-1.856815	0.292184
18	6	0	-0.344887	-3.132632	0.436323
19	1	0	-2.321165	-3.443100	1.197412
20	1	0	-2.035667	-4.254317	-0.328998
21	6	0	-2.108414	-2.346200	-2.036259
22	6	0	-1.689454	-0.292158	1.297706
23	1	0	0.334632	-3.935833	0.690126
24	1	0	-2.404667	-1.508007	-2.667350
25	1	0	-1.068978	-2.585672	-2.268236
26	1	0	-2.710088	-3.207245	-2.332948
27	1	0	-0.904936	0.352608	1.690822
28	1	0	-2.578482	0.320927	1.145187
29	1	0	-1.924949	-1.028407	2.068523
30	6	0	-3.783998	-1.747617	-0.208194
31	6	0	-4.339245	-0.531913	-0.982349
32	6	0	-5.648240	0.036688	-0.439224
33	6	0	-6.154581	1.285220	-1.185761
34	6	0	-5.619826	2.453777	-0.351845
35	6	0	-5.445841	1.833349	1.031596
36	8	0	-5.470652	0.478727	0.937997
37	1	0	-6.414163	-0.736529	-0.397627
38	1	0	-7.247381	1.302813	-1.188454
39	1	0	-5.819082	1.303902	-2.223045
40	1	0	-4.607414	2.715795	-0.681879
41	6	0	-6.471204	3.719088	-0.331041
42	1	0	-3.834165	-1.503519	0.854487
43	1	0	-4.522033	-0.811248	-2.025589
44	1	0	-3.604298	0.275441	-1.005867
45	8	0	-5.293341	2.399638	2.076921
46	1	0	-6.055025	4.447504	0.365586
47	1	0	-6.514272	4.172462	-1.323541
48	1	0	-7.492793	3.496255	-0.014171
49	1	0	1.437804	-0.882423	-1.639804
50	6	0	3.118280	0.095542	-0.771972
51	6	0	3.574492	0.168203	-2.238064

52	6	0	3.514328	1.386667	-0.005451
53	1	0	4.611499	0.496724	-2.336068
54	1	0	3.492492	-0.805153	-2.724182
55	1	0	2.952919	0.869052	-2.801203
56	6	0	3.224180	2.733602	-0.674345
57	6	0	3.867700	3.887877	0.064609
58	8	0	4.799588	3.810410	0.826199
59	8	0	3.275623	5.058921	-0.259896
60	6	0	3.843090	6.233551	0.346959
61	6	0	5.043182	-1.725115	-0.556742
62	1	0	4.017070	-0.756617	1.001218
63	6	0	5.103442	-2.887843	-1.206416
64	6	0	6.300133	-0.930196	-0.301079
65	1	0	6.048546	-3.268680	-1.576155
66	1	0	4.236102	-3.507840	-1.391891
67	1	0	6.252242	0.066686	-0.746846
68	1	0	6.452929	-0.781597	0.772744
69	1	0	7.177648	-1.436663	-0.704523
70	1	0	2.160086	2.945639	-0.765213
71	1	0	3.627932	2.767711	-1.691677
72	1	0	4.589575	1.351155	0.179913
73	1	0	3.041026	1.365386	0.977166
74	8	0	2.563519	-4.279105	1.395952
75	1	0	3.683550	-2.773115	2.098759
76	6	0	1.282156	-1.086613	2.872917
77	1	0	1.012698	-0.311281	3.590421
78	1	0	0.485182	-1.832586	2.836361
79	1	0	2.204408	-1.567461	3.215876
80	6	0	-4.702023	-2.965783	-0.423615
81	1	0	-5.715892	-2.753661	-0.078820
82	1	0	-4.768984	-3.247608	-1.477470
83	1	0	-4.359171	-3.836841	0.134467
84	1	0	4.886676	6.347475	0.054204
85	1	0	3.249001	7.066404	-0.020554
86	1	0	3.782119	6.167995	1.432877

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056792	0.084566	-1.173521
2	6	0	0.323788	0.765682	-1.117524
3	1	0	-1.084451	-0.505939	-2.090066
4	1	0	-1.827368	0.853396	-1.275790
5	1	0	0.369162	1.498477	-0.311194
6	1	0	0.480630	1.311739	-2.052635
7	6	0	3.611899	-1.100081	-0.231620
8	6	0	2.470139	-1.994932	0.318045
9	6	0	1.241943	-1.034940	0.409727
10	6	0	1.400013	-0.300151	-0.936159
11	6	0	2.906274	-2.745378	1.558066
12	1	0	2.180236	-2.757117	-0.405077
13	8	0	1.411115	-0.038857	1.438264
14	6	0	-1.960305	-3.090128	0.780047
15	6	0	-2.462254	-1.976520	-0.190799
16	6	0	-1.370536	-0.814704	0.054112
17	6	0	-0.137052	-1.648415	0.466268
18	6	0	-0.480491	-2.866923	0.872520
19	1	0	-2.419594	-2.996150	1.772814
20	1	0	-2.211959	-4.091793	0.421746
21	6	0	-2.358665	-2.548219	-1.619092
22	6	0	-1.764852	0.099393	1.238398
23	1	0	0.206633	-3.616101	1.244732
24	1	0	-2.681326	-1.843746	-2.386103
25	1	0	-1.332874	-2.842342	-1.848585
26	1	0	-2.978934	-3.441251	-1.714458
27	1	0	-0.955043	0.791044	1.466406
28	1	0	-2.653266	0.691803	1.016446
29	1	0	-1.968072	-0.476090	2.143330
30	6	0	-3.941177	-1.586275	0.135141
31	6	0	-4.523777	-0.526968	-0.825351
32	6	0	-5.815557	0.136176	-0.352667
33	6	0	-6.333607	1.247529	-1.284565
34	6	0	-5.772707	2.533545	-0.669288
35	6	0	-5.569950	2.150486	0.794101
36	8	0	-5.601476	0.799212	0.927309
37	1	0	-6.584058	-0.612356	-0.164280
38	1	0	-7.426031	1.274608	-1.264966
39	1	0	-6.023051	1.090390	-2.317852
40	1	0	-4.766662	2.726847	-1.060336
41	6	0	-6.615618	3.792853	-0.841744
42	1	0	-3.940377	-1.149634	1.135557
43	1	0	-4.739780	-0.986524	-1.795926
44	1	0	-3.790830	0.259547	-1.016321
45	8	0	-5.391666	2.881119	1.727352
46	1	0	-6.179443	4.623063	-0.285334
47	1	0	-6.678060	4.075209	-1.894760
48	1	0	-7.631280	3.635835	-0.470816
49	1	0	1.195312	-1.072199	-1.687980
50	6	0	2.912734	0.045258	-1.104717
51	6	0	3.268490	-0.019212	-2.597606

52	6	0	3.201587	1.466370	-0.554439
53	1	0	4.319240	0.199246	-2.790984
54	1	0	3.062362	-1.006316	-3.013475
55	1	0	2.676382	0.712844	-3.153726
56	6	0	4.663004	1.949986	-0.594987
57	6	0	4.740764	3.387423	-0.135632
58	8	0	4.366745	4.337973	-0.778041
59	8	0	5.263846	3.493663	1.105674
60	6	0	5.339764	4.829741	1.635415
61	6	0	4.742632	-1.889297	-0.881457
62	1	0	4.050049	-0.595480	0.636509
63	6	0	4.581240	-3.087918	-1.442446
64	6	0	6.116003	-1.266824	-0.835314
65	1	0	5.422327	-3.610249	-1.883370
66	1	0	3.629823	-3.600809	-1.489588
67	1	0	6.866886	-1.939162	-1.251296
68	1	0	6.159040	-0.329703	-1.394973
69	1	0	6.402900	-1.031010	0.194786
70	1	0	5.051803	1.928340	-1.614639
71	1	0	5.302532	1.337564	0.038435
72	1	0	2.845565	1.520516	0.474414
73	1	0	2.609252	2.179727	-1.132639
74	8	0	2.497714	-3.832372	1.886848
75	1	0	3.685932	-2.242801	2.168764
76	6	0	1.277114	-0.446039	2.792298
77	1	0	1.103858	0.460637	3.372322
78	1	0	0.437093	-1.128673	2.936296
79	1	0	2.189932	-0.923489	3.163700
80	6	0	-4.876374	-2.809272	0.193733
81	1	0	-5.867570	-2.522736	0.550183
82	1	0	-5.005148	-3.275619	-0.786385
83	1	0	-4.508006	-3.571408	0.880290
84	1	0	4.345561	5.271599	1.695423
85	1	0	5.774504	4.725752	2.626256
86	1	0	5.969902	5.453724	1.002228

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.924904	0.011897	-1.177023
2	6	0	0.444039	0.721893	-1.162557
3	1	0	-0.970015	-0.564302	-2.101633
4	1	0	-1.714113	0.765479	-1.241739
5	1	0	0.494107	1.469095	-0.369766
6	1	0	0.565805	1.254998	-2.109671
7	6	0	3.788213	-0.929570	-0.207318
8	6	0	2.718066	-1.922392	0.302496
9	6	0	1.433069	-1.031673	0.371393
10	6	0	1.537911	-0.327396	-0.995316
11	6	0	3.168918	-2.641329	1.555624
12	1	0	2.502590	-2.698415	-0.435057
13	8	0	1.556329	-0.003665	1.374629
14	6	0	-1.677980	-3.216027	0.764088
15	6	0	-2.228042	-2.122101	-0.203025
16	6	0	-1.186512	-0.914648	0.045137
17	6	0	0.082669	-1.700195	0.448248
18	6	0	-0.208436	-2.932326	0.853279
19	1	0	-2.139151	-3.144333	1.757852
20	1	0	-1.888185	-4.226282	0.403226
21	6	0	-2.100721	-2.684565	-1.633066
22	6	0	-1.617330	-0.028281	1.237775
23	1	0	0.511343	-3.652709	1.220516
24	1	0	-2.458935	-1.994680	-2.397476
25	1	0	-1.062764	-2.928974	-1.866022
26	1	0	-2.678139	-3.605728	-1.728750
27	1	0	-0.846563	0.709710	1.455750
28	1	0	-2.541198	0.511711	1.028379
29	1	0	-1.775325	-0.615862	2.144016
30	6	0	-3.723059	-1.798886	0.124386
31	6	0	-4.351939	-0.760005	-0.829675
32	6	0	-5.662175	-0.144530	-0.343737
33	6	0	-6.234741	0.941659	-1.273436
34	6	0	-5.715223	2.251454	-0.671871
35	6	0	-5.475839	1.883550	0.789836
36	8	0	-5.456824	0.532852	0.930263
37	1	0	-6.399045	-0.920816	-0.141672
38	1	0	-7.327007	0.927119	-1.238768
39	1	0	-5.932577	0.791175	-2.310194
40	1	0	-4.723841	2.482752	-1.079270
41	6	0	-6.609945	3.475759	-0.836168
42	1	0	-3.742404	-1.370338	1.128062
43	1	0	-4.559784	-1.226890	-1.798531
44	1	0	-3.649911	0.052680	-1.026438
45	8	0	-5.309538	2.625151	1.716690
46	1	0	-6.198534	4.325110	-0.289896
47	1	0	-6.699647	3.750554	-1.889201
48	1	0	-7.612761	3.280250	-0.448950
49	1	0	1.288196	-1.121669	-1.707805
50	6	0	3.049290	-0.008700	-1.270925
51	6	0	3.352416	-0.452446	-2.715859

52	6	0	3.428786	1.492106	-1.192521
53	1	0	4.389669	-0.262237	-2.997078
54	1	0	3.163179	-1.517992	-2.857443
55	1	0	2.715896	0.097400	-3.415148
56	6	0	3.417096	2.195463	0.164620
57	6	0	3.562670	3.694875	0.036107
58	8	0	3.428863	4.339872	-0.974780
59	8	0	3.848049	4.254596	1.233721
60	6	0	3.958253	5.688531	1.241337
61	6	0	5.102728	-1.552869	-0.636276
62	1	0	4.021649	-0.289086	0.648951
63	6	0	5.245532	-2.842790	-0.940836
64	6	0	6.292197	-0.625209	-0.660336
65	1	0	6.211628	-3.242168	-1.227321
66	1	0	4.426484	-3.549893	-0.916853
67	1	0	7.201268	-1.151084	-0.953775
68	1	0	6.144282	0.206358	-1.354389
69	1	0	6.458099	-0.181699	0.327094
70	1	0	4.214199	1.844232	0.823402
71	1	0	2.490526	2.005324	0.710086
72	1	0	2.764959	2.040496	-1.864114
73	1	0	4.424548	1.616191	-1.627443
74	8	0	2.805598	-3.744335	1.885701
75	1	0	3.909829	-2.096942	2.177120
76	6	0	1.456845	-0.386522	2.739577
77	1	0	1.210518	0.515942	3.299547
78	1	0	0.674943	-1.131360	2.900786
79	1	0	2.405898	-0.779160	3.118939
80	6	0	-4.603655	-3.062189	0.172764
81	1	0	-5.609469	-2.820214	0.521371
82	1	0	-4.703769	-3.530566	-0.809675
83	1	0	-4.208146	-3.809251	0.860893
84	1	0	4.758285	6.012940	0.576294
85	1	0	3.021609	6.144538	0.921275
86	1	0	4.182785	5.957601	2.270380

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022014	0.150989	-1.103712
2	6	0	0.358601	0.821602	-0.971634
3	1	0	-1.037918	-0.361984	-2.065837
4	1	0	-1.789830	0.927732	-1.152160
5	1	0	0.390690	1.487883	-0.108826
6	1	0	0.531437	1.439386	-1.858311
7	6	0	3.631019	-1.117777	-0.185604
8	6	0	2.479016	-2.045207	0.283645
9	6	0	1.250094	-1.092109	0.426262
10	6	0	1.431064	-0.257240	-0.856585
11	6	0	2.896052	-2.882497	1.473773
12	1	0	2.198906	-2.753290	-0.495889
13	8	0	1.398228	-0.176647	1.528788
14	6	0	-1.952788	-3.174317	0.568080
15	6	0	-2.438854	-1.985929	-0.318844
16	6	0	-1.355864	-0.845235	0.040889
17	6	0	-0.129041	-1.708085	0.409204
18	6	0	-0.476242	-2.955661	0.709557
19	1	0	-2.433325	-3.163963	1.555017
20	1	0	-2.192696	-4.143863	0.123436
21	6	0	-2.305857	-2.440548	-1.786430
22	6	0	-1.778471	-0.029163	1.285470
23	1	0	0.206886	-3.729848	1.035086
24	1	0	-2.611723	-1.675590	-2.500566
25	1	0	-1.276108	-2.719088	-2.017895
26	1	0	-2.925369	-3.321015	-1.965412
27	1	0	-0.972877	0.638062	1.588044
28	1	0	-2.660051	0.582912	1.089807
29	1	0	-2.004749	-0.674583	2.136268
30	6	0	-3.925769	-1.625896	0.005886
31	6	0	-4.494779	-0.501795	-0.887587
32	6	0	-5.777762	0.147680	-0.374112
33	6	0	-6.297114	1.302569	-1.250880
34	6	0	-5.720569	2.556151	-0.585597
35	6	0	-5.506312	2.107931	0.857418
36	8	0	-5.547369	0.752317	0.931827
37	1	0	-6.549363	-0.603707	-0.211245
38	1	0	-7.389066	1.336281	-1.218881
39	1	0	-5.998084	1.188841	-2.293188
40	1	0	-4.717009	2.759356	-0.978023
41	6	0	-6.555397	3.828002	-0.693738
42	1	0	-3.947715	-1.264253	1.035379
43	1	0	-4.716661	-0.900107	-1.883582
44	1	0	-3.752364	0.285742	-1.032270
45	8	0	-5.312672	2.795967	1.819506
46	1	0	-6.108314	4.629022	-0.104135
47	1	0	-6.624771	4.158301	-1.732303
48	1	0	-7.569010	3.661659	-0.321320
49	1	0	1.237971	-0.968465	-1.669017
50	6	0	2.946758	0.096294	-0.973507
51	6	0	3.324274	0.152763	-2.461632

52	6	0	3.232817	1.463630	-0.299724
53	1	0	4.380964	0.369096	-2.622991
54	1	0	3.109528	-0.791994	-2.962824
55	1	0	2.750258	0.937705	-2.962121
56	6	0	4.697778	1.940055	-0.286344
57	6	0	4.808874	3.262065	0.434989
58	8	0	5.048288	3.395339	1.609956
59	8	0	4.576022	4.303438	-0.395264
60	6	0	4.610177	5.605585	0.215513
61	6	0	4.761573	-1.862477	-0.887280
62	1	0	4.066670	-0.684805	0.721633
63	6	0	4.593523	-3.006352	-1.551074
64	6	0	6.141466	-1.263079	-0.773492
65	1	0	5.434139	-3.499390	-2.025337
66	1	0	3.636900	-3.501480	-1.652734
67	1	0	6.890838	-1.912415	-1.227188
68	1	0	6.204873	-0.287628	-1.261668
69	1	0	6.414835	-1.108385	0.275363
70	1	0	5.081803	2.057933	-1.300383
71	1	0	5.329250	1.237394	0.254547
72	1	0	2.871824	1.426495	0.727573
73	1	0	2.641613	2.223923	-0.817384
74	8	0	2.482902	-3.990247	1.716222
75	1	0	3.664877	-2.424713	2.131291
76	6	0	1.247568	-0.686154	2.846745
77	1	0	0.421946	-1.397091	2.921001
78	1	0	2.164992	-1.167973	3.200403
79	1	0	1.041831	0.170556	3.488534
80	6	0	-4.855893	-2.853004	-0.047002
81	1	0	-5.861466	-2.592803	0.289239
82	1	0	-4.945308	-3.256437	-1.058806
83	1	0	-4.508510	-3.655609	0.603431
84	1	0	4.399907	6.309136	-0.586056
85	1	0	3.856282	5.677971	0.999040
86	1	0	5.592304	5.796999	0.647056

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.857634	0.150912	-1.032277
2	6	0	0.513337	0.811110	-0.788748
3	1	0	-0.838355	-0.255553	-2.044194
4	1	0	-1.629043	0.925683	-1.023373
5	1	0	0.513717	1.390805	0.135891
6	1	0	0.699456	1.509700	-1.608679
7	6	0	3.760618	-1.143050	0.008584
8	6	0	2.620644	-2.157894	0.239632
9	6	0	1.369749	-1.237008	0.425722
10	6	0	1.596674	-0.263734	-0.748158
11	6	0	2.971126	-3.144489	1.333092
12	1	0	2.415235	-2.752327	-0.652600
13	8	0	1.465163	-0.437989	1.622286
14	6	0	-1.815085	-3.340312	0.228779
15	6	0	-2.286299	-2.061520	-0.531116
16	6	0	-1.221864	-0.964635	-0.014908
17	6	0	0.000009	-1.856815	0.292183
18	6	0	-0.344887	-3.132632	0.436323
19	1	0	-2.321164	-3.443099	1.197412
20	1	0	-2.035667	-4.254318	-0.328997
21	6	0	-2.108415	-2.346202	-2.036259
22	6	0	-1.689454	-0.292158	1.297704
23	1	0	0.334633	-3.935833	0.690127
24	1	0	-2.404669	-1.508009	-2.667351
25	1	0	-1.068978	-2.585672	-2.268236
26	1	0	-2.710088	-3.207248	-2.332947
27	1	0	-0.904935	0.352609	1.690820
28	1	0	-2.578481	0.320928	1.145185
29	1	0	-1.924949	-1.028406	2.068522
30	6	0	-3.783998	-1.747617	-0.208194
31	6	0	-4.339245	-0.531913	-0.982350
32	6	0	-5.648239	0.036688	-0.439225
33	6	0	-6.154581	1.285220	-1.185762
34	6	0	-5.619825	2.453777	-0.351844
35	6	0	-5.445841	1.833348	1.031596
36	8	0	-5.470653	0.478727	0.937997
37	1	0	-6.414163	-0.736529	-0.397628
38	1	0	-7.247380	1.302813	-1.188455
39	1	0	-5.819081	1.303903	-2.223045
40	1	0	-4.607414	2.715795	-0.681877
41	6	0	-6.471203	3.719088	-0.331040
42	1	0	-3.834164	-1.503519	0.854487
43	1	0	-4.522032	-0.811248	-2.025589
44	1	0	-3.604298	0.275441	-1.005867
45	8	0	-5.293342	2.399636	2.076922
46	1	0	-6.055025	4.447504	0.365587
47	1	0	-6.514270	4.172462	-1.323540
48	1	0	-7.492793	3.496255	-0.014171
49	1	0	1.437805	-0.882423	-1.639805
50	6	0	3.118281	0.095542	-0.771972
51	6	0	3.574493	0.168203	-2.238064

52	6	0	3.514327	1.386667	-0.005451
53	1	0	4.611500	0.496724	-2.336068
54	1	0	3.492494	-0.805153	-2.724182
55	1	0	2.952921	0.869052	-2.801203
56	6	0	3.224180	2.733602	-0.674346
57	6	0	3.867698	3.887877	0.064609
58	8	0	4.799585	3.810411	0.826201
59	8	0	3.275622	5.058921	-0.259898
60	6	0	3.843088	6.233552	0.346958
61	6	0	5.043182	-1.725115	-0.556741
62	1	0	4.017071	-0.756617	1.001218
63	6	0	5.103443	-2.887844	-1.206415
64	6	0	6.300134	-0.930196	-0.301079
65	1	0	6.048547	-3.268681	-1.576155
66	1	0	4.236102	-3.507840	-1.391890
67	1	0	6.452929	-0.781597	0.772744
68	1	0	7.177649	-1.436663	-0.704523
69	1	0	6.252243	0.066686	-0.746846
70	1	0	2.160086	2.945638	-0.765215
71	1	0	3.627933	2.767711	-1.691677
72	1	0	4.589575	1.351156	0.179914
73	1	0	3.041025	1.365386	0.977166
74	8	0	2.563520	-4.279104	1.395954
75	1	0	3.683549	-2.773114	2.098760
76	6	0	1.282156	-1.086612	2.872916
77	1	0	0.485182	-1.832584	2.836360
78	1	0	2.204408	-1.567459	3.215876
79	1	0	1.012697	-0.311279	3.590420
80	6	0	-4.702023	-2.965783	-0.423615
81	1	0	-5.715892	-2.753661	-0.078820
82	1	0	-4.768985	-3.247608	-1.477469
83	1	0	-4.359171	-3.836841	0.134467
84	1	0	4.886675	6.347475	0.054206
85	1	0	3.249001	7.066404	-0.020558
86	1	0	3.782115	6.167996	1.432876

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.924903	0.011901	-1.177021
2	6	0	0.444041	0.721896	-1.162555
3	1	0	-0.970014	-0.564299	-2.101631
4	1	0	-1.714112	0.765482	-1.241738
5	1	0	0.494109	1.469098	-0.369765
6	1	0	0.565806	1.255001	-2.109670
7	6	0	3.788214	-0.929572	-0.207321
8	6	0	2.718065	-1.922392	0.302495
9	6	0	1.433071	-1.031671	0.371392
10	6	0	1.537912	-0.327394	-0.995316
11	6	0	3.168916	-2.641330	1.555622
12	1	0	2.502587	-2.698415	-0.435058
13	8	0	1.556332	-0.003665	1.374631
14	6	0	-1.677979	-3.216022	0.764095
15	6	0	-2.228041	-2.122098	-0.203020
16	6	0	-1.186511	-0.914645	0.045139
17	6	0	0.082670	-1.700192	0.448250
18	6	0	-0.208434	-2.932322	0.853283
19	1	0	-2.139148	-3.144326	1.757860
20	1	0	-1.888185	-4.226278	0.403236
21	6	0	-2.100720	-2.684566	-1.633061
22	6	0	-1.617327	-0.028276	1.237778
23	1	0	0.511345	-3.652704	1.220520
24	1	0	-2.458936	-1.994684	-2.397472
25	1	0	-1.062762	-2.928972	-1.866018
26	1	0	-2.678135	-3.605730	-1.728742
27	1	0	-0.846558	0.709712	1.455753
28	1	0	-2.541194	0.511718	1.028381
29	1	0	-1.775325	-0.615858	2.144018
30	6	0	-3.723058	-1.798883	0.124389
31	6	0	-4.351938	-0.760003	-0.829673
32	6	0	-5.662177	-0.144532	-0.343740
33	6	0	-6.234744	0.941653	-1.273442
34	6	0	-5.715231	2.251452	-0.671877
35	6	0	-5.475852	1.883550	0.789832
36	8	0	-5.456834	0.532852	0.930260
37	1	0	-6.399045	-0.920822	-0.141678
38	1	0	-7.327010	0.927110	-1.238776
39	1	0	-5.932577	0.791169	-2.310199
40	1	0	-4.723847	2.482750	-1.079272
41	6	0	-6.609954	3.475754	-0.836181
42	1	0	-3.742404	-1.370334	1.128066
43	1	0	-4.559778	-1.226888	-1.798531
44	1	0	-3.649911	0.052684	-1.026434
45	8	0	-5.309560	2.625152	1.716686
46	1	0	-6.198546	4.325109	-0.289911
47	1	0	-6.699654	3.750544	-1.889215
48	1	0	-7.612771	3.280245	-0.448965
49	1	0	1.288196	-1.121666	-1.707806
50	6	0	3.049291	-0.008699	-1.270924
51	6	0	3.352416	-0.452442	-2.715860

52	6	0	3.428788	1.492107	-1.192518
53	1	0	4.389670	-0.262233	-2.997078
54	1	0	3.163178	-1.517988	-2.857447
55	1	0	2.715897	0.097406	-3.415147
56	6	0	3.417100	2.195462	0.164624
57	6	0	3.562670	3.694875	0.036113
58	8	0	3.428858	4.339873	-0.974772
59	8	0	3.848067	4.254592	1.233725
60	6	0	3.958274	5.688528	1.241343
61	6	0	5.102727	-1.552873	-0.636284
62	1	0	4.021654	-0.289090	0.648949
63	6	0	5.245527	-2.842793	-0.940849
64	6	0	6.292199	-0.625217	-0.660340
65	1	0	6.211622	-3.242173	-1.227335
66	1	0	4.426477	-3.549894	-0.916869
67	1	0	7.201267	-1.151092	-0.953785
68	1	0	6.144284	0.206356	-1.354385
69	1	0	6.458105	-0.181716	0.327093
70	1	0	4.214204	1.844230	0.823404
71	1	0	2.490532	2.005321	0.710091
72	1	0	2.764961	2.040499	-1.864109
73	1	0	4.424550	1.616193	-1.627441
74	8	0	2.805591	-3.744333	1.885701
75	1	0	3.909832	-2.096947	2.177116
76	6	0	1.456853	-0.386526	2.739579
77	1	0	1.210522	0.515934	3.299552
78	1	0	0.674955	-1.131369	2.900785
79	1	0	2.405908	-0.779162	3.118937
80	6	0	-4.603655	-3.062185	0.172767
81	1	0	-5.609469	-2.820208	0.521374
82	1	0	-4.703769	-3.530562	-0.809672
83	1	0	-4.208147	-3.809247	0.860897
84	1	0	4.758302	6.012935	0.576294
85	1	0	3.021629	6.144537	0.921290
86	1	0	4.182816	5.957593	2.270384

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.074232	0.190310	-1.137443
2	6	0	0.320541	0.836044	-1.027078
3	1	0	-1.099282	-0.356090	-2.080807
4	1	0	-1.825779	0.980389	-1.216596
5	1	0	0.369258	1.536051	-0.192213
6	1	0	0.509343	1.414322	-1.936688
7	6	0	3.548218	-1.124894	-0.137926
8	6	0	2.378067	-2.025112	0.350650
9	6	0	1.167646	-1.039897	0.446904
10	6	0	1.367889	-0.261002	-0.869252
11	6	0	2.769746	-2.811699	1.580115
12	1	0	2.102571	-2.761441	-0.405516
13	8	0	1.335857	-0.084242	1.511891
14	6	0	-2.073203	-3.055029	0.652381
15	6	0	-2.532350	-1.892890	-0.283302
16	6	0	-1.432092	-0.758197	0.040602
17	6	0	-0.222650	-1.628297	0.448926
18	6	0	-0.593743	-2.856796	0.795418
19	1	0	-2.560901	-2.997880	1.634332
20	1	0	-2.326828	-4.036713	0.243635
21	6	0	-2.397824	-2.405230	-1.731401
22	6	0	-1.845458	0.110009	1.252616
23	1	0	0.072665	-3.631564	1.153171
24	1	0	-2.690656	-1.664678	-2.476113
25	1	0	-1.370607	-2.705244	-1.946709
26	1	0	-3.027972	-3.283887	-1.879613
27	1	0	-1.031681	0.777982	1.531089
28	1	0	-2.717031	0.727230	1.031130
29	1	0	-2.084129	-0.498829	2.126487
30	6	0	-4.014420	-1.496439	0.019680
31	6	0	-4.552117	-0.378011	-0.898578
32	6	0	-5.861967	0.262623	-0.443512
33	6	0	-6.313106	1.456769	-1.305472
34	6	0	-5.778034	2.677290	-0.549845
35	6	0	-5.669028	2.168555	0.884659
36	8	0	-5.716914	0.810879	0.898444
37	1	0	-6.647782	-0.487561	-0.365335
38	1	0	-7.404453	1.497859	-1.348047
39	1	0	-5.942565	1.384020	-2.328336
40	1	0	-4.748009	2.887526	-0.861547
41	6	0	-6.595613	3.959688	-0.663916
42	1	0	-4.037102	-1.113592	1.041441
43	1	0	-4.728288	-0.776089	-1.903813
44	1	0	-3.808615	0.413751	-1.010663
45	8	0	-5.545220	2.814284	1.886624
46	1	0	-6.184831	4.732778	-0.013777
47	1	0	-6.591480	4.331237	-1.690767
48	1	0	-7.633365	3.788063	-0.368301
49	1	0	1.153990	-1.001384	-1.649980
50	6	0	2.889490	0.047857	-1.002417
51	6	0	3.285077	0.040566	-2.489055

52	6	0	3.233664	1.435265	-0.400925
53	1	0	4.367039	0.049014	-2.626775
54	1	0	2.893968	-0.832276	-3.013311
55	1	0	2.879069	0.924858	-2.988262
56	6	0	4.704830	1.847821	-0.469598
57	6	0	4.938708	3.245834	0.059315
58	8	0	4.094543	4.089282	0.231968
59	8	0	6.252533	3.456001	0.302830
60	6	0	6.597128	4.773635	0.765412
61	6	0	4.690106	-1.924726	-0.748317
62	1	0	3.956188	-0.643377	0.754105
63	6	0	5.950285	-1.703022	-0.373169
64	6	0	4.377468	-3.028767	-1.730775
65	1	0	6.774473	-2.269618	-0.791402
66	1	0	6.205701	-0.955658	0.369088
67	1	0	5.289353	-3.392708	-2.205334
68	1	0	3.907166	-3.878813	-1.226935
69	1	0	3.691501	-2.708176	-2.516231
70	1	0	5.079296	1.844498	-1.498236
71	1	0	5.356291	1.168165	0.081085
72	1	0	2.904724	1.465372	0.637339
73	1	0	2.649581	2.194949	-0.924775
74	8	0	2.418337	-3.943693	1.812324
75	1	0	3.462673	-2.295974	2.276252
76	6	0	1.122879	-0.517325	2.848353
77	1	0	0.948547	0.381611	3.439943
78	1	0	0.256583	-1.176048	2.935588
79	1	0	2.000733	-1.031244	3.253064
80	6	0	-4.968302	-2.705959	-0.013482
81	1	0	-5.961864	-2.425813	0.341121
82	1	0	-5.083572	-3.111103	-1.022128
83	1	0	-4.623569	-3.513160	0.632668
84	1	0	7.675649	4.761509	0.901036
85	1	0	6.311228	5.523541	0.028098
86	1	0	6.094076	4.990263	1.707486

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.066679	0.127531	-1.144170
2	6	0	0.309751	0.818421	-1.099480
3	1	0	-1.095549	-0.464479	-2.059460
4	1	0	-1.844279	0.889351	-1.241860
5	1	0	0.357481	1.554511	-0.295900
6	1	0	0.457161	1.360751	-2.038060
7	6	0	3.617261	-1.025969	-0.237910
8	6	0	2.484201	-1.928939	0.332740
9	6	0	1.253131	-0.966089	0.430690
10	6	0	1.392181	-0.241489	-0.923480
11	6	0	2.944661	-2.642909	1.577880
12	1	0	2.198941	-2.703949	-0.379540
13	8	0	1.430861	0.036321	1.450500
14	6	0	-1.926949	-3.049349	0.831950
15	6	0	-2.441269	-1.950659	-0.149890
16	6	0	-1.365109	-0.772619	0.086810
17	6	0	-0.120599	-1.588299	0.502530
18	6	0	-0.450229	-2.806339	0.920600
19	1	0	-2.387569	-2.951569	1.823570
20	1	0	-2.165919	-4.056919	0.482220
21	6	0	-2.325859	-2.532149	-1.573420
22	6	0	-1.770279	0.140861	1.268080
23	1	0	0.244941	-3.546169	1.296800
24	1	0	-2.657669	-1.838359	-2.345960
25	1	0	-1.294889	-2.811349	-1.798560
26	1	0	-2.932659	-3.434959	-1.662000
27	1	0	-0.971249	0.847241	1.490190
28	1	0	-2.667119	0.718061	1.039780
29	1	0	-1.963799	-0.433009	2.176120
30	6	0	-3.927009	-1.579229	0.169500
31	6	0	-4.518719	-0.533509	-0.800050
32	6	0	-5.839789	0.091801	-0.362470
33	6	0	-6.366599	1.186141	-1.306790
34	6	0	-5.861779	2.490661	-0.679960
35	6	0	-5.689839	2.115031	0.785150
36	8	0	-5.675629	0.772231	0.925980
37	1	0	-6.591309	-0.674689	-0.183770
38	1	0	-7.458939	1.179041	-1.316090
39	1	0	-6.021529	1.040151	-2.330040
40	1	0	-4.850449	2.711281	-1.041280
41	6	0	-6.737289	3.722001	-0.889860
42	1	0	-3.934319	-1.139749	1.168900
43	1	0	-4.703639	-0.996939	-1.774540
44	1	0	-3.804349	0.272881	-0.976960
45	8	0	-5.564609	2.852391	1.730360
46	1	0	-6.334369	4.579611	-0.349940
47	1	0	-6.786989	3.976681	-1.950150
48	1	0	-7.754759	3.542571	-0.534990
49	1	0	1.176891	-1.020619	-1.664400
50	6	0	2.899631	0.097741	-1.120060
51	6	0	3.244021	0.054591	-2.618160

52	6	0	3.232641	1.511181	-0.573200
53	1	0	4.320001	0.084001	-2.793770
54	1	0	2.854051	-0.841889	-3.100740
55	1	0	2.801851	0.914981	-3.127980
56	6	0	4.695521	1.967051	-0.753360
57	6	0	4.877931	3.352880	-0.186920
58	8	0	4.581751	4.379341	-0.757770
59	8	0	5.387681	3.327060	1.059110
60	6	0	5.552281	4.605320	1.706360
61	6	0	4.750031	-1.828409	-0.862240
62	1	0	4.051511	-0.502619	0.616780
63	6	0	6.017361	-1.577450	-0.529510
64	6	0	4.424831	-2.962279	-1.805520
65	1	0	6.837681	-2.142890	-0.957330
66	1	0	6.280661	-0.805860	0.184980
67	1	0	5.327611	-3.324920	-2.298080
68	1	0	3.983671	-3.805629	-1.265370
69	1	0	3.708681	-2.673839	-2.575910
70	1	0	4.956211	2.016440	-1.810550
71	1	0	5.383101	1.283640	-0.257820
72	1	0	2.972661	1.550831	0.484550
73	1	0	2.594871	2.236611	-1.084860
74	8	0	2.679691	-3.793169	1.850540
75	1	0	3.606681	-2.061259	2.247940
76	6	0	1.259081	-0.343499	2.810670
77	1	0	2.156841	-0.821779	3.214170
78	1	0	1.081201	0.575971	3.368480
79	1	0	0.408011	-1.013039	2.946850
80	6	0	-4.843629	-2.816259	0.230930
81	1	0	-5.838979	-2.543779	0.586610
82	1	0	-4.965069	-3.285139	-0.748720
83	1	0	-4.462739	-3.570999	0.918920
84	1	0	5.971201	4.383750	2.684020
85	1	0	6.231211	5.234820	1.132720
86	1	0	4.589761	5.105291	1.806570

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056794	0.084571	-1.173516
2	6	0	0.323787	0.765684	-1.117519
3	1	0	-1.084454	-0.505933	-2.090063
4	1	0	-1.827368	0.853401	-1.275782
5	1	0	0.369163	1.498478	-0.311187
6	1	0	0.480629	1.311743	-2.052628
7	6	0	3.611897	-1.100081	-0.231620
8	6	0	2.470137	-1.994933	0.318043
9	6	0	1.241942	-1.034942	0.409728
10	6	0	1.400011	-0.300150	-0.936157
11	6	0	2.906273	-2.745383	1.558062
12	1	0	2.180233	-2.757117	-0.405081
13	8	0	1.411113	-0.038860	1.438266
14	6	0	-1.960308	-3.090129	0.780044
15	6	0	-2.462257	-1.976517	-0.190798
16	6	0	-1.370537	-0.814703	0.054115
17	6	0	-0.137054	-1.648416	0.466267
18	6	0	-0.480494	-2.866925	0.872517
19	1	0	-2.419596	-2.996153	1.772811
20	1	0	-2.211963	-4.091793	0.421740
21	6	0	-2.358669	-2.548212	-1.619093
22	6	0	-1.764850	0.099391	1.238404
23	1	0	0.206631	-3.616104	1.244726
24	1	0	-2.681329	-1.843735	-2.386102
25	1	0	-1.332878	-2.842336	-1.848587
26	1	0	-2.978940	-3.441243	-1.714461
27	1	0	-0.955041	0.791040	1.466413
28	1	0	-2.653264	0.691804	1.016454
29	1	0	-1.968071	-0.476094	2.143335
30	6	0	-3.941179	-1.586272	0.135143
31	6	0	-4.523782	-0.526969	-0.825350
32	6	0	-5.815560	0.136178	-0.352664
33	6	0	-6.333612	1.247528	-1.284565
34	6	0	-5.772710	2.533546	-0.669294
35	6	0	-5.569949	2.150492	0.794096
36	8	0	-5.601475	0.799218	0.927308
37	1	0	-6.584061	-0.612354	-0.164272
38	1	0	-7.426036	1.274607	-1.264963
39	1	0	-6.023060	1.090385	-2.317852
40	1	0	-4.766665	2.726845	-1.060345
41	6	0	-6.615620	3.792854	-0.841752
42	1	0	-3.940377	-1.149628	1.135558
43	1	0	-4.739788	-0.986528	-1.795923
44	1	0	-3.790836	0.259545	-1.016326
45	8	0	-5.391660	2.881128	1.727344
46	1	0	-6.179443	4.623065	-0.285346
47	1	0	-6.678065	4.075206	-1.894770
48	1	0	-7.631281	3.635838	-0.470820
49	1	0	1.195308	-1.072196	-1.687980
50	6	0	2.912733	0.045258	-1.104716
51	6	0	3.268487	-0.019213	-2.597606

52	6	0	3.201588	1.466370	-0.554439
53	1	0	4.319237	0.199245	-2.790985
54	1	0	3.062358	-1.006317	-3.013473
55	1	0	2.676378	0.712842	-3.153725
56	6	0	4.663006	1.949981	-0.594985
57	6	0	4.740770	3.387418	-0.135629
58	8	0	4.366742	4.337968	-0.778034
59	8	0	5.263865	3.493658	1.105671
60	6	0	5.339788	4.829736	1.635411
61	6	0	4.742632	-1.889295	-0.881457
62	1	0	4.050046	-0.595481	0.636510
63	6	0	4.581243	-3.087918	-1.442445
64	6	0	6.116001	-1.266818	-0.835316
65	1	0	5.422330	-3.610247	-1.883368
66	1	0	3.629827	-3.600812	-1.489585
67	1	0	6.866886	-1.939155	-1.251298
68	1	0	6.159035	-0.329698	-1.394976
69	1	0	6.402898	-1.031002	0.194783
70	1	0	5.051807	1.928334	-1.614637
71	1	0	5.302532	1.337558	0.038437
72	1	0	2.845564	1.520517	0.474413
73	1	0	2.609256	2.179728	-1.132640
74	8	0	2.497712	-3.832376	1.886843
75	1	0	3.685933	-2.242808	2.168760
76	6	0	1.277108	-0.446043	2.792300
77	1	0	1.103853	0.460633	3.372324
78	1	0	0.437085	-1.128675	2.936294
79	1	0	2.189925	-0.923495	3.163703
80	6	0	-4.876375	-2.809270	0.193743
81	1	0	-5.867570	-2.522734	0.550195
82	1	0	-5.005151	-3.275620	-0.786373
83	1	0	-4.508003	-3.571404	0.880301
84	1	0	4.345585	5.271594	1.695430
85	1	0	5.774538	4.725747	2.626248
86	1	0	5.969919	5.453720	1.002218

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.033548	0.162013	-1.105224
2	6	0	0.345559	0.839687	-0.987782
3	1	0	-1.050884	-0.363228	-2.060694
4	1	0	-1.804713	0.934921	-1.160912
5	1	0	0.379866	1.518508	-0.134774
6	1	0	0.513384	1.444725	-1.884075
7	6	0	3.627108	-1.067124	-0.168394
8	6	0	2.480315	-2.001532	0.311438
9	6	0	1.247790	-1.047948	0.436354
10	6	0	1.421836	-0.233647	-0.861640
11	6	0	2.899168	-2.805466	1.521293
12	1	0	2.215059	-2.727991	-0.457845
13	8	0	1.395960	-0.111381	1.520737
14	6	0	-1.940744	-3.146776	0.614663
15	6	0	-2.435986	-1.974188	-0.288388
16	6	0	-1.360129	-0.821035	0.053334
17	6	0	-0.127483	-1.670592	0.432332
18	6	0	-0.465542	-2.916141	0.750680
19	1	0	-2.420124	-3.125373	1.601984
20	1	0	-2.174733	-4.124081	0.184227
21	6	0	-2.302554	-2.448163	-1.749667
22	6	0	-1.786899	0.010357	1.286284
23	1	0	0.222731	-3.682433	1.084558
24	1	0	-2.616208	-1.695628	-2.473567
25	1	0	-1.271181	-2.721889	-1.979694
26	1	0	-2.915543	-3.335803	-1.915105
27	1	0	-0.987621	0.691275	1.574863
28	1	0	-2.675179	0.610062	1.083659
29	1	0	-2.004131	-0.623041	2.148345
30	6	0	-3.924717	-1.620143	0.034546
31	6	0	-4.503186	-0.510081	-0.870372
32	6	0	-5.788612	0.136789	-0.359604
33	6	0	-6.319773	1.277761	-1.247414
34	6	0	-5.750777	2.543374	-0.598452
35	6	0	-5.525857	2.112892	0.848346
36	8	0	-5.556895	0.757943	0.938268
37	1	0	-6.554331	-0.617932	-0.184816
38	1	0	-7.411820	1.303346	-1.211899
39	1	0	-6.023538	1.154573	-2.289446
40	1	0	-4.750964	2.751147	-0.997967
41	6	0	-6.597411	3.806585	-0.716226
42	1	0	-3.947207	-1.247108	1.059960
43	1	0	-4.725597	-0.921298	-1.860989
44	1	0	-3.766340	0.280526	-1.026430
45	8	0	-5.332105	2.812970	1.801665
46	1	0	-6.154381	4.618065	-0.137991
47	1	0	-6.675170	4.124581	-1.758018
48	1	0	-7.607524	3.635407	-0.336561
49	1	0	1.223823	-0.959485	-1.660018
50	6	0	2.935279	0.114961	-0.992964
51	6	0	3.324003	0.169872	-2.479723

52	6	0	3.253843	1.485683	-0.340391
53	1	0	4.404898	0.207881	-2.620328
54	1	0	2.949077	-0.692609	-3.031904
55	1	0	2.897497	1.062263	-2.946570
56	6	0	4.719014	1.953749	-0.454369
57	6	0	4.928345	3.217705	0.343173
58	8	0	5.292176	3.263476	1.492890
59	8	0	4.626802	4.319673	-0.380450
60	6	0	4.749339	5.573124	0.314528
61	6	0	4.774472	-1.832016	-0.812737
62	1	0	4.039889	-0.600808	0.729250
63	6	0	6.033532	-1.608052	-0.435024
64	6	0	4.469650	-2.909200	-1.827181
65	1	0	6.862043	-2.152257	-0.874028
66	1	0	6.283072	-0.883509	0.331542
67	1	0	5.383816	-3.249376	-2.314770
68	1	0	4.010029	-3.778890	-1.347537
69	1	0	3.777958	-2.573637	-2.601384
70	1	0	4.986836	2.140940	-1.494491
71	1	0	5.399087	1.206961	-0.048184
72	1	0	2.974504	1.446701	0.712094
73	1	0	2.622833	2.246158	-0.808470
74	8	0	2.565456	-3.946285	1.735656
75	1	0	3.593722	-2.293513	2.218105
76	6	0	1.218174	-0.583198	2.849819
77	1	0	1.002078	0.291956	3.462761
78	1	0	0.388826	-1.289009	2.928623
79	1	0	2.126670	-1.056593	3.235147
80	6	0	-4.846916	-2.853866	-0.002477
81	1	0	-5.853221	-2.596406	0.333634
82	1	0	-4.936549	-3.268745	-1.009607
83	1	0	-4.493062	-3.647264	0.655745
84	1	0	4.473209	6.335959	-0.409089
85	1	0	4.080360	5.598662	1.174448
86	1	0	5.773845	5.719830	0.655543

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.872707	0.183452	-1.107184
2	6	0	0.510392	0.827533	-0.890369
3	1	0	-0.856887	-0.273819	-2.097132
4	1	0	-1.628176	0.972895	-1.143082
5	1	0	0.521555	1.456885	0.000835
6	1	0	0.712225	1.476915	-1.746095
7	6	0	3.711727	-1.152339	0.024688
8	6	0	2.550188	-2.133563	0.289961
9	6	0	1.318244	-1.178475	0.425484
10	6	0	1.571102	-0.265877	-0.792164
11	6	0	2.872996	-3.077099	1.428828
12	1	0	2.339419	-2.762539	-0.576916
13	8	0	1.429066	-0.325733	1.583071
14	6	0	-1.907369	-3.224825	0.305424
15	6	0	-2.349400	-1.970842	-0.512017
16	6	0	-1.265129	-0.873353	-0.039913
17	6	0	-0.063609	-1.774912	0.315062
18	6	0	-0.435045	-3.035635	0.515311
19	1	0	-2.424142	-3.278310	1.272434
20	1	0	-2.139340	-4.157548	-0.215560
21	6	0	-2.172173	-2.326592	-2.002192
22	6	0	-1.723559	-0.131425	1.237975
23	1	0	0.226546	-3.840252	0.809044
24	1	0	-2.445593	-1.510802	-2.671815
25	1	0	-1.138173	-2.601541	-2.218781
26	1	0	-2.794230	-3.184940	-2.261569
27	1	0	-0.925110	0.509745	1.607950
28	1	0	-2.593327	0.499591	1.050429
29	1	0	-1.984524	-0.826151	2.038253
30	6	0	-3.842605	-1.616473	-0.209645
31	6	0	-4.357853	-0.398645	-1.005960
32	6	0	-5.714572	0.144779	-0.562462
33	6	0	-6.131655	1.449318	-1.266879
34	6	0	-5.681079	2.547656	-0.298517
35	6	0	-5.671707	1.829243	1.048022
36	8	0	-5.686301	0.484723	0.853977
37	1	0	-6.483288	-0.620509	-0.660103
38	1	0	-7.217969	1.482471	-1.382814
39	1	0	-5.688315	1.537121	-2.259233
40	1	0	-4.634538	2.810964	-0.493528
41	6	0	-6.513282	3.825517	-0.284213
42	1	0	-3.898046	-1.354440	0.848574
43	1	0	-4.455887	-0.661232	-2.064889
44	1	0	-3.633809	0.417254	-0.958744
45	8	0	-5.643380	2.317247	2.142156
46	1	0	-6.170923	4.494437	0.505974
47	1	0	-6.435549	4.348468	-1.239701
48	1	0	-7.567406	3.602468	-0.102936
49	1	0	1.405969	-0.922116	-1.655298
50	6	0	3.100505	0.059196	-0.820500
51	6	0	3.573220	0.053184	-2.282404

52	6	0	3.509356	1.381394	-0.112880
53	1	0	4.623407	0.335483	-2.382342
54	1	0	3.456228	-0.935685	-2.728148
55	1	0	2.986149	0.755405	-2.879573
56	6	0	3.293075	2.697357	-0.889306
57	6	0	3.755146	3.877401	-0.067925
58	8	0	3.038964	4.608759	0.570304
59	8	0	5.100755	4.013414	-0.109633
60	6	0	5.642443	5.088944	0.677046
61	6	0	4.988879	-1.782370	-0.499840
62	1	0	3.963812	-0.725985	1.002142
63	6	0	5.033424	-2.970698	-1.102238
64	6	0	6.258502	-1.001964	-0.261983
65	1	0	5.974720	-3.384161	-1.445666
66	1	0	4.155857	-3.580248	-1.273947
67	1	0	6.405540	-0.818636	0.807507
68	1	0	7.129887	-1.538455	-0.639003
69	1	0	6.232325	-0.021655	-0.745106
70	1	0	2.242529	2.863694	-1.113051
71	1	0	3.855193	2.684343	-1.824317
72	1	0	4.575619	1.318385	0.118206
73	1	0	2.985542	1.438030	0.842494
74	8	0	2.450703	-4.203037	1.533318
75	1	0	3.579307	-2.682294	2.188666
76	6	0	1.215380	-0.905690	2.862489
77	1	0	0.395962	-1.627630	2.854942
78	1	0	2.119014	-1.397576	3.238079
79	1	0	0.964308	-0.087559	3.537825
80	6	0	-4.786092	-2.817380	-0.412908
81	1	0	-5.784607	-2.593503	-0.033640
82	1	0	-4.888349	-3.085821	-1.467676
83	1	0	-4.439850	-3.700381	0.123879
84	1	0	5.393363	4.954323	1.729391
85	1	0	6.718531	5.045630	0.528736
86	1	0	5.246140	6.045391	0.337009

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022014	0.150989	-1.103712
2	6	0	0.358601	0.821602	-0.971635
3	1	0	-1.037918	-0.361984	-2.065837
4	1	0	-1.789830	0.927732	-1.152160
5	1	0	0.390690	1.487883	-0.108827
6	1	0	0.531437	1.439386	-1.858311
7	6	0	3.631019	-1.117777	-0.185604
8	6	0	2.479016	-2.045207	0.283645
9	6	0	1.250094	-1.092109	0.426262
10	6	0	1.431064	-0.257240	-0.856585
11	6	0	2.896052	-2.882497	1.473773
12	1	0	2.198906	-2.753290	-0.495889
13	8	0	1.398228	-0.176647	1.528788
14	6	0	-1.952788	-3.174317	0.568080
15	6	0	-2.438854	-1.985929	-0.318843
16	6	0	-1.355864	-0.845235	0.040889
17	6	0	-0.129041	-1.708084	0.409204
18	6	0	-0.476242	-2.955661	0.709557
19	1	0	-2.433325	-3.163963	1.555017
20	1	0	-2.192696	-4.143863	0.123436
21	6	0	-2.305857	-2.440548	-1.786430
22	6	0	-1.778471	-0.029163	1.285470
23	1	0	0.206886	-3.729848	1.035086
24	1	0	-2.611723	-1.675590	-2.500566
25	1	0	-1.276108	-2.719088	-2.017895
26	1	0	-2.925369	-3.321015	-1.965412
27	1	0	-0.972877	0.638062	1.588044
28	1	0	-2.660051	0.582912	1.089807
29	1	0	-2.004749	-0.674583	2.136268
30	6	0	-3.925769	-1.625896	0.005886
31	6	0	-4.494779	-0.501795	-0.887587
32	6	0	-5.777762	0.147680	-0.374112
33	6	0	-6.297114	1.302569	-1.250880
34	6	0	-5.720569	2.556151	-0.585597
35	6	0	-5.506312	2.107931	0.857418
36	8	0	-5.547369	0.752317	0.931827
37	1	0	-6.549363	-0.603707	-0.211245
38	1	0	-7.389066	1.336281	-1.218881
39	1	0	-5.998085	1.188841	-2.293188
40	1	0	-4.717009	2.759356	-0.978023
41	6	0	-6.555397	3.828002	-0.693739
42	1	0	-3.947715	-1.264253	1.035379
43	1	0	-4.716661	-0.900107	-1.883582
44	1	0	-3.752364	0.285742	-1.032270
45	8	0	-5.312672	2.795967	1.819506
46	1	0	-6.108314	4.629022	-0.104136
47	1	0	-6.624771	4.158301	-1.732304
48	1	0	-7.569010	3.661659	-0.321320
49	1	0	1.237971	-0.968465	-1.669017
50	6	0	2.946758	0.096294	-0.973507
51	6	0	3.324274	0.152763	-2.461632

52	6	0	3.232817	1.463630	-0.299724
53	1	0	4.380964	0.369096	-2.622991
54	1	0	3.109528	-0.791994	-2.962824
55	1	0	2.750258	0.937705	-2.962121
56	6	0	4.697778	1.940055	-0.286344
57	6	0	4.808874	3.262065	0.434989
58	8	0	5.048288	3.395339	1.609956
59	8	0	4.576022	4.303438	-0.395264
60	6	0	4.610176	5.605585	0.215514
61	6	0	4.761573	-1.862477	-0.887280
62	1	0	4.066670	-0.684805	0.721633
63	6	0	4.593523	-3.006352	-1.551074
64	6	0	6.141466	-1.263079	-0.773492
65	1	0	5.434139	-3.499390	-2.025337
66	1	0	3.636900	-3.501480	-1.652734
67	1	0	6.890838	-1.912415	-1.227188
68	1	0	6.204873	-0.287628	-1.261669
69	1	0	6.414835	-1.108385	0.275363
70	1	0	5.081803	2.057933	-1.300384
71	1	0	5.329250	1.237394	0.254546
72	1	0	2.871824	1.426495	0.727573
73	1	0	2.641613	2.223923	-0.817384
74	8	0	2.482902	-3.990247	1.716222
75	1	0	3.664877	-2.424713	2.131291
76	6	0	1.247568	-0.686154	2.846745
77	1	0	0.421946	-1.397091	2.921001
78	1	0	2.164992	-1.167972	3.200403
79	1	0	1.041831	0.170556	3.488534
80	6	0	-4.855893	-2.853004	-0.047001
81	1	0	-5.861466	-2.592803	0.289239
82	1	0	-4.945308	-3.256437	-1.058806
83	1	0	-4.508510	-3.655609	0.603431
84	1	0	4.399907	6.309136	-0.586056
85	1	0	3.856281	5.677970	0.999040
86	1	0	5.592304	5.796999	0.647056

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.924904	0.011898	-1.177022
2	6	0	0.444039	0.721893	-1.162556
3	1	0	-0.970016	-0.564301	-2.101633
4	1	0	-1.714114	0.765479	-1.241738
5	1	0	0.494107	1.469096	-0.369765
6	1	0	0.565805	1.254998	-2.109671
7	6	0	3.788213	-0.929570	-0.207318
8	6	0	2.718066	-1.922392	0.302496
9	6	0	1.433069	-1.031673	0.371393
10	6	0	1.537911	-0.327396	-0.995316
11	6	0	3.168918	-2.641329	1.555623
12	1	0	2.502589	-2.698416	-0.435057
13	8	0	1.556329	-0.003666	1.374629
14	6	0	-1.677980	-3.216027	0.764088
15	6	0	-2.228042	-2.122101	-0.203024
16	6	0	-1.186512	-0.914648	0.045137
17	6	0	0.082669	-1.700195	0.448249
18	6	0	-0.208436	-2.932327	0.853279
19	1	0	-2.139151	-3.144334	1.757852
20	1	0	-1.888185	-4.226282	0.403226
21	6	0	-2.100721	-2.684565	-1.633066
22	6	0	-1.617330	-0.028281	1.237776
23	1	0	0.511343	-3.652709	1.220516
24	1	0	-2.458935	-1.994680	-2.397476
25	1	0	-1.062764	-2.928974	-1.866022
26	1	0	-2.678139	-3.605727	-1.728750
27	1	0	-0.846563	0.709710	1.455751
28	1	0	-2.541198	0.511711	1.028380
29	1	0	-1.775326	-0.615862	2.144017
30	6	0	-3.723059	-1.798886	0.124386
31	6	0	-4.351939	-0.760005	-0.829675
32	6	0	-5.662175	-0.144530	-0.343736
33	6	0	-6.234741	0.941659	-1.273436
34	6	0	-5.715223	2.251455	-0.671871
35	6	0	-5.475838	1.883550	0.789836
36	8	0	-5.456824	0.532853	0.930263
37	1	0	-6.399045	-0.920816	-0.141671
38	1	0	-7.327007	0.927119	-1.238768
39	1	0	-5.932577	0.791175	-2.310194
40	1	0	-4.723840	2.482752	-1.079270
41	6	0	-6.609945	3.475759	-0.836169
42	1	0	-3.742405	-1.370338	1.128063
43	1	0	-4.559784	-1.226890	-1.798531
44	1	0	-3.649911	0.052680	-1.026437
45	8	0	-5.309537	2.625152	1.716690
46	1	0	-6.198533	4.325111	-0.289896
47	1	0	-6.699647	3.750554	-1.889201
48	1	0	-7.612761	3.280250	-0.448950
49	1	0	1.288195	-1.121669	-1.707805
50	6	0	3.049289	-0.008700	-1.270925
51	6	0	3.352415	-0.452446	-2.715860

52	6	0	3.428785	1.492106	-1.192521
53	1	0	4.389668	-0.262236	-2.997079
54	1	0	3.163178	-1.517992	-2.857444
55	1	0	2.715895	0.097400	-3.415148
56	6	0	3.417097	2.195462	0.164621
57	6	0	3.562668	3.694875	0.036107
58	8	0	3.428853	4.339873	-0.974778
59	8	0	3.848057	4.254595	1.233720
60	6	0	3.958258	5.688531	1.241336
61	6	0	5.102728	-1.552869	-0.636277
62	1	0	4.021650	-0.289086	0.648951
63	6	0	5.245531	-2.842790	-0.940838
64	6	0	6.292197	-0.625210	-0.660338
65	1	0	6.211627	-3.242169	-1.227323
66	1	0	4.426483	-3.549893	-0.916854
67	1	0	7.201267	-1.151085	-0.953777
68	1	0	6.144282	0.206357	-1.354390
69	1	0	6.458099	-0.181700	0.327092
70	1	0	4.214200	1.844232	0.823401
71	1	0	2.490528	2.005323	0.710087
72	1	0	2.764959	2.040497	-1.864113
73	1	0	4.424548	1.616191	-1.627443
74	8	0	2.805598	-3.744335	1.885701
75	1	0	3.909830	-2.096942	2.177119
76	6	0	1.456846	-0.386522	2.739578
77	1	0	1.210518	0.515941	3.299547
78	1	0	0.674944	-1.131361	2.900786
79	1	0	2.405898	-0.779160	3.118939
80	6	0	-4.603656	-3.062189	0.172764
81	1	0	-5.609470	-2.820214	0.521371
82	1	0	-4.703769	-3.530566	-0.809675
83	1	0	-4.208147	-3.809251	0.860893
84	1	0	4.758285	6.012941	0.576287
85	1	0	3.021611	6.144536	0.921283
86	1	0	4.182799	5.957599	2.270377

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.951481	0.175144	-1.184440
2	6	0	0.445583	0.816551	-1.085257
3	1	0	-0.973405	-0.402677	-2.109245
4	1	0	-1.697001	0.967074	-1.293917
5	1	0	0.491304	1.540850	-0.271422
6	1	0	0.642228	1.367105	-2.010242
7	6	0	3.657974	-1.145273	-0.135714
8	6	0	2.479158	-2.014354	0.376179
9	6	0	1.275095	-1.022325	0.446744
10	6	0	1.487342	-0.279715	-0.887614
11	6	0	2.864207	-2.784861	1.620317
12	1	0	2.188325	-2.762488	-0.360870
13	8	0	1.445000	-0.042454	1.489647
14	6	0	-1.987042	-2.997976	0.708497
15	6	0	-2.432889	-1.862328	-0.264190
16	6	0	-1.320729	-0.729838	0.023752
17	6	0	-0.120671	-1.599470	0.460441
18	6	0	-0.505182	-2.812785	0.844595
19	1	0	-2.472021	-2.901565	1.688804
20	1	0	-2.254086	-3.989383	0.332941
21	6	0	-2.303755	-2.421067	-1.695594
22	6	0	-1.726442	0.182644	1.205709
23	1	0	0.152490	-3.582262	1.228286
24	1	0	-2.592977	-1.702328	-2.462852
25	1	0	-1.278313	-2.732870	-1.902036
26	1	0	-2.938322	-3.300836	-1.816580
27	1	0	-0.905384	0.850489	1.463028
28	1	0	-2.592913	0.799499	0.964180
29	1	0	-1.968705	-0.396554	2.098917
30	6	0	-3.909820	-1.438364	0.024069
31	6	0	-4.437626	-0.355275	-0.941993
32	6	0	-5.683928	0.378709	-0.474224
33	6	0	-6.225500	1.426368	-1.458231
34	6	0	-6.819054	2.506633	-0.545703
35	6	0	-6.026894	2.328351	0.747666
36	8	0	-5.380020	1.132916	0.734692
37	1	0	-6.471272	-0.329531	-0.202847
38	1	0	-6.951887	0.995489	-2.148866
39	1	0	-5.401488	1.834197	-2.049222
40	1	0	-6.626405	3.514014	-0.917120
41	6	0	-8.322603	2.358079	-0.270461
42	1	0	-3.924888	-1.011223	1.028642
43	1	0	-4.675647	-0.806462	-1.911876
44	1	0	-3.673150	0.399262	-1.133488
45	8	0	-5.958338	3.083186	1.675892
46	1	0	-8.648676	3.084356	0.475167
47	1	0	-8.892199	2.524463	-1.187029
48	1	0	-8.565897	1.359648	0.101782
49	1	0	1.280780	-1.039782	-1.651187
50	6	0	3.011964	0.027892	-1.014161
51	6	0	3.405496	-0.035677	-2.497974

52	6	0	3.325062	1.435492	-0.443933
53	1	0	4.469551	0.141579	-2.659358
54	1	0	3.173162	-1.009289	-2.931605
55	1	0	2.857710	0.724525	-3.062008
56	6	0	4.788452	1.875738	-0.440135
57	6	0	4.959209	3.305208	0.029162
58	8	0	4.088994	4.135551	0.107058
59	8	0	6.251202	3.557883	0.339951
60	6	0	6.539535	4.904354	0.756411
61	6	0	4.783055	-1.960035	-0.763601
62	1	0	4.087011	-0.661366	0.748873
63	6	0	4.602765	-3.146176	-1.345051
64	6	0	6.172552	-1.379246	-0.672146
65	1	0	5.440460	-3.687508	-1.769243
66	1	0	3.638381	-3.629829	-1.426029
67	1	0	6.915674	-2.072478	-1.067421
68	1	0	6.261663	-0.442182	-1.226575
69	1	0	6.434656	-1.155475	0.367206
70	1	0	5.231880	1.832658	-1.440568
71	1	0	5.413708	1.244319	0.192688
72	1	0	2.941579	1.495845	0.573928
73	1	0	2.761515	2.171181	-1.021336
74	8	0	2.429016	-3.868765	1.924450
75	1	0	3.632196	-2.300729	2.260277
76	6	0	1.253276	-0.455633	2.834712
77	1	0	1.098620	0.452625	3.417451
78	1	0	0.382806	-1.105359	2.946629
79	1	0	2.134077	-0.972986	3.229644
80	6	0	-4.876071	-2.637957	0.042983
81	1	0	-5.876994	-2.325360	0.347335
82	1	0	-4.967964	-3.106334	-0.940188
83	1	0	-4.560079	-3.404724	0.750348
84	1	0	6.281692	5.610845	-0.032275
85	1	0	5.977029	5.153298	1.655906
86	1	0	7.608114	4.924856	0.954972

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.117822	0.120145	-1.142479
2	6	0	0.275109	0.772340	-1.063070
3	1	0	-1.148310	-0.455742	-2.068086
4	1	0	-1.873343	0.904232	-1.239858
5	1	0	0.328258	1.498187	-0.251047
6	1	0	0.454907	1.321778	-1.991864
7	6	0	3.520990	-1.198287	-0.224893
8	6	0	2.367040	-2.015846	0.406815
9	6	0	1.143122	-1.049628	0.467056
10	6	0	1.326598	-0.315925	-0.877215
11	6	0	2.779063	-2.729943	1.673470
12	1	0	2.054592	-2.821956	-0.266220
13	8	0	1.292093	-0.053108	1.496670
14	6	0	-2.104828	-3.063048	0.761180
15	6	0	-2.566265	-1.934732	-0.212859
16	6	0	-1.463532	-0.791370	0.067549
17	6	0	-0.247516	-1.645361	0.495122
18	6	0	-0.624393	-2.859206	0.884301
19	1	0	-2.585606	-2.967927	1.743460
20	1	0	-2.362789	-4.058116	0.389315
21	6	0	-2.437419	-2.497675	-1.642611
22	6	0	-1.866335	0.111565	1.257719
23	1	0	0.032873	-3.630290	1.266947
24	1	0	-2.736173	-1.784328	-2.410840
25	1	0	-1.410303	-2.800918	-1.853664
26	1	0	-3.065843	-3.382667	-1.757367
27	1	0	-1.051505	0.789234	1.507361
28	1	0	-2.742465	0.718409	1.026411
29	1	0	-2.094020	-0.471888	2.151679
30	6	0	-4.046729	-1.526746	0.082744
31	6	0	-4.586275	-0.438467	-0.869589
32	6	0	-5.904482	0.204151	-0.441969
33	6	0	-6.350811	1.378819	-1.332730
34	6	0	-5.829872	2.616481	-0.595281
35	6	0	-5.735854	2.136855	0.850281
36	8	0	-5.777389	0.779047	0.890222
37	1	0	-6.687651	-0.548263	-0.358657
38	1	0	-7.441746	1.413970	-1.388502
39	1	0	-5.968285	1.287603	-2.349706
40	1	0	-4.797098	2.825093	-0.898930
41	6	0	-6.651471	3.892668	-0.744805
42	1	0	-4.064448	-1.109921	1.091267
43	1	0	-4.751790	-0.864477	-1.865075
44	1	0	-3.847904	0.355582	-0.996985
45	8	0	-5.627359	2.802295	1.840850
46	1	0	-6.251849	4.680391	-0.105395
47	1	0	-6.636332	4.243621	-1.778757
48	1	0	-7.691999	3.722345	-0.458372
49	1	0	1.111290	-1.084970	-1.630628
50	6	0	2.844286	-0.002946	-1.041531
51	6	0	3.186064	0.004931	-2.540202

52	6	0	3.195966	1.377589	-0.428047
53	1	0	4.252529	0.139737	-2.725314
54	1	0	2.895626	-0.926539	-3.026465
55	1	0	2.659704	0.824777	-3.037236
56	6	0	4.667936	1.786346	-0.482957
57	6	0	4.901588	3.185321	0.045231
58	8	0	4.053776	4.015843	0.257324
59	8	0	6.221005	3.411334	0.239247
60	6	0	6.565389	4.726775	0.707412
61	6	0	4.529092	-2.066257	-0.970473
62	1	0	4.063183	-0.751962	0.609922
63	6	0	4.189534	-3.099896	-1.739433
64	6	0	5.978004	-1.700170	-0.783398
65	1	0	4.943201	-3.686861	-2.251322
66	1	0	3.162319	-3.406335	-1.899528
67	1	0	6.637183	-2.388894	-1.313165
68	1	0	6.186198	-0.689144	-1.145807
69	1	0	6.238399	-1.718048	0.279193
70	1	0	5.058301	1.778707	-1.505819
71	1	0	5.308361	1.109653	0.086174
72	1	0	2.865834	1.401394	0.609198
73	1	0	2.616785	2.144788	-0.946742
74	8	0	3.880024	-2.678050	2.165546
75	1	0	2.001492	-3.368243	2.139264
76	6	0	1.145004	-0.453386	2.852775
77	1	0	0.292878	-1.123247	2.993238
78	1	0	2.050068	-0.932761	3.234832
79	1	0	0.972796	0.459219	3.423685
80	6	0	-5.002345	-2.735311	0.094303
81	1	0	-5.990733	-2.443336	0.453434
82	1	0	-5.130978	-3.167875	-0.901285
83	1	0	-4.651733	-3.525409	0.758298
84	1	0	7.648306	4.727438	0.802592
85	1	0	6.242214	5.483062	-0.007732
86	1	0	6.095411	4.923282	1.670749

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722658	0.217967	-1.064121
2	6	0	0.656621	0.856727	-0.809883
3	1	0	-0.697107	-0.198814	-2.071722
4	1	0	-1.480052	1.006198	-1.072503
5	1	0	0.655229	1.447287	0.107835
6	1	0	0.865755	1.541975	-1.635521
7	6	0	3.858233	-1.142589	0.056700
8	6	0	2.698108	-2.135411	0.283095
9	6	0	1.460497	-1.191039	0.439462
10	6	0	1.720393	-0.235922	-0.742691
11	6	0	3.015852	-3.113645	1.393733
12	1	0	2.495796	-2.737331	-0.604812
13	8	0	1.552889	-0.378997	1.627426
14	6	0	-1.754786	-3.244865	0.216091
15	6	0	-2.193735	-1.965904	-0.562494
16	6	0	-1.119679	-0.880875	-0.040745
17	6	0	0.082569	-1.789467	0.293161
18	6	0	-0.284679	-3.058319	0.444061
19	1	0	-2.277410	-3.329954	1.177692
20	1	0	-1.981952	-4.160584	-0.336353
21	6	0	-1.999910	-2.266764	-2.062468
22	6	0	-1.597161	-0.186235	1.256978
23	1	0	0.377927	-3.869883	0.715492
24	1	0	-2.277806	-1.430667	-2.704702
25	1	0	-0.960587	-2.520816	-2.278848
26	1	0	-2.607851	-3.123279	-2.359409
27	1	0	-0.808117	0.451041	1.653566
28	1	0	-2.475076	0.437568	1.084452
29	1	0	-1.852351	-0.910802	2.032813
30	6	0	-3.690136	-1.625025	-0.264307
31	6	0	-4.211340	-0.402633	-1.052355
32	6	0	-5.487773	0.219770	-0.510359
33	6	0	-6.024722	1.409006	-1.320720
34	6	0	-6.668842	2.308796	-0.258887
35	6	0	-5.909391	1.929354	1.010278
36	8	0	-5.237114	0.763947	0.817900
37	1	0	-6.265769	-0.538510	-0.388107
38	1	0	-6.721272	1.088705	-2.096866
39	1	0	-5.193673	1.925376	-1.808168
40	1	0	-6.489793	3.367821	-0.449427
41	6	0	-8.175819	2.088176	-0.061235
42	1	0	-3.750907	-1.374239	0.796452
43	1	0	-4.408899	-0.687983	-2.091736
44	1	0	-3.458185	0.386162	-1.086932
45	8	0	-5.882167	2.519378	2.053060
46	1	0	-8.540104	2.670824	0.785847
47	1	0	-8.722451	2.397967	-0.954233
48	1	0	-8.406518	1.036705	0.127879
49	1	0	1.562693	-0.862152	-1.629260
50	6	0	3.248314	0.096089	-0.749524
51	6	0	3.726979	0.139370	-2.209630

52	6	0	3.655768	1.391215	0.004336
53	1	0	4.772241	0.443988	-2.296284
54	1	0	3.631035	-0.838382	-2.684245
55	1	0	3.128974	0.845751	-2.791058
56	6	0	3.401909	2.731824	-0.690954
57	6	0	4.051977	3.887450	0.039860
58	8	0	4.951667	3.805492	0.838772
59	8	0	3.507655	5.065105	-0.339891
60	6	0	4.085953	6.240195	0.255540
61	6	0	5.139435	-1.752585	-0.481716
62	1	0	4.105854	-0.747400	1.048096
63	6	0	5.190431	-2.924541	-1.115365
64	6	0	6.405150	-0.974222	-0.218349
65	1	0	6.134548	-3.325175	-1.466237
66	1	0	4.315961	-3.532991	-1.305679
67	1	0	6.545319	-0.814027	0.855519
68	1	0	7.280107	-1.499451	-0.602951
69	1	0	6.378799	0.017317	-0.677608
70	1	0	2.343325	2.960827	-0.804076
71	1	0	3.822715	2.741922	-1.701724
72	1	0	4.726817	1.338746	0.208956
73	1	0	3.166015	1.394142	0.979048
74	8	0	2.591090	-4.241598	1.463177
75	1	0	3.720746	-2.743233	2.166819
76	6	0	1.336510	-1.007384	2.882934
77	1	0	0.523601	-1.735774	2.843483
78	1	0	2.242248	-1.504268	3.246471
79	1	0	1.073703	-0.217040	3.586408
80	6	0	-4.625853	-2.827866	-0.487510
81	1	0	-5.644468	-2.590731	-0.173442
82	1	0	-4.671059	-3.121978	-1.539074
83	1	0	-4.315145	-3.698003	0.090658
84	1	0	5.144199	6.312996	0.005452
85	1	0	3.534885	7.078895	-0.162268
86	1	0	3.976612	6.210751	1.339278

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.801397	0.042415	-1.213650
2	6	0	0.576376	0.734841	-1.203748
3	1	0	-0.842864	-0.561712	-2.120602
4	1	0	-1.579310	0.804119	-1.310592
5	1	0	0.627198	1.503872	-0.432325
6	1	0	0.716063	1.238740	-2.164322
7	6	0	3.887611	-0.930966	-0.163503
8	6	0	2.798988	-1.896112	0.360305
9	6	0	1.525571	-0.986317	0.391866
10	6	0	1.654456	-0.322615	-0.993087
11	6	0	3.227434	-2.588604	1.635891
12	1	0	2.581240	-2.687803	-0.359658
13	8	0	1.654616	0.067621	1.367231
14	6	0	-1.621256	-3.111691	0.821315
15	6	0	-2.144442	-2.042311	-0.186733
16	6	0	-1.088771	-0.841650	0.034069
17	6	0	0.164621	-1.632499	0.474931
18	6	0	-0.148355	-2.846875	0.915861
19	1	0	-2.090361	-2.999944	1.807645
20	1	0	-1.844414	-4.129886	0.491666
21	6	0	-2.008793	-2.651751	-1.596809
22	6	0	-1.521384	0.088747	1.192153
23	1	0	0.557060	-3.565468	1.313060
24	1	0	-2.349538	-1.981602	-2.386358
25	1	0	-0.971154	-2.914995	-1.809659
26	1	0	-2.595718	-3.569020	-1.670758
27	1	0	-0.741954	0.821703	1.397054
28	1	0	-2.434807	0.634265	0.952996
29	1	0	-1.697242	-0.468896	2.114180
30	6	0	-3.637584	-1.685835	0.110710
31	6	0	-4.241293	-0.685172	-0.899057
32	6	0	-5.505165	0.021045	-0.436478
33	6	0	-6.131024	0.967918	-1.471339
34	6	0	-6.741099	2.085840	-0.617057
35	6	0	-5.895536	2.039318	0.653559
36	8	0	-5.196027	0.875031	0.703254
37	1	0	-6.246413	-0.701420	-0.084593
38	1	0	-6.861017	0.455170	-2.099374
39	1	0	-5.349343	1.366611	-2.122994
40	1	0	-6.609088	3.070335	-1.067911
41	6	0	-8.225473	1.892452	-0.273713
42	1	0	-3.659944	-1.209406	1.092791
43	1	0	-4.485416	-1.203789	-1.832971
44	1	0	-3.517416	0.089138	-1.157522
45	8	0	-5.826830	2.864278	1.520157
46	1	0	-8.557793	2.655228	0.431621
47	1	0	-8.834276	1.968532	-1.176916
48	1	0	-8.409528	0.913364	0.175838
49	1	0	1.403024	-1.133938	-1.685438
50	6	0	3.172558	-0.029686	-1.259542
51	6	0	3.486066	-0.514145	-2.689141

52	6	0	3.570245	1.467919	-1.216404
53	1	0	4.528424	-0.342955	-2.963836
54	1	0	3.285641	-1.580632	-2.806247
55	1	0	2.863690	0.025093	-3.409105
56	6	0	3.551988	2.207709	0.121099
57	6	0	3.729228	3.699899	-0.045137
58	8	0	3.637020	4.318306	-1.077014
59	8	0	3.991830	4.287988	1.144222
60	6	0	4.131192	5.719035	1.114865
61	6	0	5.198671	-1.581532	-0.560837
62	1	0	4.119238	-0.271135	0.678388
63	6	0	5.328866	-2.880383	-0.831141
64	6	0	6.399604	-0.669052	-0.595683
65	1	0	6.293080	-3.298504	-1.096470
66	1	0	4.501059	-3.576818	-0.798758
67	1	0	7.304974	-1.212709	-0.867399
68	1	0	6.268239	0.147153	-1.311027
69	1	0	6.561460	-0.203586	0.382273
70	1	0	4.332677	1.859668	0.801015
71	1	0	2.614479	2.048864	0.657556
72	1	0	2.921008	2.006181	-1.910110
73	1	0	4.572232	1.567711	-1.642974
74	8	0	2.845128	-3.677395	1.990972
75	1	0	3.970807	-2.039162	2.250004
76	6	0	1.533396	-0.274727	2.740961
77	1	0	0.728144	-0.991093	2.915921
78	1	0	2.466946	-0.685201	3.139675
79	1	0	1.310119	0.650027	3.273533
80	6	0	-4.535742	-2.933337	0.209275
81	1	0	-5.551042	-2.657587	0.502107
82	1	0	-4.607272	-3.463908	-0.743521
83	1	0	-4.175863	-3.638169	0.958983
84	1	0	4.953916	6.008731	0.461591
85	1	0	3.212293	6.184346	0.758709
86	1	0	4.335520	6.012591	2.141436

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.922885	0.106433	-1.214528
2	6	0	0.461247	0.781073	-1.166528
3	1	0	-0.944232	-0.513971	-2.111327
4	1	0	-1.687295	0.876110	-1.349500
5	1	0	0.502431	1.540210	-0.384882
6	1	0	0.631370	1.293918	-2.117941
7	6	0	3.728703	-1.067729	-0.176313
8	6	0	2.575832	-1.936573	0.391015
9	6	0	1.351836	-0.968164	0.434028
10	6	0	1.529005	-0.283816	-0.936069
11	6	0	2.993578	-2.645239	1.661596
12	1	0	2.289948	-2.722351	-0.308198
13	8	0	1.514612	0.063480	1.427832
14	6	0	-1.862476	-2.997509	0.835413
15	6	0	-2.347920	-1.916243	-0.178660
16	6	0	-1.255285	-0.749423	0.039482
17	6	0	-0.030617	-1.572935	0.496011
18	6	0	-0.383186	-2.776154	0.938546
19	1	0	-2.333128	-2.868106	1.818791
20	1	0	-2.114438	-4.009740	0.508161
21	6	0	-2.228883	-2.535191	-1.586065
22	6	0	-1.663755	0.207407	1.184842
23	1	0	0.296419	-3.514422	1.344667
24	1	0	-2.543043	-1.855741	-2.378802
25	1	0	-1.200378	-2.835424	-1.794469
26	1	0	-2.847100	-3.431757	-1.659688
27	1	0	-0.856309	0.907104	1.397350
28	1	0	-2.550047	0.789987	0.930817
29	1	0	-1.875733	-0.336339	2.107557
30	6	0	-3.829070	-1.510048	0.114280
31	6	0	-4.398358	-0.493586	-0.899440
32	6	0	-5.648621	0.242699	-0.446747
33	6	0	-6.240850	1.208766	-1.483592
34	6	0	-6.835256	2.335297	-0.629642
35	6	0	-6.003031	2.264306	0.648715
36	8	0	-5.330212	1.084310	0.699454
37	1	0	-6.411267	-0.462472	-0.105810
38	1	0	-6.974956	0.715842	-2.122620
39	1	0	-5.442918	1.593093	-2.124143
40	1	0	-6.678326	3.319023	-1.074116
41	6	0	-8.326467	2.171138	-0.301159
42	1	0	-3.836764	-1.028997	1.094377
43	1	0	-4.647176	-1.004204	-1.836513
44	1	0	-3.652958	0.262903	-1.149678
45	8	0	-5.924318	3.083572	1.519802
46	1	0	-8.649615	2.937265	0.404793
47	1	0	-8.925036	2.263980	-1.209614
48	1	0	-8.534776	1.193947	0.141878
49	1	0	1.327248	-1.081291	-1.661629
50	6	0	3.045734	0.046389	-1.100599
51	6	0	3.419538	-0.078093	-2.585301

52	6	0	3.337544	1.486092	-0.602352
53	1	0	4.474715	0.124285	-2.771933
54	1	0	3.210637	-1.078821	-2.965657
55	1	0	2.841239	0.636664	-3.177390
56	6	0	4.803221	1.959126	-0.648615
57	6	0	4.885171	3.410025	-0.236552
58	8	0	4.638259	4.347952	-0.954476
59	8	0	5.243588	3.544859	1.059471
60	6	0	5.297841	4.895752	1.552260
61	6	0	4.864151	-1.886505	-0.779563
62	1	0	4.157163	-0.532389	0.678057
63	6	0	4.704369	-3.104369	-1.297921
64	6	0	6.240038	-1.269455	-0.737307
65	1	0	5.548930	-3.647115	-1.706319
66	1	0	3.750838	-3.613756	-1.340266
67	1	0	6.993449	-1.961166	-1.115165
68	1	0	6.296270	-0.355576	-1.333075
69	1	0	6.512947	-0.994180	0.286775
70	1	0	5.201226	1.898828	-1.662369
71	1	0	5.429866	1.364741	0.014808
72	1	0	2.972582	1.582728	0.420108
73	1	0	2.753881	2.178237	-1.214665
74	8	0	2.576913	-3.718923	2.022553
75	1	0	3.767389	-2.124616	2.264528
76	6	0	1.362218	-0.294418	2.793633
77	1	0	1.190570	0.633674	3.339225
78	1	0	0.514726	-0.964536	2.952097
79	1	0	2.266623	-0.766060	3.192122
80	6	0	-4.766989	-2.727861	0.215886
81	1	0	-5.771709	-2.420061	0.512795
82	1	0	-4.858865	-3.255685	-0.736718
83	1	0	-4.426977	-3.444283	0.963801
84	1	0	5.594064	4.813727	2.594915
85	1	0	6.028287	5.476187	0.989292
86	1	0	4.321239	5.371434	1.465951

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891291	0.177000	-1.150267
2	6	0	0.492187	0.842150	-1.021083
3	1	0	-0.897842	-0.366190	-2.095892
4	1	0	-1.652295	0.957333	-1.233141
5	1	0	0.518342	1.535672	-0.179779
6	1	0	0.681146	1.430201	-1.924563
7	6	0	3.740223	-1.095289	-0.135872
8	6	0	2.575736	-1.999674	0.347538
9	6	0	1.352746	-1.033265	0.447405
10	6	0	1.555251	-0.239413	-0.858411
11	6	0	2.973071	-2.803380	1.567062
12	1	0	2.299057	-2.729080	-0.413266
13	8	0	1.497468	-0.085815	1.522832
14	6	0	-1.868597	-3.084574	0.619354
15	6	0	-2.332639	-1.924567	-0.315250
16	6	0	-1.246796	-0.779796	0.021234
17	6	0	-0.031127	-1.638885	0.433492
18	6	0	-0.391820	-2.872965	0.771711
19	1	0	-2.361254	-3.034070	1.599225
20	1	0	-2.112074	-4.067415	0.207019
21	6	0	-2.182509	-2.428944	-1.764787
22	6	0	-1.680204	0.079846	1.232620
23	1	0	0.280574	-3.641201	1.131782
24	1	0	-2.478137	-1.687982	-2.508050
25	1	0	-1.150463	-2.716319	-1.973815
26	1	0	-2.801038	-3.314224	-1.922382
27	1	0	-0.872780	0.750182	1.523949
28	1	0	-2.554537	0.691051	1.004912
29	1	0	-1.920742	-0.536669	2.100999
30	6	0	-3.820541	-1.542076	-0.024778
31	6	0	-4.367059	-0.445925	-0.966009
32	6	0	-5.613102	0.270953	-0.471960
33	6	0	-6.189468	1.310256	-1.445127
34	6	0	-6.772974	2.386706	-0.521862
35	6	0	-5.948187	2.220943	0.752542
36	8	0	-5.292196	1.030684	0.729260
37	1	0	-6.384440	-0.447547	-0.182093
38	1	0	-6.927097	0.869589	-2.117400
39	1	0	-5.384152	1.725263	-2.056611
40	1	0	-6.600308	3.395019	-0.900565
41	6	0	-8.267860	2.222729	-0.210558
42	1	0	-3.852292	-1.143674	0.991066
43	1	0	-4.612043	-0.883357	-1.940422
44	1	0	-3.611191	0.318265	-1.153662
45	8	0	-5.862509	2.981006	1.675114
46	1	0	-8.583925	2.947166	0.541140
47	1	0	-8.860782	2.381145	-1.113643
48	1	0	-8.491630	1.222584	0.169193
49	1	0	1.367547	-0.974304	-1.650858
50	6	0	3.074491	0.100400	-0.966755
51	6	0	3.471942	0.111446	-2.450566

52	6	0	3.361997	1.485114	-0.329494
53	1	0	4.532909	0.312797	-2.602549
54	1	0	3.254569	-0.844956	-2.927963
55	1	0	2.912839	0.887617	-2.980801
56	6	0	4.829724	1.953115	-0.312190
57	6	0	4.939719	3.293783	0.374050
58	8	0	5.165655	3.458042	1.547796
59	8	0	4.722668	4.313217	-0.487128
60	6	0	4.755763	5.631378	0.088255
61	6	0	4.872456	-1.868719	-0.802880
62	1	0	4.168897	-0.639318	0.763331
63	6	0	4.703176	-3.030778	-1.433984
64	6	0	6.255261	-1.275342	-0.692514
65	1	0	5.545105	-3.543331	-1.884666
66	1	0	3.744178	-3.522179	-1.531108
67	1	0	7.004647	-1.942303	-1.119865
68	1	0	6.330106	-0.314748	-1.207796
69	1	0	6.519302	-1.092282	0.354168
70	1	0	5.226233	2.041350	-1.324442
71	1	0	5.450987	1.262143	0.255010
72	1	0	2.988819	1.480961	0.694016
73	1	0	2.782133	2.233566	-0.876366
74	8	0	2.552043	-3.901999	1.836350
75	1	0	3.735368	-2.329649	2.220978
76	6	0	1.317136	-0.548865	2.853729
77	1	0	1.148493	0.335971	3.467503
78	1	0	0.458767	-1.217832	2.944241
79	1	0	2.208610	-1.062291	3.228510
80	6	0	-4.760257	-2.762467	-0.047106
81	1	0	-5.774260	-2.476513	0.240391
82	1	0	-4.820953	-3.214517	-1.040191
83	1	0	-4.442936	-3.534840	0.653571
84	1	0	5.732892	5.829434	0.528058
85	1	0	4.560427	6.313786	-0.735080
86	1	0	3.991512	5.729233	0.858899

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109220	0.060790	-1.149300
2	6	0	0.271920	0.741590	-1.120460
3	1	0	-1.145960	-0.546790	-2.054200
4	1	0	-1.881690	0.826670	-1.257850
5	1	0	0.326070	1.493610	-0.332750
6	1	0	0.422410	1.263440	-2.070010
7	6	0	3.572040	-1.137611	-0.279050
8	6	0	2.445950	-1.953970	0.402170
9	6	0	1.204970	-1.009970	0.452460
10	6	0	1.347390	-0.320620	-0.919680
11	6	0	2.893980	-2.616820	1.684420
12	1	0	2.137820	-2.788440	-0.237520
13	8	0	1.354340	0.026040	1.443660
14	6	0	-1.995780	-3.074300	0.878800
15	6	0	-2.499420	-1.988090	-0.121230
16	6	0	-1.413570	-0.815160	0.097810
17	6	0	-0.172810	-1.630500	0.529310
18	6	0	-0.517670	-2.838460	0.964260
19	1	0	-2.457340	-2.956670	1.867780
20	1	0	-2.241720	-4.085650	0.544640
21	6	0	-2.388100	-2.594960	-1.534490
22	6	0	-1.812270	0.120130	1.263950
23	1	0	0.161760	-3.584710	1.357550
24	1	0	-2.714820	-1.912020	-2.318770
25	1	0	-1.359420	-2.885230	-1.755990
26	1	0	-3.000950	-3.495090	-1.609140
27	1	0	-1.009790	0.826150	1.472200
28	1	0	-2.708400	0.696280	1.031470
29	1	0	-2.005750	-0.437220	2.182320
30	6	0	-3.981490	-1.598470	0.191350
31	6	0	-4.566580	-0.565559	-0.795630
32	6	0	-5.870840	0.091401	-0.348840
33	6	0	-6.384050	1.188031	-1.300570
34	6	0	-5.842479	2.485311	-0.691420
35	6	0	-5.658759	2.120141	0.778990
36	8	0	-5.681030	0.769561	0.926500
37	1	0	-6.635810	-0.661709	-0.164210
38	1	0	-7.476790	1.206351	-1.296930
39	1	0	-6.057380	1.022201	-2.327530
40	1	0	-4.832179	2.682191	-1.069530
41	6	0	-6.692509	3.735841	-0.890800
42	1	0	-3.985720	-1.137660	1.180870
43	1	0	-4.767340	-1.045979	-1.759300
44	1	0	-3.840650	0.225500	-0.993900
45	8	0	-5.500679	2.861641	1.707000
46	1	0	-6.270959	4.575801	-0.337820
47	1	0	-6.741469	4.005471	-1.947830
48	1	0	-7.712279	3.575081	-0.533020
49	1	0	1.130920	-1.118350	-1.642080
50	6	0	2.856050	0.011400	-1.127200
51	6	0	3.168190	-0.028130	-2.631140

52	6	0	3.194840	1.419780	-0.571040
53	1	0	4.228380	0.115619	-2.842340
54	1	0	2.882260	-0.980820	-3.077110
55	1	0	2.620390	0.766020	-3.146160
56	6	0	4.665521	1.862089	-0.693340
57	6	0	4.816781	3.290269	-0.224560
58	8	0	4.411791	4.258449	-0.820990
59	8	0	5.447811	3.367929	0.967340
60	6	0	5.604701	4.694079	1.502700
61	6	0	4.585070	-2.012561	-1.009740
62	1	0	4.118960	-0.647491	0.527610
63	6	0	4.253150	-3.077471	-1.738220
64	6	0	6.029460	-1.615791	-0.854530
65	1	0	5.009930	-3.668581	-2.240600
66	1	0	3.229320	-3.406640	-1.873380
67	1	0	6.693570	-2.308821	-1.372350
68	1	0	6.214040	-0.612691	-1.250240
69	1	0	6.304170	-1.596021	0.204370
70	1	0	4.989811	1.840249	-1.735200
71	1	0	5.322800	1.220579	-0.107890
72	1	0	2.900960	1.465040	0.477310
73	1	0	2.587481	2.155870	-1.103630
74	8	0	4.003320	-2.530911	2.151920
75	1	0	2.135580	-3.249690	2.187750
76	6	0	1.244370	-0.330700	2.815500
77	1	0	0.414860	-1.019310	2.994860
78	1	0	2.170240	-0.770030	3.195620
79	1	0	1.055380	0.595500	3.358690
80	6	0	-4.909700	-2.825169	0.277190
81	1	0	-5.902290	-2.535749	0.626940
82	1	0	-5.035740	-3.314299	-0.692130
83	1	0	-4.538120	-3.569759	0.981200
84	1	0	6.121201	4.565929	2.450540
85	1	0	6.193451	5.310549	0.823850
86	1	0	4.631551	5.160419	1.654470

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722656	0.217965	-1.064127
2	6	0	0.656623	0.856726	-0.809889
3	1	0	-0.697104	-0.198818	-2.071727
4	1	0	-1.480050	1.006196	-1.072512
5	1	0	0.655230	1.447287	0.107829
6	1	0	0.865757	1.541972	-1.635528
7	6	0	3.858235	-1.142587	0.056700
8	6	0	2.698111	-2.135409	0.283097
9	6	0	1.460499	-1.191039	0.439459
10	6	0	1.720395	-0.235923	-0.742694
11	6	0	3.015856	-3.113638	1.393740
12	1	0	2.495800	-2.737333	-0.604808
13	8	0	1.552889	-0.378993	1.627422
14	6	0	-1.754785	-3.244864	0.216094
15	6	0	-2.193734	-1.965906	-0.562495
16	6	0	-1.119677	-0.880875	-0.040749
17	6	0	0.082570	-1.789467	0.293159
18	6	0	-0.284678	-3.058317	0.444062
19	1	0	-2.277409	-3.329949	1.177695
20	1	0	-1.981952	-4.160585	-0.336347
21	6	0	-1.999909	-2.266771	-2.062469
22	6	0	-1.597159	-0.186232	1.256972
23	1	0	0.377927	-3.869882	0.715496
24	1	0	-2.277806	-1.430676	-2.704705
25	1	0	-0.960586	-2.520825	-2.278847
26	1	0	-2.607850	-3.123287	-2.359406
27	1	0	-0.808116	0.451048	1.653557
28	1	0	-2.475076	0.437567	1.084446
29	1	0	-1.852346	-0.910797	2.032810
30	6	0	-3.690135	-1.625025	-0.264309
31	6	0	-4.211336	-0.402630	-1.052354
32	6	0	-5.487772	0.219771	-0.510361
33	6	0	-6.024717	1.409013	-1.320716
34	6	0	-6.668842	2.308794	-0.258878
35	6	0	-5.909396	1.929344	1.010286
36	8	0	-5.237119	0.763939	0.817904
37	1	0	-6.265769	-0.538509	-0.388117
38	1	0	-6.721263	1.088717	-2.096868
39	1	0	-5.193665	1.925386	-1.808155
40	1	0	-6.489792	3.367822	-0.449410
41	6	0	-8.175820	2.088173	-0.061235
42	1	0	-3.750907	-1.374242	0.796450
43	1	0	-4.408890	-0.687974	-2.091736
44	1	0	-3.458182	0.386166	-1.086923
45	8	0	-5.882181	2.519359	2.053074
46	1	0	-8.540109	2.670813	0.785850
47	1	0	-8.722448	2.397970	-0.954232
48	1	0	-8.406518	1.036700	0.127869
49	1	0	1.562695	-0.862154	-1.629263
50	6	0	3.248316	0.096089	-0.749528
51	6	0	3.726980	0.139365	-2.209635

52	6	0	3.655769	1.391217	0.004330
53	1	0	4.772243	0.443984	-2.296289
54	1	0	3.631037	-0.838389	-2.684246
55	1	0	3.128976	0.845744	-2.791065
56	6	0	3.401910	2.731825	-0.690963
57	6	0	4.051978	3.887451	0.039850
58	8	0	4.951664	3.805493	0.838766
59	8	0	3.507645	5.065105	-0.339891
60	6	0	4.085936	6.240195	0.255549
61	6	0	5.139438	-1.752584	-0.481713
62	1	0	4.105855	-0.747395	1.048094
63	6	0	5.190436	-2.924541	-1.115359
64	6	0	6.405151	-0.974215	-0.218348
65	1	0	6.134554	-3.325173	-1.466231
66	1	0	4.315968	-3.532991	-1.305674
67	1	0	6.545320	-0.814018	0.855519
68	1	0	7.280110	-1.499443	-0.602949
69	1	0	6.378797	0.017322	-0.677610
70	1	0	2.343326	2.960827	-0.804086
71	1	0	3.822716	2.741921	-1.701733
72	1	0	4.726818	1.338749	0.208950
73	1	0	3.166015	1.394145	0.979042
74	8	0	2.591092	-4.241591	1.463190
75	1	0	3.720750	-2.743223	2.166824
76	6	0	1.336515	-1.007380	2.882931
77	1	0	0.523608	-1.735772	2.843483
78	1	0	2.242255	-1.504261	3.246467
79	1	0	1.073707	-0.217036	3.586404
80	6	0	-4.625853	-2.827864	-0.487517
81	1	0	-5.644468	-2.590729	-0.173450
82	1	0	-4.671058	-3.121973	-1.539082
83	1	0	-4.315147	-3.698003	0.090648
84	1	0	3.976589	6.210745	1.339286
85	1	0	5.144183	6.313002	0.005465
86	1	0	3.534865	7.078894	-0.162259

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.263002	0.287461	-1.157174
2	6	0	0.076790	1.046069	-1.107159
3	1	0	-1.279654	-0.270106	-2.094414
4	1	0	-2.079020	1.013032	-1.211665
5	1	0	0.098134	1.748458	-0.273310
6	1	0	0.175626	1.634725	-2.024555
7	6	0	3.489709	-0.664572	-0.375596
8	6	0	2.411608	-1.633413	0.177672
9	6	0	1.134975	-0.747436	0.331194
10	6	0	1.219365	0.040710	-0.989516
11	6	0	2.923352	-2.393579	1.382844
12	1	0	2.139953	-2.390591	-0.557999
13	8	0	1.260669	0.224899	1.384600
14	6	0	-1.931839	-3.001426	0.698505
15	6	0	-2.521153	-1.887247	-0.220433
16	6	0	-1.493460	-0.672115	0.042818
17	6	0	-0.203804	-1.444629	0.395783
18	6	0	-0.465644	-2.694897	0.764659
19	1	0	-2.371173	-2.968771	1.704025
20	1	0	-2.134049	-4.003394	0.310624
21	6	0	-2.418305	-2.402768	-1.669981
22	6	0	-1.912798	0.174155	1.268419
23	1	0	0.273453	-3.414410	1.093125
24	1	0	-2.794570	-1.690553	-2.404702
25	1	0	-1.383655	-2.633541	-1.929893
26	1	0	-2.992612	-3.323882	-1.784140
27	1	0	-1.141570	0.906941	1.500974
28	1	0	-2.842802	0.715504	1.089907
29	1	0	-2.053874	-0.443505	2.157383
30	6	0	-4.013668	-1.597291	0.148598
31	6	0	-4.681110	-0.550637	-0.770314
32	6	0	-5.986309	0.039503	-0.241988
33	6	0	-6.604909	1.119608	-1.149186
34	6	0	-6.086082	2.434906	-0.559732
35	6	0	-5.798438	2.066250	0.893190
36	8	0	-5.755112	0.715745	1.028360
37	1	0	-6.703696	-0.749960	-0.021755
38	1	0	-7.695187	1.088438	-1.079269
39	1	0	-6.334137	0.976754	-2.195646
40	1	0	-5.110623	2.680957	-0.995981
41	6	0	-7.002133	3.647039	-0.693744
42	1	0	-4.017398	-1.189687	1.161092
43	1	0	-4.907669	-1.004743	-1.741033
44	1	0	-3.994635	0.274245	-0.971024
45	8	0	-5.617112	2.808115	1.817029
46	1	0	-6.586726	4.500620	-0.157131
47	1	0	-7.126829	3.923340	-1.742870
48	1	0	-7.990277	3.436552	-0.277759
49	1	0	1.043118	-0.715011	-1.764728
50	6	0	2.707575	0.480873	-1.176865
51	6	0	3.016562	0.498630	-2.682183

52	6	0	2.924435	1.897336	-0.575755
53	1	0	4.047132	0.780265	-2.902161
54	1	0	2.849890	-0.480013	-3.133947
55	1	0	2.367251	1.218736	-3.188666
56	6	0	4.302739	2.562833	-0.698384
57	6	0	5.263412	2.312080	0.444313
58	8	0	5.009255	1.763378	1.488492
59	8	0	6.477938	2.832761	0.164379
60	6	0	7.464661	2.719670	1.205222
61	6	0	4.624318	-1.373029	-1.105274
62	1	0	3.938605	-0.173673	0.490967
63	6	0	4.498720	-2.552651	-1.713677
64	6	0	5.966793	-0.686505	-1.076365
65	1	0	5.345799	-3.013534	-2.208669
66	1	0	3.572058	-3.110235	-1.745518
67	1	0	6.725731	-1.278008	-1.589721
68	1	0	5.934337	0.297114	-1.551666
69	1	0	6.293841	-0.526904	-0.044517
70	1	0	4.170210	3.650485	-0.716883
71	1	0	4.816193	2.335617	-1.634301
72	1	0	2.639881	1.883017	0.474905
73	1	0	2.216840	2.560286	-1.079807
74	8	0	2.581574	-3.510947	1.688002
75	1	0	3.691424	-1.868079	1.986904
76	6	0	1.234243	-0.236263	2.727831
77	1	0	0.943454	0.614491	3.344543
78	1	0	0.513229	-1.044422	2.870880
79	1	0	2.223312	-0.573207	3.053701
80	6	0	-4.871818	-2.876170	0.189787
81	1	0	-5.875729	-2.657519	0.558955
82	1	0	-4.980326	-3.329526	-0.798855
83	1	0	-4.452023	-3.627627	0.858489
84	1	0	7.664082	1.672087	1.429445
85	1	0	8.356291	3.202888	0.814066
86	1	0	7.122000	3.219773	2.110668

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.924902	0.011902	-1.177020
2	6	0	0.444043	0.721895	-1.162551
3	1	0	-0.970013	-0.564295	-2.101632
4	1	0	-1.714110	0.765484	-1.241735
5	1	0	0.494111	1.469096	-0.369760
6	1	0	0.565810	1.255001	-2.109665
7	6	0	3.788214	-0.929571	-0.207312
8	6	0	2.718065	-1.922393	0.302500
9	6	0	1.433069	-1.031675	0.371395
10	6	0	1.537913	-0.327396	-0.995312
11	6	0	3.168916	-2.641331	1.555628
12	1	0	2.502591	-2.698417	-0.435053
13	8	0	1.556327	-0.003670	1.374635
14	6	0	-1.677983	-3.216027	0.764081
15	6	0	-2.228042	-2.122098	-0.203030
16	6	0	-1.186512	-0.914647	0.045137
17	6	0	0.082668	-1.700196	0.448248
18	6	0	-0.208438	-2.932328	0.853275
19	1	0	-2.139155	-3.144337	1.757844
20	1	0	-1.888188	-4.226281	0.403215
21	6	0	-2.100719	-2.684557	-1.633073
22	6	0	-1.617332	-0.028283	1.237777
23	1	0	0.511339	-3.652713	1.220510
24	1	0	-2.458930	-1.994668	-2.397481
25	1	0	-1.062763	-2.928967	-1.866028
26	1	0	-2.678139	-3.605718	-1.728762
27	1	0	-0.846565	0.709707	1.455755
28	1	0	-2.541199	0.511710	1.028380
29	1	0	-1.775330	-0.615867	2.144016
30	6	0	-3.723060	-1.798883	0.124381
31	6	0	-4.351939	-0.759998	-0.829678
32	6	0	-5.662177	-0.144529	-0.343741
33	6	0	-6.234742	0.941664	-1.273437
34	6	0	-5.715229	2.251457	-0.671864
35	6	0	-5.475850	1.883546	0.789843
36	8	0	-5.456834	0.532847	0.930263
37	1	0	-6.399047	-0.920818	-0.141683
38	1	0	-7.327009	0.927122	-1.238772
39	1	0	-5.932575	0.791185	-2.310194
40	1	0	-4.723845	2.482758	-1.079257
41	6	0	-6.609952	3.475761	-0.836159
42	1	0	-3.742405	-1.370338	1.128058
43	1	0	-4.559780	-1.226879	-1.798537
44	1	0	-3.649912	0.052689	-1.026434
45	8	0	-5.309556	2.625142	1.716702
46	1	0	-6.198543	4.325112	-0.289883
47	1	0	-6.699651	3.750559	-1.889191
48	1	0	-7.612768	3.280250	-0.448944
49	1	0	1.288195	-1.121667	-1.707802
50	6	0	3.049292	-0.008703	-1.270921
51	6	0	3.352416	-0.452454	-2.715855

52	6	0	3.428790	1.492103	-1.192523
53	1	0	4.389670	-0.262247	-2.997074
54	1	0	3.163177	-1.518000	-2.857436
55	1	0	2.715898	0.097392	-3.415145
56	6	0	3.417102	2.195466	0.164615
57	6	0	3.562679	3.694878	0.036094
58	8	0	3.428878	4.339870	-0.974796
59	8	0	3.848054	4.254603	1.233708
60	6	0	3.958262	5.688538	1.241317
61	6	0	5.102729	-1.552870	-0.636267
62	1	0	4.021647	-0.289086	0.648957
63	6	0	5.245534	-2.842791	-0.940827
64	6	0	6.292199	-0.625211	-0.660324
65	1	0	6.211631	-3.242170	-1.227310
66	1	0	4.426486	-3.549894	-0.916846
67	1	0	7.201270	-1.151085	-0.953761
68	1	0	6.144285	0.206357	-1.354376
69	1	0	6.458098	-0.181702	0.327107
70	1	0	4.214203	1.844237	0.823399
71	1	0	2.490531	2.005332	0.710081
72	1	0	2.764966	2.040492	-1.864119
73	1	0	4.424554	1.616184	-1.627444
74	8	0	2.805597	-3.744337	1.885705
75	1	0	3.909828	-2.096944	2.177124
76	6	0	1.456847	-0.386530	2.739582
77	1	0	1.210521	0.515931	3.299555
78	1	0	0.674947	-1.131370	2.900790
79	1	0	2.405901	-0.779169	3.118940
80	6	0	-4.603658	-3.062185	0.172755
81	1	0	-5.609471	-2.820209	0.521363
82	1	0	-4.703772	-3.530559	-0.809686
83	1	0	-4.208150	-3.809250	0.860882
84	1	0	4.758284	6.012942	0.576259
85	1	0	3.021614	6.144547	0.921270
86	1	0	4.182813	5.957610	2.270355

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960672	0.216039	-1.156766
2	6	0	0.435481	0.859981	-1.054185
3	1	0	-0.982700	-0.352123	-2.087514
4	1	0	-1.708649	1.006874	-1.256627
5	1	0	0.482298	1.578226	-0.234891
6	1	0	0.630336	1.417404	-1.975493
7	6	0	3.653015	-1.092603	-0.110954
8	6	0	2.477561	-1.976598	0.395062
9	6	0	1.270851	-0.984345	0.466332
10	6	0	1.478481	-0.236318	-0.866440
11	6	0	2.863408	-2.736518	1.642851
12	1	0	2.200406	-2.728946	-0.344552
13	8	0	1.440340	-0.006389	1.510473
14	6	0	-1.978924	-2.979843	0.712067
15	6	0	-2.428453	-1.842395	-0.257195
16	6	0	-1.326587	-0.702644	0.042596
17	6	0	-0.121945	-1.566722	0.477659
18	6	0	-0.498875	-2.784618	0.854332
19	1	0	-2.468784	-2.891496	1.690683
20	1	0	-2.237362	-3.971205	0.330536
21	6	0	-2.286946	-2.392410	-1.690812
22	6	0	-1.744477	0.198199	1.229185
23	1	0	0.162832	-3.552775	1.234261
24	1	0	-2.577856	-1.671860	-2.455675
25	1	0	-1.257963	-2.694968	-1.893376
26	1	0	-2.913868	-3.276442	-1.819896
27	1	0	-0.930918	0.872928	1.492482
28	1	0	-2.615805	0.808305	0.988157
29	1	0	-1.984124	-0.388174	2.118365
30	6	0	-3.910351	-1.431904	0.024809
31	6	0	-4.441467	-0.349171	-0.939900
32	6	0	-5.693674	0.376045	-0.474330
33	6	0	-6.240485	1.419856	-1.459526
34	6	0	-6.842339	2.496656	-0.548380
35	6	0	-6.051151	2.323967	0.746316
36	8	0	-5.396957	1.132350	0.735007
37	1	0	-6.476600	-0.337575	-0.204245
38	1	0	-6.963009	0.984018	-2.151094
39	1	0	-5.418219	1.832737	-2.049443
40	1	0	-6.655497	3.505083	-0.919917
41	6	0	-8.345381	2.338671	-0.275583
42	1	0	-3.934912	-1.009593	1.031214
43	1	0	-4.673444	-0.799306	-1.911730
44	1	0	-3.681103	0.410656	-1.126923
45	8	0	-5.988484	3.079590	1.674252
46	1	0	-8.677381	3.063355	0.468973
47	1	0	-8.914399	2.500833	-1.193262
48	1	0	-8.582982	1.338955	0.096900
49	1	0	1.265344	-0.993946	-1.630710
50	6	0	3.001324	0.064527	-1.001109
51	6	0	3.400677	0.026490	-2.486214

52	6	0	3.349670	1.462573	-0.426790
53	1	0	4.482970	0.030684	-2.621585
54	1	0	3.009247	-0.855897	-2.993968
55	1	0	2.997068	0.901281	-3.003745
56	6	0	4.822522	1.867881	-0.503419
57	6	0	5.062844	3.273140	0.002794
58	8	0	4.221809	4.121197	0.167692
59	8	0	6.378610	3.483667	0.236105
60	6	0	6.728358	4.806856	0.678433
61	6	0	4.792259	-1.910728	-0.701524
62	1	0	4.061568	-0.594287	0.771448
63	6	0	6.052423	-1.688022	-0.326818
64	6	0	4.477064	-3.032048	-1.663273
65	1	0	6.875048	-2.266834	-0.731183
66	1	0	6.309224	-0.927279	0.401251
67	1	0	5.388447	-3.409080	-2.128514
68	1	0	4.001762	-3.870187	-1.144408
69	1	0	3.794448	-2.723380	-2.456363
70	1	0	5.195836	1.845698	-1.532203
71	1	0	5.471715	1.194490	0.057666
72	1	0	3.020361	1.514847	0.610434
73	1	0	2.768421	2.213744	-0.965804
74	8	0	2.509486	-3.862707	1.898645
75	1	0	3.554522	-2.206765	2.330193
76	6	0	1.217970	-0.407794	2.855055
77	1	0	1.050486	0.505761	3.425857
78	1	0	0.344707	-1.055650	2.953168
79	1	0	2.088908	-0.921592	3.274710
80	6	0	-4.866743	-2.639520	0.032592
81	1	0	-5.872846	-2.335803	0.328781
82	1	0	-4.946145	-3.106205	-0.952446
83	1	0	-4.550783	-3.405356	0.741004
84	1	0	7.807470	4.794147	0.809289
85	1	0	6.440751	5.547016	-0.068017
86	1	0	6.230116	5.037936	1.619631

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.902836	0.191249	-1.148367
2	6	0	0.479725	0.862051	-1.033472
3	1	0	-0.911433	-0.363153	-2.087529
4	1	0	-1.666756	0.968000	-1.237511
5	1	0	0.509075	1.566162	-0.200992
6	1	0	0.663620	1.438780	-1.945227
7	6	0	3.736081	-1.044979	-0.120664
8	6	0	2.576355	-1.956549	0.372578
9	6	0	1.350663	-0.989332	0.457459
10	6	0	1.545651	-0.214925	-0.861995
11	6	0	2.976002	-2.729302	1.608875
12	1	0	2.313233	-2.702581	-0.378558
13	8	0	1.497676	-0.023184	1.515608
14	6	0	-1.859206	-3.052360	0.668648
15	6	0	-2.331067	-1.908521	-0.282076
16	6	0	-1.251247	-0.752731	0.036179
17	6	0	-0.030257	-1.599629	0.457739
18	6	0	-0.383240	-2.830721	0.814250
19	1	0	-2.350148	-2.989588	1.648665
20	1	0	-2.098470	-4.042325	0.271320
21	6	0	-2.179673	-2.432511	-1.724420
22	6	0	-1.687773	0.121206	1.236137
23	1	0	0.293673	-3.591627	1.181833
24	1	0	-2.482024	-1.704348	-2.477534
25	1	0	-1.145847	-2.715145	-1.931071
26	1	0	-2.791938	-3.324406	-1.868537
27	1	0	-0.886355	0.804816	1.513072
28	1	0	-2.569059	0.719844	1.002564
29	1	0	-1.918742	-0.483703	2.115141
30	6	0	-3.820794	-1.530965	0.005381
31	6	0	-4.374953	-0.450032	-0.948835
32	6	0	-5.625984	0.263670	-0.462894
33	6	0	-6.210160	1.287234	-1.447895
34	6	0	-6.802393	2.369255	-0.536763
35	6	0	-5.975505	2.225223	0.738889
36	8	0	-5.310243	1.039812	0.729183
37	1	0	-6.392097	-0.456863	-0.164411
38	1	0	-6.944073	0.833125	-2.115269
39	1	0	-5.408013	1.701782	-2.063847
40	1	0	-6.638668	3.374586	-0.927163
41	6	0	-8.295653	2.195891	-0.222634
42	1	0	-3.853593	-1.119959	1.016186
43	1	0	-4.616846	-0.900704	-1.917966
44	1	0	-3.624518	0.317248	-1.145516
45	8	0	-5.894968	2.996693	1.652362
46	1	0	-8.617581	2.926024	0.521017
47	1	0	-8.890367	2.338979	-1.127089
48	1	0	-8.510618	1.198205	0.168507
49	1	0	1.351183	-0.962718	-1.640756
50	6	0	3.062930	0.118290	-0.986052
51	6	0	3.468525	0.129184	-2.469225

52	6	0	3.385389	1.505012	-0.369501
53	1	0	4.551200	0.155777	-2.597991
54	1	0	3.093740	-0.745373	-3.002219
55	1	0	3.053544	1.011350	-2.964931
56	6	0	4.855862	1.957544	-0.479061
57	6	0	5.065992	3.243378	0.282509
58	8	0	5.427261	3.321705	1.431302
59	8	0	4.768236	4.324621	-0.473269
60	6	0	4.890199	5.597272	0.185884
61	6	0	4.884451	-1.836299	-0.730122
62	1	0	4.141998	-0.556770	0.768337
63	6	0	6.140787	-1.612607	-0.343268
64	6	0	4.582284	-2.936556	-1.720164
65	1	0	6.969898	-2.174575	-0.758110
66	1	0	6.387206	-0.870193	0.407038
67	1	0	5.498424	-3.293303	-2.191985
68	1	0	4.114218	-3.791845	-1.223098
69	1	0	3.898502	-2.615935	-2.507509
70	1	0	5.137992	2.111533	-1.520931
71	1	0	5.524822	1.218001	-0.042387
72	1	0	3.093226	1.499574	0.680196
73	1	0	2.766740	2.256532	-0.867472
74	8	0	2.631875	-3.861468	1.851205
75	1	0	3.666798	-2.203092	2.298808
76	6	0	1.294102	-0.451485	2.855305
77	1	0	0.436265	-1.120510	2.947974
78	1	0	2.179850	-0.950874	3.260334
79	1	0	1.110563	0.448671	3.442035
80	6	0	-4.753351	-2.757084	0.000027
81	1	0	-5.768262	-2.473635	0.286714
82	1	0	-4.813975	-3.221304	-0.987429
83	1	0	-4.430112	-3.519260	0.709128
84	1	0	4.615406	6.339308	-0.559544
85	1	0	4.219944	5.647459	1.043721
86	1	0	5.914245	5.753348	0.524144

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.801400	0.042420	-1.213640
2	6	0	0.576370	0.734840	-1.203740
3	1	0	-0.842870	-0.561710	-2.120590
4	1	0	-1.579320	0.804120	-1.310590
5	1	0	0.627190	1.503870	-0.432320
6	1	0	0.716060	1.238740	-2.164320
7	6	0	3.887610	-0.930970	-0.163510
8	6	0	2.798980	-1.896110	0.360300
9	6	0	1.525570	-0.986320	0.391870
10	6	0	1.654450	-0.322610	-0.993080
11	6	0	3.227440	-2.588610	1.635880
12	1	0	2.581230	-2.687800	-0.359660
13	8	0	1.654620	0.067620	1.367230
14	6	0	-1.621260	-3.111690	0.821330
15	6	0	-2.144450	-2.042310	-0.186720
16	6	0	-1.088780	-0.841650	0.034080
17	6	0	0.164620	-1.632500	0.474940
18	6	0	-0.148360	-2.846870	0.915880
19	1	0	-2.090360	-2.999940	1.807660
20	1	0	-1.844420	-4.129880	0.491680
21	6	0	-2.008790	-2.651750	-1.596800
22	6	0	-1.521390	0.088750	1.192160
23	1	0	0.557060	-3.565460	1.313080
24	1	0	-2.349540	-1.981610	-2.386350
25	1	0	-0.971160	-2.915000	-1.809640
26	1	0	-2.595720	-3.569020	-1.670740
27	1	0	-0.741960	0.821710	1.397060
28	1	0	-2.434810	0.634270	0.953000
29	1	0	-1.697240	-0.468890	2.114190
30	6	0	-3.637590	-1.685830	0.110720
31	6	0	-4.241290	-0.685170	-0.899050
32	6	0	-5.505170	0.021050	-0.436480
33	6	0	-6.131020	0.967920	-1.471350
34	6	0	-6.741090	2.085840	-0.617070
35	6	0	-5.895540	2.039320	0.653550
36	8	0	-5.196030	0.875030	0.703250
37	1	0	-6.246420	-0.701420	-0.084600
38	1	0	-6.861010	0.455170	-2.099380
39	1	0	-5.349340	1.366610	-2.123000
40	1	0	-6.609080	3.070340	-1.067930
41	6	0	-8.225470	1.892470	-0.273730
42	1	0	-3.659950	-1.209400	1.092800
43	1	0	-4.485410	-1.203790	-1.832970
44	1	0	-3.517420	0.089140	-1.157520
45	8	0	-5.826830	2.864290	1.520140
46	1	0	-8.557790	2.655240	0.431600
47	1	0	-8.834270	1.968540	-1.176940
48	1	0	-8.409530	0.913380	0.175820
49	1	0	1.403010	-1.133940	-1.685430
50	6	0	3.172550	-0.029690	-1.259540
51	6	0	3.486050	-0.514140	-2.689140

52	6	0	3.570240	1.467920	-1.216400
53	1	0	4.528410	-0.342950	-2.963840
54	1	0	3.285630	-1.580630	-2.806250
55	1	0	2.863670	0.025100	-3.409110
56	6	0	3.551990	2.207710	0.121100
57	6	0	3.729250	3.699900	-0.045130
58	8	0	3.637050	4.318300	-1.077010
59	8	0	3.991840	4.287980	1.144230
60	6	0	4.131220	5.719030	1.114870
61	6	0	5.198660	-1.581540	-0.560850
62	1	0	4.119240	-0.271140	0.678380
63	6	0	5.328860	-2.880390	-0.831150
64	6	0	6.399600	-0.669060	-0.595700
65	1	0	6.293070	-3.298510	-1.096490
66	1	0	4.501050	-3.576820	-0.798770
67	1	0	7.304970	-1.212720	-0.867410
68	1	0	6.268230	0.147140	-1.311050
69	1	0	6.561450	-0.203580	0.382250
70	1	0	4.332670	1.859650	0.801020
71	1	0	2.614480	2.048870	0.657550
72	1	0	2.921010	2.006180	-1.910110
73	1	0	4.572230	1.567710	-1.642970
74	8	0	2.845140	-3.677400	1.990960
75	1	0	3.970820	-2.039170	2.249990
76	6	0	1.533400	-0.274730	2.740960
77	1	0	0.728090	-0.991030	2.915930
78	1	0	2.466920	-0.685270	3.139660
79	1	0	1.310200	0.650040	3.273540
80	6	0	-4.535750	-2.933340	0.209290
81	1	0	-5.551050	-2.657590	0.502120
82	1	0	-4.607280	-3.463910	-0.743510
83	1	0	-4.175870	-3.638170	0.958990
84	1	0	4.335540	6.012580	2.141440
85	1	0	4.953950	6.008710	0.461600
86	1	0	3.212330	6.184350	0.758700

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.033548	0.162012	-1.105223
2	6	0	0.345559	0.839687	-0.987782
3	1	0	-1.050885	-0.363228	-2.060693
4	1	0	-1.804713	0.934920	-1.160910
5	1	0	0.379866	1.518508	-0.134773
6	1	0	0.513384	1.444725	-1.884075
7	6	0	3.627110	-1.067123	-0.168395
8	6	0	2.480317	-2.001532	0.311437
9	6	0	1.247792	-1.047948	0.436353
10	6	0	1.421837	-0.233647	-0.861640
11	6	0	2.899172	-2.805465	1.521292
12	1	0	2.215062	-2.727990	-0.457845
13	8	0	1.395960	-0.111381	1.520737
14	6	0	-1.940742	-3.146778	0.614662
15	6	0	-2.435984	-1.974190	-0.288387
16	6	0	-1.360128	-0.821036	0.053335
17	6	0	-0.127481	-1.670593	0.432331
18	6	0	-0.465540	-2.916142	0.750678
19	1	0	-2.420121	-3.125376	1.601983
20	1	0	-2.174730	-4.124083	0.184226
21	6	0	-2.302553	-2.448163	-1.749667
22	6	0	-1.786898	0.010355	1.286285
23	1	0	0.222733	-3.682434	1.084555
24	1	0	-2.616209	-1.695627	-2.473566
25	1	0	-1.271181	-2.721887	-1.979695
26	1	0	-2.915542	-3.335803	-1.915106
27	1	0	-0.987620	0.691273	1.574864
28	1	0	-2.675179	0.610060	1.083661
29	1	0	-2.004129	-0.623044	2.148346
30	6	0	-3.924715	-1.620145	0.034547
31	6	0	-4.503186	-0.510084	-0.870370
32	6	0	-5.788611	0.136787	-0.359600
33	6	0	-6.319776	1.277755	-1.247412
34	6	0	-5.750781	2.543371	-0.598454
35	6	0	-5.525857	2.112893	0.848344
36	8	0	-5.556891	0.757944	0.938269
37	1	0	-6.554329	-0.617935	-0.184808
38	1	0	-7.411823	1.303338	-1.211896
39	1	0	-6.023542	1.154566	-2.289443
40	1	0	-4.750972	2.751148	-0.997972
41	6	0	-6.597421	3.806579	-0.716227
42	1	0	-3.947205	-1.247110	1.059961
43	1	0	-4.725598	-0.921300	-1.860986
44	1	0	-3.766340	0.280523	-1.026430
45	8	0	-5.332102	2.812973	1.801662
46	1	0	-6.154391	4.618063	-0.137997
47	1	0	-6.675186	4.124571	-1.758021
48	1	0	-7.607532	3.635399	-0.336558
49	1	0	1.223823	-0.959485	-1.660018
50	6	0	2.935279	0.114962	-0.992965
51	6	0	3.324003	0.169874	-2.479724

52	6	0	3.253842	1.485684	-0.340391
53	1	0	4.404898	0.207883	-2.620329
54	1	0	2.949077	-0.692607	-3.031905
55	1	0	2.897496	1.062264	-2.946570
56	6	0	4.719014	1.953751	-0.454369
57	6	0	4.928343	3.217708	0.343172
58	8	0	5.292183	3.263481	1.492887
59	8	0	4.626789	4.319674	-0.380448
60	6	0	4.749324	5.573125	0.314530
61	6	0	4.774474	-1.832013	-0.812738
62	1	0	4.039890	-0.600806	0.729249
63	6	0	6.033534	-1.608048	-0.435024
64	6	0	4.469655	-2.909198	-1.827182
65	1	0	6.862046	-2.152252	-0.874028
66	1	0	6.283073	-0.883504	0.331542
67	1	0	5.383821	-3.249374	-2.314769
68	1	0	4.010032	-3.778887	-1.347539
69	1	0	3.777964	-2.573634	-2.601387
70	1	0	4.986835	2.140941	-1.494491
71	1	0	5.399087	1.206963	-0.048183
72	1	0	2.974503	1.446702	0.712094
73	1	0	2.622832	2.246159	-0.808470
74	8	0	2.565459	-3.946284	1.735657
75	1	0	3.593727	-2.293513	2.218102
76	6	0	1.218177	-0.583199	2.849819
77	1	0	0.388830	-1.289012	2.928623
78	1	0	2.126674	-1.056593	3.235145
79	1	0	1.002080	0.291954	3.462761
80	6	0	-4.846913	-2.853869	-0.002475
81	1	0	-5.853220	-2.596409	0.333634
82	1	0	-4.936545	-3.268749	-1.009605
83	1	0	-4.493060	-3.647266	0.655748
84	1	0	4.473181	6.335959	-0.409085
85	1	0	4.080353	5.598659	1.174456
86	1	0	5.773833	5.719839	0.655534

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.943782	0.160880	-1.177805
2	6	0	0.442276	0.832597	-1.131258
3	1	0	-0.971883	-0.448747	-2.081825
4	1	0	-1.707839	0.933168	-1.298672
5	1	0	0.491113	1.584905	-0.343294
6	1	0	0.609251	1.352886	-2.079214
7	6	0	3.711048	-1.028479	-0.172101
8	6	0	2.559909	-1.901405	0.403843
9	6	0	1.338976	-0.925842	0.453859
10	6	0	1.507055	-0.237694	-0.915968
11	6	0	2.983867	-2.595768	1.677553
12	1	0	2.276430	-2.692767	-0.291445
13	8	0	1.510751	0.103236	1.448137
14	6	0	-1.868919	-2.963195	0.854050
15	6	0	-2.356157	-1.881181	-0.158726
16	6	0	-1.270924	-0.709075	0.068442
17	6	0	-0.042742	-1.530238	0.520214
18	6	0	-0.390524	-2.736133	0.958938
19	1	0	-2.342077	-2.837707	1.836714
20	1	0	-2.116268	-3.975547	0.523827
21	6	0	-2.226268	-2.494700	-1.567583
22	6	0	-1.685892	0.236582	1.220657
23	1	0	0.291630	-3.474898	1.360425
24	1	0	-2.541389	-1.814931	-2.359572
25	1	0	-1.194781	-2.787210	-1.772135
26	1	0	-2.838178	-3.395067	-1.646841
27	1	0	-0.883785	0.941475	1.436801
28	1	0	-2.576234	0.814360	0.969836
29	1	0	-1.893955	-0.314170	2.140044
30	6	0	-3.841130	-1.484935	0.127999
31	6	0	-4.411014	-0.469638	-0.886516
32	6	0	-5.669778	0.256184	-0.440832
33	6	0	-6.261292	1.220728	-1.479413
34	6	0	-6.871134	2.339852	-0.626634
35	6	0	-6.047845	2.271715	0.657692
36	8	0	-5.365833	1.096876	0.709865
37	1	0	-6.429854	-0.455376	-0.107543
38	1	0	-6.986441	0.724145	-2.125785
39	1	0	-5.461322	1.613385	-2.112308
40	1	0	-6.718750	3.326118	-1.067032
41	6	0	-8.363446	2.162797	-0.310045
42	1	0	-3.857138	-1.006530	1.109298
43	1	0	-4.649510	-0.979399	-1.826731
44	1	0	-3.669482	0.293015	-1.129448
45	8	0	-5.982086	3.088814	1.531790
46	1	0	-8.698248	2.924539	0.395207
47	1	0	-8.955642	2.253085	-1.222920
48	1	0	-8.567342	1.182870	0.128996
49	1	0	1.290361	-1.032462	-1.640302
50	6	0	3.022248	0.076799	-1.098502
51	6	0	3.389554	-0.018858	-2.588708

52	6	0	3.363401	1.503119	-0.592342
53	1	0	4.468336	-0.007157	-2.748052
54	1	0	2.998017	-0.926992	-3.048465
55	1	0	2.964852	0.828513	-3.133979
56	6	0	4.835641	1.933475	-0.744884
57	6	0	5.007586	3.358084	-0.275391
58	8	0	4.658667	4.335613	-0.891203
59	8	0	5.582243	3.421679	0.946658
60	6	0	5.746048	4.744828	1.487800
61	6	0	4.846172	-1.860233	-0.751590
62	1	0	4.135735	-0.484137	0.674520
63	6	0	6.110927	-1.606705	-0.413594
64	6	0	4.525179	-3.027078	-1.655306
65	1	0	6.932039	-2.193869	-0.808893
66	1	0	6.372439	-0.811003	0.274259
67	1	0	5.431821	-3.414557	-2.121175
68	1	0	4.070456	-3.846480	-1.090137
69	1	0	3.823681	-2.762887	-2.447978
70	1	0	5.136109	1.907678	-1.792862
71	1	0	5.499626	1.283183	-0.178003
72	1	0	3.073238	1.584830	0.455449
73	1	0	2.753798	2.220885	-1.146894
74	8	0	2.648059	-3.711470	1.995865
75	1	0	3.685184	-2.027031	2.321825
76	6	0	1.330031	-0.242210	2.814435
77	1	0	1.145164	0.690662	3.347504
78	1	0	0.480166	-0.911583	2.961489
79	1	0	2.226133	-0.708444	3.236397
80	6	0	-4.771856	-2.708883	0.221679
81	1	0	-5.780092	-2.408059	0.513697
82	1	0	-4.855146	-3.235143	-0.732585
83	1	0	-4.431588	-3.424803	0.969959
84	1	0	6.215762	4.606574	2.458343
85	1	0	6.379496	5.345957	0.836034
86	1	0	4.778397	5.234426	1.594781

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.916276	0.513081	-0.739347
2	6	0	0.422784	1.070123	-0.220523
3	1	0	-0.807738	0.384898	-1.816821
4	1	0	-1.692304	1.269527	-0.594144
5	1	0	0.341962	1.394303	0.818388
6	1	0	0.667229	1.952094	-0.817419
7	6	0	3.608916	-1.065194	0.310012
8	6	0	2.462888	-2.090753	0.176212
9	6	0	1.193314	-1.233819	0.490863
10	6	0	1.507976	0.007319	-0.369739
11	6	0	2.734728	-3.331111	1.000812
12	1	0	2.337634	-2.430811	-0.853396
13	8	0	1.184001	-0.772576	1.858185
14	6	0	-1.945556	-3.173077	-0.507973
15	6	0	-2.357748	-1.736594	-0.955740
16	6	0	-1.356083	-0.823147	-0.082287
17	6	0	-0.155644	-1.780269	0.090325
18	6	0	-0.501069	-3.045875	-0.126107
19	1	0	-2.535244	-3.512342	0.353652
20	1	0	-2.107385	-3.911857	-1.297409
21	6	0	-2.041426	-1.629695	-2.461186
22	6	0	-1.942638	-0.509304	1.314722
23	1	0	0.160064	-3.897217	-0.028792
24	1	0	-2.284884	-0.653364	-2.880351
25	1	0	-0.983718	-1.819729	-2.652315
26	1	0	-2.608476	-2.376135	-3.020158
27	1	0	-1.200260	-0.002629	1.929717
28	1	0	-2.818114	0.137866	1.251245
29	1	0	-2.239640	-1.417823	1.841860
30	6	0	-3.881655	-1.493421	-0.699891
31	6	0	-4.372355	-0.110729	-1.180651
32	6	0	-5.729278	0.321864	-0.629773
33	6	0	-6.168288	1.731548	-1.068762
34	6	0	-5.723459	2.631905	0.088140
35	6	0	-5.676106	1.669141	1.271363
36	8	0	-5.683342	0.386274	0.825262
37	1	0	-6.492331	-0.419861	-0.861942
38	1	0	-7.255636	1.771080	-1.171380
39	1	0	-5.732738	2.012257	-2.028005
40	1	0	-4.686564	2.953568	-0.065863
41	6	0	-6.582514	3.862553	0.359885
42	1	0	-4.031080	-1.532894	0.380551
43	1	0	-4.457247	-0.108064	-2.272687
44	1	0	-3.643974	0.662760	-0.928544
45	8	0	-5.625823	1.940299	2.437846
46	1	0	-6.238647	4.376919	1.257760
47	1	0	-6.535868	4.559703	-0.479328
48	1	0	-7.627541	3.582348	0.511889
49	1	0	1.428417	-0.358390	-1.400398
50	6	0	3.025479	0.339086	-0.177414
51	6	0	3.600712	0.777356	-1.532694

52	6	0	3.329406	1.386499	0.931198
53	1	0	4.656457	1.045072	-1.469590
54	1	0	3.511674	-0.020839	-2.271518
55	1	0	3.061744	1.645527	-1.918524
56	6	0	3.110310	2.881398	0.626089
57	6	0	4.136489	3.576051	-0.242296
58	8	0	3.878511	4.340562	-1.139553
59	8	0	5.403204	3.289696	0.135820
60	6	0	6.438680	3.962978	-0.601701
61	6	0	4.939803	-1.498621	-0.277201
62	1	0	3.777631	-0.952581	1.387153
63	6	0	5.064148	-2.448027	-1.204616
64	6	0	6.162354	-0.817585	0.287302
65	1	0	6.039884	-2.731039	-1.582518
66	1	0	4.219750	-2.981918	-1.620564
67	1	0	6.232633	-0.985895	1.367222
68	1	0	7.075140	-1.193870	-0.176083
69	1	0	6.130074	0.265468	0.143133
70	1	0	3.132873	3.414747	1.583491
71	1	0	2.140195	3.085636	0.181401
72	1	0	4.370300	1.268593	1.237941
73	1	0	2.724803	1.130518	1.801944
74	8	0	2.335191	-4.438896	0.735782
75	1	0	3.380712	-3.177890	1.890516
76	6	0	0.895201	-1.717667	2.878774
77	1	0	0.094619	-2.402528	2.591109
78	1	0	1.781146	-2.301096	3.151311
79	1	0	0.578598	-1.146547	3.751868
80	6	0	-4.764888	-2.600413	-1.306359
81	1	0	-5.809721	-2.463598	-1.021060
82	1	0	-4.723378	-2.605167	-2.398559
83	1	0	-4.473650	-3.590700	-0.956177
84	1	0	7.375033	3.625859	-0.164090
85	1	0	6.389199	3.696426	-1.657264
86	1	0	6.335205	5.043134	-0.502611

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022009	0.150986	-1.103725
2	6	0	0.358606	0.821600	-0.971646
3	1	0	-1.037910	-0.361992	-2.065847
4	1	0	-1.789825	0.927728	-1.152178
5	1	0	0.390692	1.487886	-0.108842
6	1	0	0.531446	1.439380	-1.858324
7	6	0	3.631022	-1.117776	-0.185594
8	6	0	2.479018	-2.045202	0.283658
9	6	0	1.250096	-1.092103	0.426266
10	6	0	1.431070	-0.257242	-0.856586
11	6	0	2.896051	-2.882488	1.473791
12	1	0	2.198910	-2.753289	-0.495872
13	8	0	1.398229	-0.176635	1.528786
14	6	0	-1.952783	-3.174316	0.568076
15	6	0	-2.438848	-1.985930	-0.318851
16	6	0	-1.355861	-0.845233	0.040881
17	6	0	-0.129039	-1.708079	0.409206
18	6	0	-0.476239	-2.955655	0.709563
19	1	0	-2.433327	-3.163964	1.555010
20	1	0	-2.192684	-4.143863	0.123430
21	6	0	-2.305848	-2.440549	-1.786436
22	6	0	-1.778475	-0.029155	1.285456
23	1	0	0.206889	-3.729838	1.035102
24	1	0	-2.611707	-1.675591	-2.500574
25	1	0	-1.276099	-2.719095	-2.017897
26	1	0	-2.925364	-3.321014	-1.965420
27	1	0	-0.972880	0.638068	1.588035
28	1	0	-2.660050	0.582924	1.089786
29	1	0	-2.004763	-0.674572	2.136255
30	6	0	-3.925765	-1.625899	0.005875
31	6	0	-4.494775	-0.501800	-0.887600
32	6	0	-5.777761	0.147673	-0.374129
33	6	0	-6.297104	1.302572	-1.250889
34	6	0	-5.720559	2.556145	-0.585589
35	6	0	-5.506315	2.107911	0.857423
36	8	0	-5.547377	0.752298	0.931819
37	1	0	-6.549364	-0.603714	-0.211274
38	1	0	-7.389055	1.336287	-1.218895
39	1	0	-5.998069	1.188852	-2.293197
40	1	0	-4.716994	2.759348	-0.978004
41	6	0	-6.555378	3.828002	-0.693726
42	1	0	-3.947714	-1.264255	1.035368
43	1	0	-4.716654	-0.900112	-1.883596
44	1	0	-3.752361	0.285740	-1.032280
45	8	0	-5.312681	2.795940	1.819519
46	1	0	-6.108299	4.629010	-0.104106
47	1	0	-6.624734	4.158317	-1.732287
48	1	0	-7.568998	3.661659	-0.321326
49	1	0	1.237980	-0.968472	-1.669014
50	6	0	2.946763	0.096293	-0.973505
51	6	0	3.324284	0.152756	-2.461629

52	6	0	3.232819	1.463632	-0.299727
53	1	0	4.380975	0.369085	-2.622986
54	1	0	3.109536	-0.792001	-2.962818
55	1	0	2.750272	0.937699	-2.962122
56	6	0	4.697780	1.940059	-0.286351
57	6	0	4.808882	3.262069	0.434979
58	8	0	5.048356	3.395350	1.609933
59	8	0	4.575953	4.303437	-0.395261
60	6	0	4.610102	5.605583	0.215516
61	6	0	4.761578	-1.862480	-0.887262
62	1	0	4.066671	-0.684798	0.721643
63	6	0	4.593527	-3.006352	-1.551060
64	6	0	6.141472	-1.263086	-0.773464
65	1	0	5.434145	-3.499394	-2.025317
66	1	0	3.636903	-3.501476	-1.652726
67	1	0	6.890846	-1.912429	-1.227145
68	1	0	6.204889	-0.287642	-1.261650
69	1	0	6.414830	-1.108384	0.275392
70	1	0	5.081802	2.057939	-1.300393
71	1	0	5.329255	1.237397	0.254535
72	1	0	2.871829	1.426498	0.727572
73	1	0	2.641615	2.223922	-0.817387
74	8	0	2.482897	-3.990234	1.716245
75	1	0	3.664878	-2.424704	2.131308
76	6	0	1.247541	-0.686127	2.846744
77	1	0	2.164911	-1.168063	3.200381
78	1	0	1.041929	0.170611	3.488535
79	1	0	0.421832	-1.396960	2.921022
80	6	0	-4.855885	-2.853009	-0.047014
81	1	0	-5.861458	-2.592811	0.289228
82	1	0	-4.945299	-3.256441	-1.058819
83	1	0	-4.508500	-3.655615	0.603418
84	1	0	4.399745	6.309127	-0.586035
85	1	0	3.856262	5.677937	0.999100
86	1	0	5.592254	5.797035	0.646985

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028842	0.533532	-0.832104
2	6	0	0.315304	1.114791	-0.356523
3	1	0	-0.926034	0.316202	-1.895760
4	1	0	-1.799728	1.304067	-0.745858
5	1	0	0.237651	1.503675	0.659450
6	1	0	0.579002	1.959169	-1.000195
7	6	0	3.512869	-1.020162	0.199092
8	6	0	2.330494	-2.024390	0.250953
9	6	0	1.076693	-1.136185	0.523194
10	6	0	1.385812	0.030634	-0.435419
11	6	0	2.626816	-3.177469	1.185854
12	1	0	2.151399	-2.472893	-0.726095
13	8	0	1.083053	-0.585369	1.855998
14	6	0	-2.088567	-3.115133	-0.303156
15	6	0	-2.493742	-1.712606	-0.854147
16	6	0	-1.473669	-0.742899	-0.065181
17	6	0	-0.281651	-1.697343	0.173298
18	6	0	-0.640465	-2.972193	0.057277
19	1	0	-2.673948	-3.385207	0.585508
20	1	0	-2.262698	-3.909531	-1.033991
21	6	0	-2.196663	-1.723492	-2.366946
22	6	0	-2.043412	-0.312222	1.307295
23	1	0	0.013831	-3.819679	0.217200
24	1	0	-2.443139	-0.781327	-2.857133
25	1	0	-1.142019	-1.931609	-2.556035
26	1	0	-2.773165	-2.508695	-2.859119
27	1	0	-1.289315	0.230959	1.874729
28	1	0	-2.910767	0.340052	1.199460
29	1	0	-2.348217	-1.171612	1.907364
30	6	0	-4.012646	-1.439451	-0.598654
31	6	0	-4.499888	-0.088643	-1.166492
32	6	0	-5.848534	0.388938	-0.632867
33	6	0	-6.282677	1.768787	-1.161760
34	6	0	-5.810516	2.741787	-0.076761
35	6	0	-5.762942	1.863204	1.170120
36	8	0	-5.788375	0.552558	0.814076
37	1	0	-6.618358	-0.361688	-0.806680
38	1	0	-7.371333	1.811966	-1.248413
39	1	0	-5.861614	1.978893	-2.145318
40	1	0	-4.770851	3.035306	-0.265198
41	6	0	-6.647882	4.001693	0.117017
42	1	0	-4.149623	-1.404884	0.483632
43	1	0	-4.596266	-0.158810	-2.255258
44	1	0	-3.764625	0.695304	-0.974488
45	8	0	-5.699694	2.213822	2.314530
46	1	0	-6.285066	4.573605	0.971650
47	1	0	-6.602232	4.636671	-0.770254
48	1	0	-7.694803	3.749142	0.301202
49	1	0	1.295817	-0.415158	-1.433584
50	6	0	2.898939	0.380927	-0.277727
51	6	0	3.441065	0.846651	-1.636752

52	6	0	3.080109	1.490111	0.792393
53	1	0	4.510205	1.062962	-1.610385
54	1	0	3.289947	0.085341	-2.403581
55	1	0	2.931940	1.759766	-1.952627
56	6	0	4.503019	1.984379	1.088934
57	6	0	5.030461	3.017362	0.117217
58	8	0	4.377693	3.893257	-0.393596
59	8	0	6.361275	2.877927	-0.081888
60	6	0	6.971209	3.867782	-0.930435
61	6	0	4.724966	-1.560649	-0.553464
62	1	0	3.838559	-0.871749	1.234734
63	6	0	4.644458	-2.457912	-1.536297
64	6	0	6.079120	-1.062575	-0.111856
65	1	0	5.538742	-2.818089	-2.031431
66	1	0	3.709673	-2.871342	-1.890904
67	1	0	6.879656	-1.598564	-0.622948
68	1	0	6.212950	0.003017	-0.313933
69	1	0	6.213531	-1.199819	0.966286
70	1	0	5.224042	1.175511	1.190068
71	1	0	4.488177	2.496658	2.058016
72	1	0	2.644811	1.131241	1.723717
73	1	0	2.496115	2.361854	0.489970
74	8	0	2.203531	-4.299998	1.054291
75	1	0	3.315157	-2.944108	2.025853
76	6	0	0.792252	-1.458260	2.938490
77	1	0	0.482263	-0.828010	3.772426
78	1	0	-0.012745	-2.156387	2.699460
79	1	0	1.675951	-2.027650	3.245945
80	6	0	-4.912189	-2.577234	-1.118558
81	1	0	-5.951264	-2.415765	-0.825072
82	1	0	-4.889379	-2.651674	-2.208834
83	1	0	-4.620315	-3.545225	-0.711332
84	1	0	6.836796	4.863797	-0.509359
85	1	0	8.025770	3.607076	-0.970092
86	1	0	6.529848	3.839097	-1.926289

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.772208	0.226223	-1.109993
2	6	0	0.614874	0.862206	-0.894629
3	1	0	-0.757931	-0.236167	-2.097634
4	1	0	-1.521164	1.021440	-1.149811
5	1	0	0.628056	1.497747	-0.007912
6	1	0	0.822820	1.504253	-1.754451
7	6	0	3.801185	-1.130935	0.042706
8	6	0	2.632880	-2.103112	0.311824
9	6	0	1.406508	-1.139265	0.437250
10	6	0	1.668183	-0.237085	-0.786357
11	6	0	2.946932	-3.039887	1.458511
12	1	0	2.420628	-2.737058	-0.551046
13	8	0	1.520286	-0.278869	1.588666
14	6	0	-1.830027	-3.168183	0.320801
15	6	0	-2.263048	-1.916964	-0.504875
16	6	0	-1.173956	-0.821507	-0.036934
17	6	0	0.021185	-1.727842	0.326964
18	6	0	-0.357064	-2.985706	0.532707
19	1	0	-2.348337	-3.212492	1.287512
20	1	0	-2.067474	-4.102667	-0.194761
21	6	0	-2.086334	-2.280786	-1.993117
22	6	0	-1.634286	-0.066536	1.232640
23	1	0	0.299381	-3.792122	0.832964
24	1	0	-2.357950	-1.467232	-2.666275
25	1	0	-1.052816	-2.558806	-2.207963
26	1	0	-2.709548	-3.139356	-2.249189
27	1	0	-0.834338	0.575473	1.598199
28	1	0	-2.503208	0.563417	1.038051
29	1	0	-1.896260	-0.754387	2.038943
30	6	0	-3.753789	-1.550186	-0.208214
31	6	0	-4.265523	-0.348787	-1.033156
32	6	0	-5.544345	0.293525	-0.520362
33	6	0	-6.050885	1.481699	-1.351967
34	6	0	-6.702043	2.400868	-0.311222
35	6	0	-5.977549	2.019634	0.977804
36	8	0	-5.313333	0.845882	0.807557
37	1	0	-6.333706	-0.454408	-0.407302
38	1	0	-6.737804	1.162834	-2.137264
39	1	0	-5.204489	1.981888	-1.829612
40	1	0	-6.499647	3.454930	-0.506044
41	6	0	-8.216713	2.209271	-0.145427
42	1	0	-3.804782	-1.263619	0.843868
43	1	0	-4.455863	-0.660968	-2.066202
44	1	0	-3.508422	0.435332	-1.082655
45	8	0	-5.969765	2.614351	2.018061
46	1	0	-8.588705	2.804905	0.689168
47	1	0	-8.737724	2.522140	-1.052566
48	1	0	-8.470693	1.163595	0.046052
49	1	0	1.500889	-0.898525	-1.645128
50	6	0	3.199685	0.077821	-0.813342
51	6	0	3.676026	0.057045	-2.273914

52	6	0	3.616319	1.402632	-0.115251
53	1	0	4.728199	0.332137	-2.373208
54	1	0	3.554091	-0.934737	-2.711774
55	1	0	3.094766	0.757858	-2.878365
56	6	0	3.406594	2.714747	-0.899957
57	6	0	3.889449	3.895575	-0.091784
58	8	0	3.188948	4.633793	0.555747
59	8	0	5.235132	4.023475	-0.157264
60	6	0	5.796234	5.099180	0.615301
61	6	0	5.076167	-1.772620	-0.472964
62	1	0	4.052815	-0.698807	1.017729
63	6	0	5.115486	-2.965677	-1.066310
64	6	0	6.349735	-0.997949	-0.237312
65	1	0	6.055376	-3.387233	-1.403719
66	1	0	4.234791	-3.571207	-1.236306
67	1	0	7.219097	-1.542689	-0.607141
68	1	0	6.330835	-0.021526	-0.728539
69	1	0	6.494447	-0.806707	0.831106
70	1	0	2.355626	2.890329	-1.114551
71	1	0	3.959480	2.688885	-1.840146
72	1	0	4.682583	1.334868	0.114718
73	1	0	3.094202	1.468981	0.840411
74	8	0	2.519970	-4.163546	1.569087
75	1	0	3.651326	-2.642407	2.218767
76	6	0	1.295034	-0.846175	2.871611
77	1	0	0.465394	-1.556327	2.867368
78	1	0	2.190432	-1.348181	3.253611
79	1	0	1.053876	-0.019292	3.539853
80	6	0	-4.703058	-2.750357	-0.384144
81	1	0	-5.715032	-2.495174	-0.063277
82	1	0	-4.764534	-3.074992	-1.425904
83	1	0	-4.391882	-3.605981	0.215157
84	1	0	6.869482	5.048489	0.449660
85	1	0	5.400369	6.056522	0.277221
86	1	0	5.563540	4.971169	1.672216

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.010514	0.536273	-0.813797
2	6	0	0.339164	1.106279	-0.338798
3	1	0	-0.912728	0.328575	-1.879827
4	1	0	-1.777012	1.309992	-0.717664
5	1	0	0.269457	1.489255	0.680020
6	1	0	0.606321	1.952579	-0.978416
7	6	0	3.518709	-1.038658	0.240209
8	6	0	2.336753	-2.049032	0.262673
9	6	0	1.086731	-1.150869	0.530426
10	6	0	1.401397	0.015297	-0.427735
11	6	0	2.615649	-3.198841	1.202809
12	1	0	2.178198	-2.493154	-0.721072
13	8	0	1.098163	-0.596991	1.861743
14	6	0	-2.081685	-3.115237	-0.311236
15	6	0	-2.481009	-1.708073	-0.855546
16	6	0	-1.461193	-0.745296	-0.057427
17	6	0	-0.272874	-1.704802	0.178996
18	6	0	-0.634266	-2.978019	0.054365
19	1	0	-2.670802	-3.388548	0.573927
20	1	0	-2.255632	-3.904816	-1.047257
21	6	0	-2.178654	-1.710980	-2.367250
22	6	0	-2.034641	-0.321074	1.315516
23	1	0	0.017128	-3.829135	0.208088
24	1	0	-2.421933	-0.765599	-2.852728
25	1	0	-1.123732	-1.919901	-2.553959
26	1	0	-2.754825	-2.492320	-2.865907
27	1	0	-1.283064	0.222594	1.885845
28	1	0	-2.902811	0.329969	1.207844
29	1	0	-2.339389	-1.182715	1.912341
30	6	0	-3.999975	-1.432717	-0.603575
31	6	0	-4.481761	-0.077017	-1.164414
32	6	0	-5.830143	0.401082	-0.630533
33	6	0	-6.259347	1.785545	-1.151355
34	6	0	-5.788095	2.750201	-0.058512
35	6	0	-5.745001	1.863140	1.182490
36	8	0	-5.772410	0.554899	0.817515
37	1	0	-6.601728	-0.346204	-0.810923
38	1	0	-7.347617	1.831909	-1.241017
39	1	0	-5.834804	2.001139	-2.132221
40	1	0	-4.747508	3.043307	-0.242386
41	6	0	-6.623846	4.010147	0.141941
42	1	0	-4.140488	-1.404668	0.478439
43	1	0	-4.576131	-0.140510	-2.253760
44	1	0	-3.744455	0.703516	-0.966270
45	8	0	-5.683359	2.205737	2.329379
46	1	0	-6.262052	4.575535	1.001322
47	1	0	-6.575040	4.651129	-0.740828
48	1	0	-7.671608	3.758075	0.321937
49	1	0	1.299927	-0.428247	-1.425863
50	6	0	2.917110	0.348728	-0.280328
51	6	0	3.468267	0.812073	-1.638571

52	6	0	3.147883	1.464856	0.772596
53	1	0	4.557019	0.894230	-1.634625
54	1	0	3.194112	0.127819	-2.442683
55	1	0	3.064724	1.794740	-1.889981
56	6	0	4.597529	1.937933	0.959144
57	6	0	5.008379	3.089976	0.066618
58	8	0	4.265219	3.896420	-0.436170
59	8	0	6.351970	3.144222	-0.065939
60	6	0	6.859914	4.251571	-0.830694
61	6	0	4.761027	-1.606207	-0.431864
62	1	0	3.793862	-0.866537	1.283683
63	6	0	5.948986	-1.527795	0.169418
64	6	0	4.628098	-2.338754	-1.746048
65	1	0	6.843664	-1.936746	-0.286052
66	1	0	6.070974	-1.060427	1.139840
67	1	0	5.610508	-2.559397	-2.164868
68	1	0	4.107218	-3.291549	-1.610739
69	1	0	4.063482	-1.772487	-2.488119
70	1	0	5.326202	1.135572	0.848259
71	1	0	4.723786	2.315771	1.980340
72	1	0	2.765566	1.113622	1.729890
73	1	0	2.552526	2.338040	0.498762
74	8	0	2.288432	-4.344198	1.002838
75	1	0	3.198783	-2.943906	2.111353
76	6	0	0.767657	-1.451228	2.948615
77	1	0	1.640839	-2.010257	3.300407
78	1	0	0.422061	-0.808181	3.758582
79	1	0	-0.025169	-2.156541	2.691432
80	6	0	-4.900624	-2.564787	-1.133900
81	1	0	-5.940167	-2.402719	-0.842467
82	1	0	-4.874688	-2.631773	-2.224591
83	1	0	-4.612438	-3.536278	-0.732403
84	1	0	7.940570	4.133760	-0.830222
85	1	0	6.470844	4.222003	-1.848108
86	1	0	6.576183	5.196483	-0.367676

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.801400	0.042419	-1.213639
2	6	0	0.576373	0.734845	-1.203739
3	1	0	-0.842868	-0.561707	-2.120592
4	1	0	-1.579313	0.804123	-1.310579
5	1	0	0.627198	1.503874	-0.432316
6	1	0	0.716058	1.238746	-2.164313
7	6	0	3.887611	-0.930966	-0.163509
8	6	0	2.798989	-1.896112	0.360303
9	6	0	1.525573	-0.986315	0.391869
10	6	0	1.654453	-0.322612	-0.993084
11	6	0	3.227439	-2.588603	1.635887
12	1	0	2.581237	-2.687802	-0.359660
13	8	0	1.654621	0.067621	1.367234
14	6	0	-1.621254	-3.111689	0.821325
15	6	0	-2.144441	-2.042310	-0.186725
16	6	0	-1.088771	-0.841647	0.034079
17	6	0	0.164622	-1.632496	0.474938
18	6	0	-0.148353	-2.846872	0.915871
19	1	0	-2.090359	-2.999941	1.807654
20	1	0	-1.844412	-4.129884	0.491677
21	6	0	-2.008789	-2.651750	-1.596800
22	6	0	-1.521384	0.088746	1.192165
23	1	0	0.557062	-3.565464	1.313069
24	1	0	-2.349532	-1.981601	-2.386350
25	1	0	-0.971150	-2.914994	-1.809647
26	1	0	-2.595714	-3.569019	-1.670751
27	1	0	-0.741957	0.821705	1.397065
28	1	0	-2.434810	0.634262	0.953010
29	1	0	-1.697239	-0.468898	2.114192
30	6	0	-3.637583	-1.685834	0.110716
31	6	0	-4.241290	-0.685175	-0.899056
32	6	0	-5.505165	0.021042	-0.436482
33	6	0	-6.131023	0.967910	-1.471348
34	6	0	-6.741101	2.085836	-0.617073
35	6	0	-5.895547	2.039314	0.653549
36	8	0	-5.196033	0.875031	0.703248
37	1	0	-6.246413	-0.701423	-0.084597
38	1	0	-6.861013	0.455160	-2.099384
39	1	0	-5.349340	1.366603	-2.123003
40	1	0	-6.609086	3.070329	-1.067929
41	6	0	-8.225477	1.892451	-0.273739
42	1	0	-3.659945	-1.209401	1.092795
43	1	0	-4.485410	-1.203795	-1.832968
44	1	0	-3.517414	0.089135	-1.157521
45	8	0	-5.826838	2.864281	1.520141
46	1	0	-8.557800	2.655228	0.431592
47	1	0	-8.834275	1.968529	-1.176945
48	1	0	-8.409537	0.913363	0.175814
49	1	0	1.403019	-1.133934	-1.685435
50	6	0	3.172554	-0.029683	-1.259544
51	6	0	3.486057	-0.514139	-2.689145

52	6	0	3.570242	1.467921	-1.216403
53	1	0	4.528415	-0.342948	-2.963842
54	1	0	3.285632	-1.580626	-2.806253
55	1	0	2.863679	0.025100	-3.409105
56	6	0	3.551992	2.207707	0.121102
57	6	0	3.729235	3.699898	-0.045130
58	8	0	3.637030	4.318307	-1.077005
59	8	0	3.991828	4.287984	1.144232
60	6	0	4.131189	5.719031	1.114879
61	6	0	5.198668	-1.581534	-0.560849
62	1	0	4.119243	-0.271136	0.678382
63	6	0	5.328860	-2.880385	-0.831155
64	6	0	6.399602	-0.669055	-0.595701
65	1	0	6.293072	-3.298507	-1.096489
66	1	0	4.501052	-3.576819	-0.798766
67	1	0	7.304969	-1.212711	-0.867428
68	1	0	6.268231	0.147154	-1.311040
69	1	0	6.561466	-0.203594	0.382255
70	1	0	4.332683	1.859662	0.801014
71	1	0	2.614485	2.048863	0.657563
72	1	0	2.921002	2.006186	-1.910104
73	1	0	4.572227	1.567714	-1.642978
74	8	0	2.845136	-3.677395	1.990969
75	1	0	3.970815	-2.039161	2.249997
76	6	0	1.533409	-0.274728	2.740964
77	1	0	0.728157	-0.991093	2.915928
78	1	0	2.466961	-0.685204	3.139671
79	1	0	1.310137	0.650025	3.273539
80	6	0	-4.535742	-2.933336	0.209284
81	1	0	-5.551042	-2.657585	0.502114
82	1	0	-4.607270	-3.463910	-0.743511
83	1	0	-4.175863	-3.638165	0.958994
84	1	0	4.953917	6.008730	0.461610
85	1	0	3.212292	6.184342	0.758718
86	1	0	4.335511	6.012585	2.141452

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002358	0.148951	-1.160396
2	6	0	0.393807	0.795248	-1.089155
3	1	0	-1.031646	-0.447616	-2.073008
4	1	0	-1.752376	0.935294	-1.277850
5	1	0	0.446778	1.539170	-0.293788
6	1	0	0.581149	1.322065	-2.029436
7	6	0	3.625085	-1.171158	-0.186898
8	6	0	2.463677	-1.965587	0.460246
9	6	0	1.244518	-0.991930	0.490028
10	6	0	1.438404	-0.293793	-0.871676
11	6	0	2.866155	-2.649780	1.746290
12	1	0	2.149748	-2.786770	-0.193578
13	8	0	1.393341	0.029394	1.494977
14	6	0	-2.012822	-2.984310	0.814840
15	6	0	-2.463844	-1.878837	-0.189021
16	6	0	-1.358873	-0.732045	0.069525
17	6	0	-0.149049	-1.580181	0.525438
18	6	0	-0.532353	-2.783213	0.941203
19	1	0	-2.497945	-2.862671	1.792030
20	1	0	-2.273891	-3.987004	0.466137
21	6	0	-2.328402	-2.475470	-1.604551
22	6	0	-1.768374	0.202729	1.232671
23	1	0	0.119652	-3.547158	1.346443
24	1	0	-2.624567	-1.780192	-2.390208
25	1	0	-1.299685	-2.781228	-1.803637
26	1	0	-2.954158	-3.364428	-1.702302
27	1	0	-0.954871	0.887432	1.467981
28	1	0	-2.644610	0.801116	0.980885
29	1	0	-1.997927	-0.357935	2.140977
30	6	0	-3.944226	-1.457860	0.086125
31	6	0	-4.477275	-0.404274	-0.909016
32	6	0	-5.737616	0.323326	-0.469917
33	6	0	-6.279237	1.344951	-1.480892
34	6	0	-6.897194	2.435098	-0.596743
35	6	0	-6.119016	2.291904	0.709370
36	8	0	-5.457215	1.104091	0.727374
37	1	0	-6.520030	-0.388900	-0.194818
38	1	0	-6.991620	0.891850	-2.171858
39	1	0	-5.452957	1.751573	-2.069536
40	1	0	-6.712226	3.437388	-0.985397
41	6	0	-8.402153	2.273187	-0.337215
42	1	0	-3.963845	-1.004154	1.078925
43	1	0	-4.699829	-0.880047	-1.870746
44	1	0	-3.720879	0.355857	-1.109674
45	8	0	-6.070880	3.064676	1.623722
46	1	0	-8.746565	3.010046	0.389511
47	1	0	-8.961915	2.414160	-1.264018
48	1	0	-8.637933	1.279385	0.051902
49	1	0	1.222116	-1.080459	-1.606384
50	6	0	2.958583	0.006567	-1.036845
51	6	0	3.308190	-0.025450	-2.533226

52	6	0	3.316130	1.399809	-0.456080
53	1	0	4.376866	0.095491	-2.714967
54	1	0	3.012660	-0.966435	-2.997598
55	1	0	2.791810	0.786141	-3.053782
56	6	0	4.789896	1.800609	-0.522777
57	6	0	5.031088	3.210105	-0.027103
58	8	0	4.187193	4.047599	0.172597
59	8	0	6.352529	3.436404	0.153356
60	6	0	6.703229	4.760430	0.591617
61	6	0	4.631422	-2.064355	-0.904562
62	1	0	4.165966	-0.706197	0.638579
63	6	0	4.289755	-3.116132	-1.647592
64	6	0	6.081452	-1.701471	-0.720204
65	1	0	5.042692	-3.720483	-2.139963
66	1	0	3.261628	-3.421090	-1.804756
67	1	0	6.739358	-2.407431	-1.228432
68	1	0	6.296761	-0.701429	-1.108074
69	1	0	6.336611	-1.692627	0.343774
70	1	0	5.178051	1.767112	-1.545878
71	1	0	5.428486	1.134231	0.060507
72	1	0	2.987227	1.449341	0.580646
73	1	0	2.739447	2.157064	-0.991824
74	8	0	3.964916	-2.590656	2.242586
75	1	0	2.083518	-3.273000	2.223911
76	6	0	1.235373	-0.336032	2.859437
77	1	0	0.376711	-0.994932	3.011172
78	1	0	2.134109	-0.813564	3.258522
79	1	0	1.067863	0.591826	3.406664
80	6	0	-4.901714	-2.663660	0.135509
81	1	0	-5.904100	-2.350744	0.434180
82	1	0	-4.992086	-3.156208	-0.835927
83	1	0	-4.580151	-3.411185	0.860871
84	1	0	7.786647	4.759900	0.681020
85	1	0	6.378409	5.502371	-0.137683
86	1	0	6.238924	4.978753	1.552995

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.074231	0.190309	-1.137446
2	6	0	0.320540	0.836045	-1.027080
3	1	0	-1.099278	-0.356093	-2.080809
4	1	0	-1.825779	0.980387	-1.216603
5	1	0	0.369257	1.536053	-0.192215
6	1	0	0.509344	1.414322	-1.936690
7	6	0	3.548218	-1.124894	-0.137927
8	6	0	2.378067	-2.025110	0.350650
9	6	0	1.167646	-1.039895	0.446905
10	6	0	1.367890	-0.261001	-0.869252
11	6	0	2.769748	-2.811698	1.580115
12	1	0	2.102570	-2.761439	-0.405516
13	8	0	1.335857	-0.084241	1.511892
14	6	0	-2.073204	-3.055025	0.652386
15	6	0	-2.532350	-1.892889	-0.283301
16	6	0	-1.432092	-0.758195	0.040601
17	6	0	-0.222651	-1.628294	0.448929
18	6	0	-0.593744	-2.856791	0.795425
19	1	0	-2.560903	-2.997873	1.634336
20	1	0	-2.326829	-4.036710	0.243643
21	6	0	-2.397823	-2.405235	-1.731397
22	6	0	-1.845460	0.110014	1.252612
23	1	0	0.072663	-3.631559	1.153180
24	1	0	-2.690659	-1.664687	-2.476113
25	1	0	-1.370605	-2.705246	-1.946705
26	1	0	-3.027967	-3.283895	-1.879606
27	1	0	-1.031682	0.777987	1.531086
28	1	0	-2.717032	0.727235	1.031123
29	1	0	-2.084133	-0.498822	2.126484
30	6	0	-4.014420	-1.496437	0.019680
31	6	0	-4.552116	-0.378009	-0.898579
32	6	0	-5.861969	0.262624	-0.443519
33	6	0	-6.313101	1.456773	-1.305478
34	6	0	-5.778033	2.677291	-0.549842
35	6	0	-5.669038	2.168550	0.884661
36	8	0	-5.716926	0.810874	0.898440
37	1	0	-6.647785	-0.487560	-0.365352
38	1	0	-7.404448	1.497864	-1.348061
39	1	0	-5.942552	1.384027	-2.328339
40	1	0	-4.748006	2.887528	-0.861536
41	6	0	-6.595612	3.959690	-0.663913
42	1	0	-4.037103	-1.113590	1.041440
43	1	0	-4.728282	-0.776085	-1.903815
44	1	0	-3.808615	0.413754	-1.010660
45	8	0	-5.545237	2.814274	1.886630
46	1	0	-6.184834	4.732777	-0.013769
47	1	0	-6.591470	4.331243	-1.690763
48	1	0	-7.633366	3.788064	-0.368308
49	1	0	1.153990	-1.001383	-1.649979
50	6	0	2.889490	0.047859	-1.002418
51	6	0	3.285076	0.040568	-2.489055

52	6	0	3.233666	1.435266	-0.400926
53	1	0	4.367038	0.049015	-2.626777
54	1	0	2.893965	-0.832272	-3.013313
55	1	0	2.879069	0.924862	-2.988261
56	6	0	4.704833	1.847822	-0.469605
57	6	0	4.938714	3.245833	0.059312
58	8	0	4.094553	4.089287	0.231955
59	8	0	6.252539	3.455991	0.302842
60	6	0	6.597140	4.773623	0.765425
61	6	0	4.690104	-1.924726	-0.748319
62	1	0	3.956190	-0.643377	0.754103
63	6	0	5.950284	-1.703025	-0.373171
64	6	0	4.377465	-3.028766	-1.730778
65	1	0	6.774472	-2.269622	-0.791404
66	1	0	6.205702	-0.955662	0.369087
67	1	0	5.289348	-3.392708	-2.205339
68	1	0	3.907162	-3.878812	-1.226937
69	1	0	3.691495	-2.708174	-2.516231
70	1	0	5.079291	1.844504	-1.498246
71	1	0	5.356297	1.168162	0.081070
72	1	0	2.904732	1.465371	0.637340
73	1	0	2.649581	2.194950	-0.924772
74	8	0	2.418340	-3.943692	1.812323
75	1	0	3.462676	-2.295973	2.276250
76	6	0	1.122876	-0.517325	2.848353
77	1	0	0.948562	0.381612	3.439946
78	1	0	0.256568	-1.176033	2.935588
79	1	0	2.000721	-1.031262	3.253061
80	6	0	-4.968303	-2.705957	-0.013481
81	1	0	-5.961863	-2.425812	0.341131
82	1	0	-5.083580	-3.111097	-1.022127
83	1	0	-4.623565	-3.513161	0.632664
84	1	0	7.675660	4.761492	0.901050
85	1	0	6.311244	5.523532	0.028112
86	1	0	6.094089	4.990253	1.707500

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.982850	0.081065	-1.189414
2	6	0	0.403810	0.751187	-1.176254
3	1	0	-1.017876	-0.560091	-2.070803
4	1	0	-1.747547	0.848902	-1.332046
5	1	0	0.457210	1.534501	-0.419803
6	1	0	0.566775	1.231849	-2.145228
7	6	0	3.682659	-1.111706	-0.221563
8	6	0	2.544015	-1.887425	0.486106
9	6	0	1.308436	-0.935905	0.479815
10	6	0	1.468973	-0.309701	-0.920347
11	6	0	2.974329	-2.493664	1.801948
12	1	0	2.237658	-2.748959	-0.117669
13	8	0	1.451934	0.143117	1.424997
14	6	0	-1.904767	-2.970070	0.950079
15	6	0	-2.392549	-1.921939	-0.096625
16	6	0	-1.305006	-0.743953	0.088208
17	6	0	-0.073241	-1.545978	0.567395
18	6	0	-0.427100	-2.735583	1.043919
19	1	0	-2.377035	-2.812947	1.928341
20	1	0	-2.151228	-3.992646	0.652129
21	6	0	-2.268168	-2.582350	-1.484703
22	6	0	-1.716997	0.239989	1.209252
23	1	0	0.244882	-3.468234	1.473862
24	1	0	-2.587052	-1.928714	-2.296716
25	1	0	-1.237398	-2.880393	-1.685340
26	1	0	-2.879791	-3.485227	-1.531957
27	1	0	-0.916514	0.954530	1.396166
28	1	0	-2.611186	0.804289	0.942530
29	1	0	-1.918499	-0.279145	2.148463
30	6	0	-3.876167	-1.515243	0.182570
31	6	0	-4.449509	-0.532510	-0.861547
32	6	0	-5.706667	0.206417	-0.432749
33	6	0	-6.295102	1.150175	-1.492179
34	6	0	-6.901233	2.289636	-0.663881
35	6	0	-6.079796	2.245868	0.622552
36	8	0	-5.400952	1.070134	0.699864
37	1	0	-6.468909	-0.496031	-0.085236
38	1	0	-7.022146	0.642205	-2.127451
39	1	0	-5.494058	1.526247	-2.133721
40	1	0	-6.744355	3.265595	-1.125141
41	6	0	-8.394597	2.125529	-0.345304
42	1	0	-3.887362	-1.004713	1.147521
43	1	0	-4.691470	-1.071194	-1.784535
44	1	0	-3.708503	0.221826	-1.130189
45	8	0	-6.012741	3.080165	1.479919
46	1	0	-8.726872	2.903429	0.343289
47	1	0	-8.985417	2.198974	-1.260553
48	1	0	-8.603028	1.155959	0.114140
49	1	0	1.252353	-1.136865	-1.608707
50	6	0	2.982169	0.001397	-1.128408
51	6	0	3.309447	-0.109716	-2.625490

52	6	0	3.327754	1.430357	-0.632349
53	1	0	4.374288	0.007030	-2.829788
54	1	0	3.013230	-1.077040	-3.031456
55	1	0	2.780525	0.668996	-3.182257
56	6	0	4.802724	1.855292	-0.769345
57	6	0	4.966399	3.294820	-0.342896
58	8	0	4.643427	4.252124	-1.003464
59	8	0	5.499985	3.397197	0.894111
60	6	0	5.651174	4.736343	1.397418
61	6	0	4.694757	-2.029233	-0.899822
62	1	0	4.226548	-0.587716	0.565564
63	6	0	4.358859	-3.120114	-1.586812
64	6	0	6.141861	-1.644508	-0.740292
65	1	0	5.114447	-3.741838	-2.052681
66	1	0	3.332454	-3.441045	-1.722541
67	1	0	6.804062	-2.367385	-1.218258
68	1	0	6.345503	-0.661631	-1.175526
69	1	0	6.401304	-1.583001	0.320859
70	1	0	5.125944	1.797498	-1.809477
71	1	0	5.451725	1.225438	-0.162037
72	1	0	3.030315	1.522357	0.411942
73	1	0	2.726707	2.146232	-1.198824
74	8	0	4.080981	-2.398243	2.274066
75	1	0	2.204926	-3.093648	2.328283
76	6	0	1.329445	-0.152737	2.810107
77	1	0	0.499160	-0.834327	3.011743
78	1	0	2.252451	-0.573350	3.217686
79	1	0	1.133991	0.796072	3.310285
80	6	0	-4.807321	-2.734779	0.320113
81	1	0	-5.813950	-2.423252	0.606032
82	1	0	-4.895067	-3.292265	-0.615848
83	1	0	-4.465345	-3.426161	1.090555
84	1	0	6.085178	4.627666	2.388123
85	1	0	6.310625	5.313468	0.749677
86	1	0	4.682841	5.233023	1.453644

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022012	0.150986	-1.103718
2	6	0	0.358604	0.821599	-0.971640
3	1	0	-1.037915	-0.361990	-2.065842
4	1	0	-1.789827	0.927728	-1.152168
5	1	0	0.390691	1.487882	-0.108833
6	1	0	0.531442	1.439381	-1.858317
7	6	0	3.631020	-1.117777	-0.185597
8	6	0	2.479017	-2.045206	0.283652
9	6	0	1.250095	-1.092109	0.426264
10	6	0	1.431067	-0.257243	-0.856585
11	6	0	2.896051	-2.882496	1.473782
12	1	0	2.198910	-2.753291	-0.495881
13	8	0	1.398229	-0.176643	1.528788
14	6	0	-1.952785	-3.174320	0.568074
15	6	0	-2.438851	-1.985930	-0.318848
16	6	0	-1.355863	-0.845236	0.040884
17	6	0	-0.129040	-1.708084	0.409204
18	6	0	-0.476241	-2.955661	0.709556
19	1	0	-2.433326	-3.163970	1.555010
20	1	0	-2.192689	-4.143865	0.123426
21	6	0	-2.305853	-2.440546	-1.786435
22	6	0	-1.778474	-0.029161	1.285462
23	1	0	0.206888	-3.729847	1.035088
24	1	0	-2.611719	-1.675587	-2.500571
25	1	0	-1.276103	-2.719085	-2.017900
26	1	0	-2.925364	-3.321014	-1.965420
27	1	0	-0.972878	0.638059	1.588042
28	1	0	-2.660048	0.582920	1.089793
29	1	0	-2.004762	-0.674579	2.136259
30	6	0	-3.925767	-1.625900	0.005880
31	6	0	-4.494776	-0.501796	-0.887589
32	6	0	-5.777760	0.147677	-0.374112
33	6	0	-6.297112	1.302571	-1.250873
34	6	0	-5.720564	2.556148	-0.585585
35	6	0	-5.506308	2.107922	0.857428
36	8	0	-5.547367	0.752309	0.931831
37	1	0	-6.549360	-0.603711	-0.211248
38	1	0	-7.389064	1.336284	-1.218870
39	1	0	-5.998086	1.188847	-2.293183
40	1	0	-4.717002	2.759351	-0.978009
41	6	0	-6.555387	3.828003	-0.693721
42	1	0	-3.947716	-1.264262	1.035375
43	1	0	-4.716658	-0.900104	-1.883586
44	1	0	-3.752361	0.285743	-1.032268
45	8	0	-5.312667	2.795956	1.819519
46	1	0	-6.108304	4.629016	-0.104108
47	1	0	-6.624752	4.158313	-1.732283
48	1	0	-7.569003	3.661661	-0.321312
49	1	0	1.237976	-0.968470	-1.669015
50	6	0	2.946761	0.096292	-0.973505
51	6	0	3.324281	0.152758	-2.461628

52	6	0	3.232817	1.463630	-0.299725
53	1	0	4.380972	0.369089	-2.622984
54	1	0	3.109535	-0.791998	-2.962820
55	1	0	2.750268	0.937701	-2.962120
56	6	0	4.697777	1.940061	-0.286356
57	6	0	4.808876	3.262072	0.434974
58	8	0	5.048338	3.395351	1.609930
59	8	0	4.575970	4.303441	-0.395271
60	6	0	4.610124	5.605588	0.215507
61	6	0	4.761576	-1.862479	-0.887269
62	1	0	4.066669	-0.684802	0.721639
63	6	0	4.593525	-3.006348	-1.551071
64	6	0	6.141469	-1.263082	-0.773476
65	1	0	5.434143	-3.499386	-2.025334
66	1	0	3.636902	-3.501472	-1.652739
67	1	0	6.890844	-1.912422	-1.227161
68	1	0	6.204881	-0.287636	-1.261663
69	1	0	6.414832	-1.108378	0.275378
70	1	0	5.081792	2.057940	-1.300399
71	1	0	5.329256	1.237402	0.254528
72	1	0	2.871832	1.426494	0.727575
73	1	0	2.641607	2.223920	-0.817381
74	8	0	2.482895	-3.990242	1.716234
75	1	0	3.664880	-2.424714	2.131297
76	6	0	1.247560	-0.686144	2.846745
77	1	0	0.421897	-1.397032	2.921014
78	1	0	2.164960	-1.168018	3.200391
79	1	0	1.041884	0.170579	3.488536
80	6	0	-4.855889	-2.853008	-0.047015
81	1	0	-5.861464	-2.592810	0.289223
82	1	0	-4.945300	-3.256438	-1.058822
83	1	0	-4.508508	-3.655616	0.603416
84	1	0	4.399792	6.309135	-0.586051
85	1	0	3.856270	5.677953	0.999074
86	1	0	5.592270	5.797028	0.646993

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.846125	0.142327	-1.045697
2	6	0	0.517133	0.823684	-0.815774
3	1	0	-0.820130	-0.289836	-2.046780
4	1	0	-1.626523	0.907932	-1.057961
5	1	0	0.510608	1.422986	0.096198
6	1	0	0.696929	1.506302	-1.650512
7	6	0	3.785108	-1.088397	0.018168
8	6	0	2.649331	-2.104968	0.287663
9	6	0	1.394246	-1.183285	0.449210
10	6	0	1.612034	-0.238276	-0.750480
11	6	0	3.006752	-3.042904	1.417500
12	1	0	2.449947	-2.735403	-0.580871
13	8	0	1.482160	-0.351991	1.623647
14	6	0	-1.764054	-3.328629	0.301168
15	6	0	-2.250206	-2.074379	-0.489975
16	6	0	-1.199918	-0.951196	-0.000888
17	6	0	0.031564	-1.820362	0.331052
18	6	0	-0.297158	-3.096535	0.506118
19	1	0	-2.271309	-3.414990	1.270719
20	1	0	-1.971231	-4.258162	-0.235648
21	6	0	-2.068062	-2.393337	-1.987755
22	6	0	-1.678398	-0.250297	1.292749
23	1	0	0.391452	-3.886032	0.778895
24	1	0	-2.373076	-1.573761	-2.638851
25	1	0	-1.025926	-2.626844	-2.213799
26	1	0	-2.659973	-3.267904	-2.263683
27	1	0	-0.903161	0.414771	1.670004
28	1	0	-2.574104	0.348092	1.122040
29	1	0	-1.906826	-0.968524	2.082392
30	6	0	-3.752011	-1.771968	-0.174931
31	6	0	-4.320831	-0.579604	-0.974777
32	6	0	-5.641794	-0.020515	-0.450728
33	6	0	-6.155037	1.213416	-1.216595
34	6	0	-5.642665	2.397577	-0.390646
35	6	0	-5.475053	1.794904	1.001380
36	8	0	-5.483304	0.439004	0.922942
37	1	0	-6.399085	-0.802146	-0.408195
38	1	0	-7.247866	1.218056	-1.230665
39	1	0	-5.808973	1.224324	-2.250511
40	1	0	-4.630276	2.668318	-0.713608
41	6	0	-6.509452	3.652587	-0.392455
42	1	0	-3.806211	-1.505961	0.882262
43	1	0	-4.492848	-0.880363	-2.013897
44	1	0	-3.597499	0.237858	-1.008538
45	8	0	-5.339320	2.374558	2.041622
46	1	0	-6.108846	4.393862	0.299718
47	1	0	-6.548357	4.094161	-1.390427
48	1	0	-7.531300	3.420954	-0.082815
49	1	0	1.456004	-0.881317	-1.625609
50	6	0	3.129449	0.127367	-0.788015
51	6	0	3.589700	0.208041	-2.251552

52	6	0	3.545469	1.420511	-0.035340
53	1	0	4.656823	0.427600	-2.328081
54	1	0	3.398183	-0.722967	-2.786064
55	1	0	3.046780	0.992448	-2.783999
56	6	0	3.232863	2.769172	-0.687906
57	6	0	3.822256	3.928262	0.087436
58	8	0	4.658248	3.852846	0.952867
59	8	0	3.298695	5.102377	-0.332766
60	6	0	3.817398	6.280829	0.308636
61	6	0	5.065443	-1.688992	-0.537679
62	1	0	4.046603	-0.672724	0.993355
63	6	0	6.248428	-1.259016	-0.095844
64	6	0	4.989408	-2.804865	-1.551545
65	1	0	7.178086	-1.660818	-0.482857
66	1	0	6.329468	-0.493737	0.667572
67	1	0	5.982154	-3.047932	-1.931947
68	1	0	4.574835	-3.713919	-1.104889
69	1	0	4.353444	-2.556966	-2.403955
70	1	0	2.164213	2.953771	-0.794730
71	1	0	3.651388	2.836895	-1.696938
72	1	0	4.628369	1.377693	0.107683
73	1	0	3.107700	1.399043	0.963051
74	8	0	2.705028	-4.211988	1.460333
75	1	0	3.625917	-2.605321	2.226624
76	6	0	1.272180	-0.954978	2.893679
77	1	0	0.944100	-0.162870	3.567292
78	1	0	0.505613	-1.732001	2.858170
79	1	0	2.197438	-1.383471	3.291777
80	6	0	-4.654923	-3.005665	-0.364598
81	1	0	-5.670454	-2.799650	-0.021243
82	1	0	-4.720603	-3.308876	-1.412568
83	1	0	-4.300201	-3.861474	0.209499
84	1	0	4.891464	6.363496	0.143440
85	1	0	3.293885	7.115896	-0.149991
86	1	0	3.622865	6.248014	1.380317

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.142325	-0.299479	-1.198669
2	6	0	-0.203370	-1.048366	-1.170736
3	1	0	1.154009	0.303343	-2.107778
4	1	0	1.950973	-1.028642	-1.296103
5	1	0	-0.223147	-1.788197	-0.369947
6	1	0	-0.316432	-1.593263	-2.113270
7	6	0	-3.593679	0.661207	-0.335502
8	6	0	-2.501727	1.590879	0.256329
9	6	0	-1.233716	0.684550	0.359969
10	6	0	-1.335336	-0.039740	-0.995823
11	6	0	-2.998818	2.299683	1.498216
12	1	0	-2.225655	2.378944	-0.444458
13	8	0	-1.364997	-0.334291	1.367726
14	6	0	1.860916	2.883353	0.819478
15	6	0	2.427872	1.815738	-0.166046
16	6	0	1.392057	0.597416	0.044965
17	6	0	0.113333	1.363369	0.449087
18	6	0	0.391521	2.589517	0.881630
19	1	0	2.307946	2.788904	1.817771
20	1	0	2.072453	3.903012	0.486291
21	6	0	2.310571	2.409397	-1.584487
22	6	0	1.817059	-0.313504	1.221256
23	1	0	-0.337140	3.298335	1.253901
24	1	0	2.669491	1.733893	-2.361275
25	1	0	1.274287	2.661262	-1.816487
26	1	0	2.891056	3.330948	-1.658261
27	1	0	1.038594	-1.046372	1.429243
28	1	0	2.737358	-0.856382	1.001653
29	1	0	1.976634	0.259709	2.136712
30	6	0	3.921484	1.489871	0.164003
31	6	0	4.569136	0.511797	-0.840928
32	6	0	5.829428	-0.183731	-0.353372
33	6	0	6.509110	-1.087562	-1.392930
34	6	0	7.106711	-2.222375	-0.552519
35	6	0	6.217424	-2.227633	0.688901
36	8	0	5.497523	-1.076833	0.749486
37	1	0	6.543484	0.541609	0.045811
38	1	0	7.252583	-0.543494	-1.977342
39	1	0	5.758653	-1.477500	-2.085417
40	1	0	7.005491	-3.194241	-1.037482
41	6	0	8.575291	-2.018551	-0.152108
42	1	0	3.932672	1.005819	1.142483
43	1	0	4.832367	1.048076	-1.759583
44	1	0	3.864778	-0.268943	-1.132137
45	8	0	6.133147	-3.080343	1.526913
46	1	0	8.895091	-2.798413	0.540225
47	1	0	9.215928	-2.056968	-1.035518
48	1	0	8.728561	-1.051707	0.333984
49	1	0	-1.158357	0.749836	-1.736383
50	6	0	-2.828534	-0.456456	-1.191709
51	6	0	-3.147177	-0.406589	-2.694234

52	6	0	-3.057730	-1.896062	-0.652469
53	1	0	-4.180833	-0.672385	-2.919126
54	1	0	-2.976958	0.589544	-3.104231
55	1	0	-2.505775	-1.108477	-3.235153
56	6	0	-4.445377	-2.538330	-0.796721
57	6	0	-5.393241	-2.332681	0.365455
58	8	0	-5.124038	-1.838131	1.432630
59	8	0	-6.616285	-2.825249	0.071531
60	6	0	-7.592641	-2.751490	1.125547
61	6	0	-4.721916	1.414570	-1.029124
62	1	0	-4.045379	0.136903	0.509628
63	6	0	-4.582638	2.615363	-1.591356
64	6	0	-6.073738	0.746285	-1.019291
65	1	0	-5.425443	3.107516	-2.063040
66	1	0	-3.648139	3.160568	-1.606488
67	1	0	-6.400265	0.556155	0.007608
68	1	0	-6.825784	1.365263	-1.509831
69	1	0	-6.055983	-0.221087	-1.527376
70	1	0	-4.327440	-3.625185	-0.871554
71	1	0	-4.963255	-2.256544	-1.715134
72	1	0	-2.767269	-1.932861	0.395988
73	1	0	-2.360890	-2.543823	-1.190218
74	8	0	-2.643113	3.397850	1.853297
75	1	0	-3.770522	1.755371	2.080747
76	6	0	-1.314629	0.061262	2.730531
77	1	0	-0.552520	0.823205	2.909626
78	1	0	-2.284082	0.433463	3.076473
79	1	0	-1.068138	-0.832398	3.304216
80	6	0	4.790436	2.754992	0.291935
81	1	0	5.808021	2.497145	0.593602
82	1	0	4.862361	3.301023	-0.652115
83	1	0	4.405366	3.440416	1.047072
84	1	0	-7.777366	-1.713857	1.402473
85	1	0	-8.493402	-3.204552	0.719492
86	1	0	-7.248314	-3.299177	2.002392

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.001112	0.511250	-0.792553
2	6	0	0.339569	1.101275	-0.317677
3	1	0	-0.906206	0.319182	-1.861807
4	1	0	-1.782025	1.268320	-0.680477
5	1	0	0.266011	1.468726	0.706641
6	1	0	0.584070	1.962019	-0.947632
7	6	0	3.571825	-0.995711	0.169569
8	6	0	2.405884	-2.018967	0.204996
9	6	0	1.141322	-1.156421	0.507231
10	6	0	1.424507	0.034540	-0.429482
11	6	0	2.727510	-3.190075	1.109394
12	1	0	2.226454	-2.446799	-0.781301
13	8	0	1.152067	-0.631936	1.850952
14	6	0	-2.005458	-3.161804	-0.326349
15	6	0	-2.431674	-1.755852	-0.851539
16	6	0	-1.420185	-0.787649	-0.050384
17	6	0	-0.212456	-1.729691	0.159126
18	6	0	-0.555845	-3.006858	0.023516
19	1	0	-2.579402	-3.452031	0.563359
20	1	0	-2.177119	-3.946728	-1.067866
21	6	0	-2.141290	-1.737121	-2.365714
22	6	0	-1.985726	-0.396080	1.335622
23	1	0	0.111038	-3.848158	0.162279
24	1	0	-2.401859	-0.789932	-2.838547
25	1	0	-1.085217	-1.929159	-2.563531
26	1	0	-2.710613	-2.520618	-2.868862
27	1	0	-1.234547	0.143304	1.910606
28	1	0	-2.862733	0.246509	1.249582
29	1	0	-2.273918	-1.273775	1.917138
30	6	0	-3.952697	-1.504717	-0.585945
31	6	0	-4.461677	-0.158347	-1.145659
32	6	0	-5.801889	0.309618	-0.583271
33	6	0	-6.270174	1.674847	-1.121126
34	6	0	-5.783311	2.671691	-0.064700
35	6	0	-5.684663	1.813265	1.193309
36	8	0	-5.703336	0.497014	0.858712
37	1	0	-6.565714	-0.454108	-0.723326
38	1	0	-7.361258	1.701126	-1.178968
39	1	0	-5.878855	1.875186	-2.118864
40	1	0	-4.754733	2.979720	-0.287609
41	6	0	-6.636307	3.920170	0.135202
42	1	0	-4.084144	-1.476949	0.497171
43	1	0	-4.580174	-0.231753	-2.232047
44	1	0	-3.729154	0.632230	-0.970857
45	8	0	-5.589978	2.183111	2.329503
46	1	0	-6.258905	4.510901	0.970508
47	1	0	-6.627597	4.542375	-0.762215
48	1	0	-7.672911	3.652775	0.353561
49	1	0	1.330981	-0.391483	-1.435748
50	6	0	2.935127	0.402505	-0.280485
51	6	0	3.455178	0.896991	-1.638455

52	6	0	3.107236	1.498290	0.804693
53	1	0	4.519889	1.130140	-1.624604
54	1	0	3.304636	0.146043	-2.415531
55	1	0	2.919611	1.802674	-1.936217
56	6	0	4.529931	1.960936	1.172104
57	6	0	5.240793	2.854353	0.181061
58	8	0	6.349455	2.664292	-0.260189
59	8	0	4.502075	3.938926	-0.135010
60	6	0	5.112497	4.865931	-1.049825
61	6	0	4.792950	-1.499815	-0.594052
62	1	0	3.895138	-0.862273	1.207949
63	6	0	4.721995	-2.373691	-1.598632
64	6	0	6.137829	-0.992509	-0.137087
65	1	0	5.620212	-2.709425	-2.103616
66	1	0	3.791920	-2.790199	-1.962455
67	1	0	6.946349	-1.494097	-0.670080
68	1	0	6.255017	0.082493	-0.294371
69	1	0	6.276687	-1.173464	0.934414
70	1	0	5.192383	1.124040	1.382932
71	1	0	4.452569	2.544234	2.095842
72	1	0	2.640455	1.135414	1.719513
73	1	0	2.540766	2.379781	0.497460
74	8	0	2.308044	-4.312088	0.962408
75	1	0	3.430663	-2.970037	1.940560
76	6	0	0.889114	-1.531628	2.918595
77	1	0	0.587105	-0.922912	3.771222
78	1	0	0.087169	-2.232700	2.677802
79	1	0	1.783557	-2.098248	3.198627
80	6	0	-4.839263	-2.652053	-1.106972
81	1	0	-5.882247	-2.496318	-0.824255
82	1	0	-4.806101	-2.732868	-2.196476
83	1	0	-4.544291	-3.615446	-0.691153
84	1	0	5.332031	4.375802	-1.998065
85	1	0	4.383834	5.660658	-1.188282
86	1	0	6.037325	5.261234	-0.630496

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.057634	0.510668	-0.818268
2	6	0	0.288257	1.095542	-0.352036
3	1	0	-0.962717	0.298965	-1.883682
4	1	0	-1.832224	1.276105	-0.721829
5	1	0	0.218424	1.485361	0.664089
6	1	0	0.545609	1.939345	-0.998528
7	6	0	3.509152	-1.046376	0.088017
8	6	0	2.325514	-2.028382	0.286122
9	6	0	1.063376	-1.146892	0.534664
10	6	0	1.360020	0.013890	-0.436065
11	6	0	2.633244	-3.131264	1.271883
12	1	0	2.115374	-2.560653	-0.648107
13	8	0	1.050236	-0.578454	1.859713
14	6	0	-2.099262	-3.146026	-0.294310
15	6	0	-2.507222	-1.745398	-0.847359
16	6	0	-1.493158	-0.771289	-0.054786
17	6	0	-0.293831	-1.717864	0.185355
18	6	0	-0.652535	-2.992248	0.066553
19	1	0	-2.685142	-3.416339	0.593755
20	1	0	-2.268600	-3.941389	-1.025140
21	6	0	-2.205091	-1.755904	-2.359166
22	6	0	-2.066994	-0.348839	1.318485
23	1	0	-0.004448	-3.846293	0.221321
24	1	0	-2.456546	-0.815806	-2.850284
25	1	0	-1.148478	-1.956071	-2.545914
26	1	0	-2.775137	-2.544996	-2.852652
27	1	0	-1.318217	0.201514	1.885557
28	1	0	-2.940577	0.294609	1.209547
29	1	0	-2.364102	-1.211447	1.917904
30	6	0	-4.028253	-1.479770	-0.596621
31	6	0	-4.520298	-0.131258	-1.165369
32	6	0	-5.875212	0.336298	-0.638301
33	6	0	-6.312271	1.717433	-1.161435
34	6	0	-5.855924	2.685599	-0.065320
35	6	0	-5.812103	1.798526	1.175566
36	8	0	-5.825937	0.489826	0.809683
37	1	0	-6.640051	-0.416776	-0.823236
38	1	0	-7.400253	1.754867	-1.258090
39	1	0	-5.883315	1.936926	-2.139517
40	1	0	-4.816937	2.988067	-0.242911
41	6	0	-6.704042	3.937979	0.130620
42	1	0	-4.168652	-1.446020	0.485215
43	1	0	-4.609962	-0.199889	-2.254774
44	1	0	-3.791114	0.656845	-0.967531
45	8	0	-5.759854	2.140501	2.322908
46	1	0	-6.352069	4.506583	0.991938
47	1	0	-6.656077	4.579389	-0.751858
48	1	0	-7.750474	3.676526	0.304841
49	1	0	1.261951	-0.441008	-1.430502
50	6	0	2.871721	0.366909	-0.304936
51	6	0	3.370712	0.924312	-1.646065

52	6	0	3.103298	1.411965	0.819359
53	1	0	4.448463	1.096688	-1.647380
54	1	0	3.161003	0.238679	-2.467375
55	1	0	2.886123	1.879167	-1.861033
56	6	0	4.548063	1.878428	1.049343
57	6	0	5.006827	3.000479	0.144017
58	8	0	4.314577	3.899859	-0.264536
59	8	0	6.329888	2.910268	-0.121778
60	6	0	6.881221	3.978883	-0.911671
61	6	0	4.590799	-1.606617	-0.830638
62	1	0	3.974676	-0.928141	1.067422
63	6	0	4.331191	-2.274715	-1.953837
64	6	0	6.013901	-1.377467	-0.393698
65	1	0	5.132638	-2.654696	-2.576607
66	1	0	3.325066	-2.467318	-2.308126
67	1	0	6.721754	-1.860653	-1.068447
68	1	0	6.258234	-0.311301	-0.361895
69	1	0	6.169474	-1.772982	0.614522
70	1	0	5.269378	1.063075	1.009564
71	1	0	4.620307	2.290626	2.062537
72	1	0	2.725209	0.998309	1.752146
73	1	0	2.505023	2.300218	0.605079
74	8	0	3.683332	-3.261924	1.852744
75	1	0	1.828825	-3.879606	1.420735
76	6	0	0.776330	-1.437152	2.959138
77	1	0	0.477031	-0.792299	3.785785
78	1	0	-0.038181	-2.133126	2.742926
79	1	0	1.662784	-1.999818	3.264394
80	6	0	-4.920252	-2.622158	-1.119627
81	1	0	-5.960886	-2.465613	-0.829463
82	1	0	-4.893680	-2.696551	-2.209793
83	1	0	-4.625797	-3.589000	-0.711281
84	1	0	6.403845	4.013323	-1.890703
85	1	0	6.737315	4.935969	-0.410859
86	1	0	7.939924	3.752263	-1.009324

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.154972	0.196670	1.189353
2	6	0	-0.210662	0.914144	1.215326
3	1	0	1.225963	-0.376826	2.114088
4	1	0	1.949681	0.946394	1.226641
5	1	0	-0.280859	1.661126	0.423466
6	1	0	-0.299569	1.446698	2.167124
7	6	0	-3.593206	-0.712994	0.355059
8	6	0	-2.542939	-1.706388	-0.194581
9	6	0	-1.251952	-0.830715	-0.291279
10	6	0	-1.315394	-0.128547	1.079563
11	6	0	-3.035748	-2.410748	-1.441591
12	1	0	-2.312110	-2.491850	0.528327
13	8	0	-1.375315	0.199433	-1.290270
14	6	0	1.830132	-3.039446	-0.768681
15	6	0	2.414387	-1.949718	0.183069
16	6	0	1.374630	-0.735243	-0.037351
17	6	0	0.089375	-1.512910	-0.401516
18	6	0	0.360105	-2.746969	-0.814235
19	1	0	2.262089	-2.968881	-1.775479
20	1	0	2.045417	-4.051215	-0.415023
21	6	0	2.321406	-2.512531	1.615666
22	6	0	1.777637	0.145563	-1.243775
23	1	0	-0.375673	-3.461465	-1.160768
24	1	0	2.701482	-1.824907	2.371566
25	1	0	1.288555	-2.752933	1.874044
26	1	0	2.897227	-3.436259	1.696063
27	1	0	1.006665	0.889194	-1.440222
28	1	0	2.712506	0.677290	-1.062799
29	1	0	1.902215	-0.445161	-2.153233
30	6	0	3.902214	-1.635740	-0.183787
31	6	0	4.565256	-0.610516	0.762018
32	6	0	5.864535	0.002497	0.245189
33	6	0	6.476245	1.067361	1.174824
34	6	0	5.949169	2.391732	0.613481
35	6	0	5.659277	2.051730	-0.845959
36	8	0	5.624806	0.704156	-1.009574
37	1	0	6.587904	-0.775997	0.006414
38	1	0	7.566660	1.044460	1.104471
39	1	0	6.206463	0.900842	2.218046
40	1	0	4.973654	2.624008	1.057101
41	6	0	6.859589	3.605465	0.769901
42	1	0	3.897220	-1.198224	-1.183818
43	1	0	4.798302	-1.089429	1.719197
44	1	0	3.874037	0.204012	0.987777
45	8	0	5.469250	2.811579	-1.753288
46	1	0	6.438555	4.467734	0.251902
47	1	0	6.985711	3.860854	1.824130
48	1	0	7.847656	3.408419	0.347212
49	1	0	-1.050116	-0.925449	1.783313
50	6	0	-2.817218	0.196055	1.401163
51	6	0	-3.077962	-0.250950	2.853984

52	6	0	-3.184633	1.703029	1.348801
53	1	0	-4.102077	-0.046829	3.171911
54	1	0	-2.902937	-1.320433	2.980814
55	1	0	-2.408109	0.281110	3.536237
56	6	0	-3.131101	2.467787	-0.002200
57	6	0	-4.476345	2.597208	-0.673757
58	8	0	-4.903809	1.883365	-1.551036
59	8	0	-5.185759	3.629025	-0.163764
60	6	0	-6.493415	3.832064	-0.727456
61	6	0	-4.887579	-1.347933	0.832261
62	1	0	-3.862245	-0.066967	-0.485378
63	6	0	-5.010887	-2.641559	1.130891
64	6	0	-6.084736	-0.433042	0.906954
65	1	0	-5.963947	-3.048662	1.448782
66	1	0	-4.191223	-3.345352	1.068772
67	1	0	-6.976428	-0.974200	1.225631
68	1	0	-5.923267	0.389601	1.609795
69	1	0	-6.281034	0.022180	-0.067776
70	1	0	-2.459246	1.974592	-0.699502
71	1	0	-2.763489	3.477509	0.187450
72	1	0	-2.511244	2.213144	2.041951
73	1	0	-4.178771	1.830518	1.784180
74	8	0	-2.678795	-3.509340	-1.794675
75	1	0	-3.797412	-1.861279	-2.030411
76	6	0	-1.361923	-0.190187	-2.658344
77	1	0	-1.036778	0.679818	-3.229504
78	1	0	-0.669815	-1.015036	-2.840699
79	1	0	-2.362136	-0.471533	-3.000645
80	6	0	4.771102	-2.905029	-0.268083
81	1	0	5.769984	-2.666966	-0.638776
82	1	0	4.891888	-3.385809	0.706067
83	1	0	4.352405	-3.640588	-0.954853
84	1	0	-6.420743	4.014480	-1.799207
85	1	0	-7.123590	2.959593	-0.556185
86	1	0	-6.898417	4.702077	-0.216788

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.902839	0.191250	-1.148359
2	6	0	0.479720	0.862054	-1.033465
3	1	0	-0.911437	-0.363154	-2.087520
4	1	0	-1.666760	0.968000	-1.237503
5	1	0	0.509072	1.566163	-0.200984
6	1	0	0.663613	1.438783	-1.945221
7	6	0	3.736079	-1.044979	-0.120670
8	6	0	2.576354	-1.956548	0.372574
9	6	0	1.350663	-0.989331	0.457461
10	6	0	1.545647	-0.214922	-0.861993
11	6	0	2.976004	-2.729307	1.608867
12	1	0	2.313227	-2.702577	-0.378564
13	8	0	1.497678	-0.023183	1.515610
14	6	0	-1.859206	-3.052359	0.668655
15	6	0	-2.331067	-1.908519	-0.282068
16	6	0	-1.251249	-0.752730	0.036188
17	6	0	-0.030257	-1.599627	0.457747
18	6	0	-0.383241	-2.830718	0.814260
19	1	0	-2.350150	-2.989589	1.648671
20	1	0	-2.098468	-4.042323	0.271325
21	6	0	-2.179670	-2.432507	-1.724412
22	6	0	-1.687774	0.121208	1.236145
23	1	0	0.293673	-3.591625	1.181842
24	1	0	-2.482016	-1.704342	-2.477526
25	1	0	-1.145843	-2.715142	-1.931061
26	1	0	-2.791937	-3.324401	-1.868533
27	1	0	-0.886361	0.804825	1.513073
28	1	0	-2.569068	0.719837	1.002576
29	1	0	-1.918733	-0.483701	2.115154
30	6	0	-3.820795	-1.530966	0.005387
31	6	0	-4.374953	-0.450035	-0.948833
32	6	0	-5.625984	0.263669	-0.462896
33	6	0	-6.210156	1.287232	-1.447901
34	6	0	-6.802387	2.369257	-0.536773
35	6	0	-5.975501	2.225226	0.738881
36	8	0	-5.310244	1.039812	0.729181
37	1	0	-6.392098	-0.456862	-0.164414
38	1	0	-6.944070	0.833123	-2.115274
39	1	0	-5.408007	1.701776	-2.063854
40	1	0	-6.638659	3.374587	-0.927176
41	6	0	-8.295647	2.195896	-0.222644
42	1	0	-3.853595	-1.119957	1.016190
43	1	0	-4.616846	-0.900711	-1.917964
44	1	0	-3.624518	0.317243	-1.145517
45	8	0	-5.894959	2.996699	1.652352
46	1	0	-8.617575	2.926033	0.521003
47	1	0	-8.890361	2.338981	-1.127100
48	1	0	-8.510613	1.198212	0.168501
49	1	0	1.351177	-0.962714	-1.640755
50	6	0	3.062926	0.118292	-0.986055
51	6	0	3.468514	0.129188	-2.469229

52	6	0	3.385390	1.505013	-0.369503
53	1	0	4.551189	0.155776	-2.598000
54	1	0	3.093723	-0.745366	-3.002223
55	1	0	3.053534	1.011356	-2.964931
56	6	0	4.855861	1.957547	-0.479074
57	6	0	5.065996	3.243374	0.282507
58	8	0	5.427264	3.321689	1.431302
59	8	0	4.768240	4.324623	-0.473259
60	6	0	4.890208	5.597267	0.185907
61	6	0	4.884446	-1.836299	-0.730133
62	1	0	4.142000	-0.556772	0.768330
63	6	0	6.140782	-1.612615	-0.343278
64	6	0	4.582274	-2.936553	-1.720178
65	1	0	6.969891	-2.174585	-0.758123
66	1	0	6.387206	-0.870207	0.407032
67	1	0	5.498411	-3.293298	-2.192006
68	1	0	4.114211	-3.791844	-1.223112
69	1	0	3.898487	-2.615928	-2.507518
70	1	0	5.137979	2.111546	-1.520946
71	1	0	5.524827	1.218000	-0.042414
72	1	0	3.093235	1.499572	0.680196
73	1	0	2.766737	2.256535	-0.867466
74	8	0	2.631863	-3.861467	1.851203
75	1	0	3.666817	-2.203106	2.298790
76	6	0	1.294109	-0.451487	2.855306
77	1	0	0.436277	-1.120519	2.947976
78	1	0	2.179861	-0.950869	3.260335
79	1	0	1.110563	0.448667	3.442038
80	6	0	-4.753349	-2.757086	0.000035
81	1	0	-5.768261	-2.473639	0.286723
82	1	0	-4.813974	-3.221307	-0.987421
83	1	0	-4.430108	-3.519261	0.709135
84	1	0	4.615468	6.339314	-0.559529
85	1	0	4.219914	5.647466	1.043713
86	1	0	5.914242	5.753313	0.524216

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960669	0.216038	-1.156768
2	6	0	0.435484	0.859981	-1.054188
3	1	0	-0.982697	-0.352123	-2.087516
4	1	0	-1.708646	1.006875	-1.256630
5	1	0	0.482301	1.578227	-0.234895
6	1	0	0.630339	1.417403	-1.975498
7	6	0	3.653017	-1.092604	-0.110954
8	6	0	2.477562	-1.976597	0.395062
9	6	0	1.270853	-0.984344	0.466331
10	6	0	1.478483	-0.236318	-0.866442
11	6	0	2.863407	-2.736517	1.642853
12	1	0	2.200408	-2.728947	-0.344551
13	8	0	1.440342	-0.006389	1.510471
14	6	0	-1.978923	-2.979841	0.712067
15	6	0	-2.428452	-1.842393	-0.257196
16	6	0	-1.326585	-0.702643	0.042595
17	6	0	-0.121942	-1.566722	0.477657
18	6	0	-0.498873	-2.784617	0.854331
19	1	0	-2.468781	-2.891495	1.690683
20	1	0	-2.237361	-3.971204	0.330536
21	6	0	-2.286947	-2.392408	-1.690812
22	6	0	-1.744473	0.198200	1.229184
23	1	0	0.162833	-3.552774	1.234262
24	1	0	-2.577864	-1.671860	-2.455674
25	1	0	-1.257964	-2.694960	-1.893379
26	1	0	-2.913866	-3.276443	-1.819895
27	1	0	-0.930914	0.872931	1.492476
28	1	0	-2.615802	0.808304	0.988159
29	1	0	-1.984113	-0.388172	2.118365
30	6	0	-3.910349	-1.431901	0.024810
31	6	0	-4.441464	-0.349167	-0.939898
32	6	0	-5.693675	0.376045	-0.474331
33	6	0	-6.240483	1.419858	-1.459526
34	6	0	-6.842345	2.496653	-0.548381
35	6	0	-6.051164	2.323961	0.746320
36	8	0	-5.396966	1.132347	0.735010
37	1	0	-6.476600	-0.337578	-0.204254
38	1	0	-6.963001	0.984020	-2.151101
39	1	0	-5.418214	1.832744	-2.049437
40	1	0	-6.655499	3.505083	-0.919911
41	6	0	-8.345388	2.338669	-0.275594
42	1	0	-3.934910	-1.009591	1.031215
43	1	0	-4.673436	-0.799299	-1.911730
44	1	0	-3.681099	0.410662	-1.126916
45	8	0	-5.988508	3.079578	1.674261
46	1	0	-8.677392	3.063349	0.468962
47	1	0	-8.914401	2.500835	-1.193275
48	1	0	-8.582992	1.338952	0.096884
49	1	0	1.265348	-0.993946	-1.630712
50	6	0	3.001327	0.064528	-1.001109
51	6	0	3.400682	0.026492	-2.486214

52	6	0	3.349672	1.462573	-0.426788
53	1	0	4.482976	0.030685	-2.621583
54	1	0	3.009252	-0.855893	-2.993970
55	1	0	2.997075	0.901285	-3.003744
56	6	0	4.822525	1.867879	-0.503414
57	6	0	5.062847	3.273138	0.002797
58	8	0	4.221811	4.121196	0.167694
59	8	0	6.378613	3.483666	0.236109
60	6	0	6.728361	4.806855	0.678437
61	6	0	4.792260	-1.910729	-0.701526
62	1	0	4.061571	-0.594289	0.771448
63	6	0	6.052424	-1.688020	-0.326825
64	6	0	4.477063	-3.032048	-1.663275
65	1	0	6.875049	-2.266829	-0.731194
66	1	0	6.309227	-0.927276	0.401242
67	1	0	5.388444	-3.409072	-2.128527
68	1	0	4.001774	-3.870192	-1.144407
69	1	0	3.794435	-2.723384	-2.456356
70	1	0	5.195843	1.845695	-1.532196
71	1	0	5.471716	1.194490	0.057677
72	1	0	3.020362	1.514846	0.610435
73	1	0	2.768425	2.213744	-0.965802
74	8	0	2.509477	-3.862702	1.898651
75	1	0	3.554524	-2.206765	2.330192
76	6	0	1.217975	-0.407794	2.855054
77	1	0	1.050469	0.505759	3.425853
78	1	0	0.344726	-1.055669	2.953166
79	1	0	2.088924	-0.921571	3.274713
80	6	0	-4.866743	-2.639516	0.032590
81	1	0	-5.872846	-2.335797	0.328777
82	1	0	-4.946144	-3.106201	-0.952447
83	1	0	-4.550785	-3.405353	0.741004
84	1	0	6.230118	5.037936	1.619634
85	1	0	7.807472	4.794146	0.809294
86	1	0	6.440756	5.547015	-0.068014

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.923725	0.021682	-1.165718
2	6	0	0.440622	0.741014	-1.154559
3	1	0	-0.965304	-0.558945	-2.087746
4	1	0	-1.718436	0.769163	-1.233159
5	1	0	0.485619	1.491678	-0.365009
6	1	0	0.561216	1.271006	-2.103596
7	6	0	3.794520	-0.884867	-0.193851
8	6	0	2.731308	-1.883233	0.332199
9	6	0	1.441352	-0.995236	0.391596
10	6	0	1.540272	-0.301434	-0.981969
11	6	0	3.184592	-2.572374	1.597929
12	1	0	2.525013	-2.674836	-0.391273
13	8	0	1.557055	0.040694	1.386678
14	6	0	-1.650985	-3.203085	0.794205
15	6	0	-2.208790	-2.120103	-0.181115
16	6	0	-1.178893	-0.901336	0.061243
17	6	0	0.096411	-1.673340	0.471781
18	6	0	-0.184135	-2.905487	0.883873
19	1	0	-2.114713	-3.129180	1.786597
20	1	0	-1.851619	-4.217329	0.439200
21	6	0	-2.072912	-2.690417	-1.607231
22	6	0	-1.620520	-0.011882	1.247580
23	1	0	0.540970	-3.618744	1.255235
24	1	0	-2.435768	-2.008641	-2.376668
25	1	0	-1.032120	-2.926346	-1.836316
26	1	0	-2.641355	-3.617599	-1.698352
27	1	0	-0.858412	0.736283	1.461154
28	1	0	-2.549855	0.516403	1.033112
29	1	0	-1.773526	-0.594766	2.157667
30	6	0	-3.707473	-1.808525	0.140961
31	6	0	-4.343693	-0.782024	-0.821588
32	6	0	-5.659167	-0.173291	-0.341210
33	6	0	-6.238664	0.902530	-1.278644
34	6	0	-5.728732	2.219950	-0.685532
35	6	0	-5.488415	1.863627	0.778870
36	8	0	-5.460317	0.513952	0.928460
37	1	0	-6.390462	-0.953751	-0.134945
38	1	0	-7.330815	0.880543	-1.244505
39	1	0	-5.934782	0.747202	-2.314188
40	1	0	-4.738503	2.455160	-1.093509
41	6	0	-6.631463	3.437062	-0.859192
42	1	0	-3.732963	-1.373285	1.141598
43	1	0	-4.546947	-1.257898	-1.787031
44	1	0	-3.647976	0.034685	-1.023886
45	8	0	-5.328140	2.612441	1.700921
46	1	0	-6.226173	4.292967	-0.318615
47	1	0	-6.722004	3.703802	-1.914216
48	1	0	-7.633306	3.237645	-0.471466
49	1	0	1.289603	-1.103504	-1.685531
50	6	0	3.047172	0.014720	-1.266234
51	6	0	3.347221	-0.408895	-2.718459

52	6	0	3.461005	1.505336	-1.185873
53	1	0	4.403969	-0.287962	-2.963852
54	1	0	3.068260	-1.446614	-2.907840
55	1	0	2.773830	0.213365	-3.411266
56	6	0	3.400385	2.235722	0.156500
57	6	0	3.560091	3.731535	0.001443
58	8	0	3.396810	4.363703	-1.013228
59	8	0	3.891029	4.306083	1.180268
60	6	0	4.010377	5.739239	1.162876
61	6	0	5.122132	-1.499255	-0.607579
62	1	0	4.015682	-0.227648	0.648057
63	6	0	6.261556	-0.858553	-0.341945
64	6	0	5.144624	-2.847910	-1.284670
65	1	0	7.222784	-1.263675	-0.637046
66	1	0	6.274979	0.092068	0.179393
67	1	0	6.161240	-3.115748	-1.574728
68	1	0	4.773121	-3.632225	-0.618169
69	1	0	4.520619	-2.875479	-2.180267
70	1	0	4.164691	1.892457	0.856076
71	1	0	2.449311	2.067050	0.665902
72	1	0	2.851902	2.063014	-1.900406
73	1	0	4.485153	1.581543	-1.565579
74	8	0	2.908064	-3.709759	1.897152
75	1	0	3.850514	-1.977916	2.256035
76	6	0	1.433136	-0.322355	2.755702
77	1	0	2.384534	-0.675238	3.166260
78	1	0	1.140783	0.579841	3.293672
79	1	0	0.672595	-1.090353	2.909475
80	6	0	-4.576458	-3.079514	0.196240
81	1	0	-5.585813	-2.843883	0.538866
82	1	0	-4.668390	-3.556758	-0.782707
83	1	0	-4.176868	-3.817203	0.892116
84	1	0	4.272547	6.021727	2.179349
85	1	0	4.788625	6.048307	0.465503
86	1	0	3.066024	6.196887	0.868817

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.846123	0.142324	-1.045702
2	6	0	0.517133	0.823684	-0.815777
3	1	0	-0.820124	-0.289844	-2.046783
4	1	0	-1.626523	0.907927	-1.057971
5	1	0	0.510604	1.422987	0.096194
6	1	0	0.696931	1.506300	-1.650515
7	6	0	3.785110	-1.088398	0.018165
8	6	0	2.649330	-2.104965	0.287666
9	6	0	1.394247	-1.183280	0.449215
10	6	0	1.612035	-0.238274	-0.750478
11	6	0	3.006752	-3.042899	1.417503
12	1	0	2.449942	-2.735401	-0.580867
13	8	0	1.482165	-0.351985	1.623652
14	6	0	-1.764051	-3.328626	0.301181
15	6	0	-2.250202	-2.074381	-0.489969
16	6	0	-1.199918	-0.951195	-0.000889
17	6	0	0.031566	-1.820358	0.331061
18	6	0	-0.297156	-3.096529	0.506134
19	1	0	-2.271309	-3.414983	1.270731
20	1	0	-1.971226	-4.258163	-0.235629
21	6	0	-2.068059	-2.393349	-1.987748
22	6	0	-1.678401	-0.250290	1.292743
23	1	0	0.391454	-3.886024	0.778917
24	1	0	-2.373076	-1.573779	-2.638849
25	1	0	-1.025921	-2.626854	-2.213791
26	1	0	-2.659967	-3.267920	-2.263669
27	1	0	-0.903167	0.414781	1.669996
28	1	0	-2.574108	0.348097	1.122029
29	1	0	-1.906830	-0.968513	2.082390
30	6	0	-3.752008	-1.771968	-0.174925
31	6	0	-4.320830	-0.579609	-0.974777
32	6	0	-5.641794	-0.020518	-0.450730
33	6	0	-6.155037	1.213408	-1.216603
34	6	0	-5.642668	2.397574	-0.390658
35	6	0	-5.475055	1.794907	1.001371
36	8	0	-5.483305	0.439006	0.922937
37	1	0	-6.399084	-0.802150	-0.408195
38	1	0	-7.247865	1.218046	-1.230675
39	1	0	-5.808970	1.224313	-2.250518
40	1	0	-4.630281	2.668316	-0.713621
41	6	0	-6.509459	3.652582	-0.392473
42	1	0	-3.806206	-1.505956	0.882265
43	1	0	-4.492849	-0.880373	-2.013896
44	1	0	-3.597499	0.237854	-1.008544
45	8	0	-5.339334	2.374563	2.041612
46	1	0	-6.108855	4.393863	0.299697
47	1	0	-6.548366	4.094149	-1.390449
48	1	0	-7.531307	3.420949	-0.082832
49	1	0	1.456007	-0.881318	-1.625605
50	6	0	3.129448	0.127370	-0.788013
51	6	0	3.589698	0.208053	-2.251550

52	6	0	3.545468	1.420512	-0.035333
53	1	0	4.656819	0.427622	-2.328078
54	1	0	3.398189	-0.722954	-2.786065
55	1	0	3.046772	0.992458	-2.783995
56	6	0	3.232847	2.769175	-0.687887
57	6	0	3.822258	3.928263	0.087445
58	8	0	4.658264	3.852843	0.952863
59	8	0	3.298694	5.102379	-0.332748
60	6	0	3.817410	6.280831	0.308646
61	6	0	5.065436	-1.688999	-0.537695
62	1	0	4.046617	-0.672727	0.993349
63	6	0	6.248428	-1.259028	-0.095876
64	6	0	4.989383	-2.804874	-1.551557
65	1	0	7.178080	-1.660834	-0.482899
66	1	0	6.329480	-0.493749	0.667538
67	1	0	5.982122	-3.047935	-1.931986
68	1	0	4.574831	-3.713931	-1.104887
69	1	0	4.353393	-2.556986	-2.403950
70	1	0	2.164195	2.953773	-0.794683
71	1	0	3.651345	2.836903	-1.696929
72	1	0	4.628370	1.377699	0.107678
73	1	0	3.107710	1.399035	0.963062
74	8	0	2.705061	-4.211993	1.460318
75	1	0	3.625924	-2.605317	2.226623
76	6	0	1.272173	-0.954968	2.893684
77	1	0	0.944084	-0.162859	3.567292
78	1	0	0.505608	-1.731993	2.858170
79	1	0	2.197427	-1.383457	3.291793
80	6	0	-4.654920	-3.005667	-0.364582
81	1	0	-5.670451	-2.799651	-0.021228
82	1	0	-4.720601	-3.308886	-1.412550
83	1	0	-4.300197	-3.861471	0.209520
84	1	0	4.891476	6.363488	0.143446
85	1	0	3.293903	7.115899	-0.149984
86	1	0	3.622881	6.248024	1.380328

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.970113	-0.053450	-1.185439
2	6	0	0.400815	0.650093	-1.205051
3	1	0	-1.022532	-0.666276	-2.085728
4	1	0	-1.757999	0.698878	-1.275781
5	1	0	0.458473	1.427549	-0.442825
6	1	0	0.522221	1.144238	-2.173064
7	6	0	3.757973	-1.004475	-0.252392
8	6	0	2.686359	-1.924904	0.369492
9	6	0	1.396203	-1.038795	0.397524
10	6	0	1.492087	-0.394129	-0.999275
11	6	0	3.124806	-2.557539	1.670941
12	1	0	2.446657	-2.763504	-0.294458
13	8	0	1.514010	0.032264	1.352551
14	6	0	-1.732768	-3.196266	0.887296
15	6	0	-2.278476	-2.139018	-0.121662
16	6	0	-1.228564	-0.928844	0.074147
17	6	0	0.041514	-1.701593	0.504238
18	6	0	-0.262262	-2.913295	0.958097
19	1	0	-2.190535	-3.082142	1.878443
20	1	0	-1.948609	-4.218816	0.566610
21	6	0	-2.158577	-2.760169	-1.528009
22	6	0	-1.648988	0.004873	1.233709
23	1	0	0.443473	-3.632199	1.355723
24	1	0	-2.515748	-2.099880	-2.318366
25	1	0	-1.122284	-3.017360	-1.754905
26	1	0	-2.740244	-3.681994	-1.584708
27	1	0	-0.875814	0.749129	1.418281
28	1	0	-2.572833	0.537320	1.006766
29	1	0	-1.803865	-0.546232	2.163085
30	6	0	-3.770181	-1.793945	0.198605
31	6	0	-4.396218	-0.790407	-0.793794
32	6	0	-5.710502	-0.161513	-0.336010
33	6	0	-6.266411	0.908909	-1.293606
34	6	0	-5.748773	2.227712	-0.710138
35	6	0	-5.531913	1.886974	0.761573
36	8	0	-5.519293	0.538468	0.927386
37	1	0	-6.452736	-0.931567	-0.129772
38	1	0	-7.359048	0.899534	-1.272616
39	1	0	-5.951753	0.737662	-2.323423
40	1	0	-4.750329	2.445732	-1.107563
41	6	0	-6.634229	3.453222	-0.911152
42	1	0	-3.782050	-1.323776	1.183630
43	1	0	-4.598024	-1.289514	-1.747707
44	1	0	-3.694314	0.016396	-1.013469
45	8	0	-5.376349	2.644630	1.676927
46	1	0	-6.225683	4.310942	-0.375956
47	1	0	-6.707431	3.707641	-1.970536
48	1	0	-7.643483	3.270879	-0.534429
49	1	0	1.238481	-1.219802	-1.674919
50	6	0	2.996914	-0.086155	-1.304603
51	6	0	3.258451	-0.517464	-2.761669

52	6	0	3.401871	1.409443	-1.235388
53	1	0	4.292497	-0.341433	-3.062697
54	1	0	3.049793	-1.577397	-2.914006
55	1	0	2.615117	0.053598	-3.437625
56	6	0	3.401763	2.132979	0.110846
57	6	0	3.635821	3.618659	-0.040131
58	8	0	3.577333	4.249532	-1.067356
59	8	0	3.907172	4.187427	1.156722
60	6	0	4.104132	5.611444	1.139722
61	6	0	5.005697	-1.708529	-0.757690
62	1	0	4.086882	-0.357368	0.561631
63	6	0	5.021036	-2.951096	-1.235516
64	6	0	6.275695	-0.903043	-0.667833
65	1	0	5.941847	-3.403908	-1.584334
66	1	0	4.134683	-3.571127	-1.296629
67	1	0	7.126956	-1.445211	-1.081319
68	1	0	6.188474	0.049361	-1.199665
69	1	0	6.494936	-0.662474	0.377328
70	1	0	4.162053	1.747548	0.793237
71	1	0	2.455294	2.004693	0.638849
72	1	0	2.755653	1.965089	-1.918585
73	1	0	4.403335	1.502628	-1.665803
74	8	0	4.152828	-2.305218	2.249160
75	1	0	2.436856	-3.321648	2.087026
76	6	0	1.412052	-0.275361	2.740002
77	1	0	2.367198	-0.610520	3.148219
78	1	0	1.123830	0.649537	3.240431
79	1	0	0.646695	-1.030661	2.934399
80	6	0	-4.657714	-3.048688	0.304205
81	1	0	-5.658399	-2.786338	0.652371
82	1	0	-4.770337	-3.555333	-0.657714
83	1	0	-4.260778	-3.770603	1.018012
84	1	0	4.306932	5.889552	2.170914
85	1	0	4.946300	5.872407	0.499146
86	1	0	3.209573	6.116179	0.775158

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.093964	0.133266	-1.141612
2	6	0	0.299343	0.784274	-1.060439
3	1	0	-1.121107	-0.447788	-2.064112
4	1	0	-1.848710	0.917074	-1.246812
5	1	0	0.350676	1.515799	-0.253479
6	1	0	0.484971	1.326419	-1.992408
7	6	0	3.543651	-1.178345	-0.187588
8	6	0	2.386153	-1.992683	0.448830
9	6	0	1.159196	-1.023461	0.489861
10	6	0	1.348129	-0.304419	-0.861649
11	6	0	2.775914	-2.686229	1.734323
12	1	0	2.071034	-2.804046	-0.217140
13	8	0	1.301265	-0.016368	1.508351
14	6	0	-2.088665	-3.039454	0.776115
15	6	0	-2.544545	-1.918326	-0.208703
16	6	0	-1.445673	-0.771347	0.072047
17	6	0	-0.231145	-1.620819	0.514437
18	6	0	-0.609720	-2.832174	0.909562
19	1	0	-2.577677	-2.939303	1.753807
20	1	0	-2.341509	-4.037367	0.408367
21	6	0	-2.404205	-2.490662	-1.633657
22	6	0	-1.858120	0.138256	1.253827
23	1	0	0.045225	-3.599375	1.303702
24	1	0	-2.699803	-1.783574	-2.408877
25	1	0	-1.374715	-2.792212	-1.835502
26	1	0	-3.029300	-3.378235	-1.746436
27	1	0	-1.047430	0.821171	1.502743
28	1	0	-2.735198	0.740161	1.013716
29	1	0	-2.088283	-0.439752	2.150610
30	6	0	-4.028001	-1.511881	0.073951
31	6	0	-4.561270	-0.424389	-0.882504
32	6	0	-5.895096	0.200656	-0.477335
33	6	0	-6.328764	1.386341	-1.359796
34	6	0	-5.839782	2.616081	-0.587873
35	6	0	-5.777959	2.112561	0.851202
36	8	0	-5.806822	0.753923	0.866967
37	1	0	-6.673618	-0.559416	-0.426797
38	1	0	-7.418076	1.412343	-1.444494
39	1	0	-5.918135	1.316175	-2.367453
40	1	0	-4.801803	2.840383	-0.861020
41	6	0	-6.670628	3.886400	-0.736651
42	1	0	-4.054565	-1.094786	1.082142
43	1	0	-4.702869	-0.845898	-1.883579
44	1	0	-3.829401	0.378443	-0.990886
45	8	0	-5.701617	2.761792	1.855417
46	1	0	-6.295150	4.667126	-0.074441
47	1	0	-6.633464	4.254875	-1.763916
48	1	0	-7.716114	3.700999	-0.479124
49	1	0	1.130897	-1.080548	-1.607361
50	6	0	2.864921	0.001668	-1.024658
51	6	0	3.221090	0.006772	-2.521288

52	6	0	3.227677	1.385050	-0.423215
53	1	0	4.297120	0.056506	-2.687494
54	1	0	2.854833	-0.883487	-3.034460
55	1	0	2.767380	0.873229	-3.010480
56	6	0	4.702874	1.781636	-0.501205
57	6	0	4.951044	3.186245	0.003224
58	8	0	4.114866	4.039062	0.170077
59	8	0	6.268362	3.390787	0.231989
60	6	0	6.625576	4.710740	0.676863
61	6	0	4.557797	-2.046139	-0.920068
62	1	0	4.083064	-0.718028	0.639659
63	6	0	5.864540	-1.832688	-0.776398
64	6	0	4.073086	-3.187252	-1.784022
65	1	0	6.598011	-2.434767	-1.300941
66	1	0	6.250747	-1.064349	-0.117892
67	1	0	4.882337	-3.570724	-2.406398
68	1	0	3.713900	-4.020114	-1.170460
69	1	0	3.248589	-2.901648	-2.441353
70	1	0	5.079059	1.755381	-1.528790
71	1	0	5.346243	1.106780	0.065603
72	1	0	2.909805	1.417608	0.617774
73	1	0	2.647410	2.151926	-0.941278
74	8	0	3.846330	-2.578922	2.280329
75	1	0	2.008404	-3.362563	2.163648
76	6	0	1.131524	-0.395094	2.869074
77	1	0	2.035234	-0.853648	3.277019
78	1	0	0.933027	0.524767	3.419501
79	1	0	0.286330	-1.074706	3.003401
80	6	0	-4.981929	-2.721909	0.078643
81	1	0	-5.970398	-2.433243	0.440007
82	1	0	-5.110091	-3.148931	-0.919448
83	1	0	-4.629937	-3.515402	0.737834
84	1	0	6.339500	5.454616	-0.066572
85	1	0	6.131222	4.941415	1.620228
86	1	0	7.704973	4.692472	0.804820

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891294	0.176995	-1.150270
2	6	0	0.492183	0.842147	-1.021087
3	1	0	-0.897847	-0.366196	-2.095895
4	1	0	-1.652299	0.957327	-1.233143
5	1	0	0.518338	1.535668	-0.179784
6	1	0	0.681141	1.430197	-1.924568
7	6	0	3.740221	-1.095286	-0.135874
8	6	0	2.575737	-1.999671	0.347538
9	6	0	1.352744	-1.033266	0.447401
10	6	0	1.555248	-0.239415	-0.858417
11	6	0	2.973074	-2.803374	1.567065
12	1	0	2.299060	-2.729080	-0.413264
13	8	0	1.497463	-0.085809	1.522824
14	6	0	-1.868596	-3.084576	0.619359
15	6	0	-2.332641	-1.924572	-0.315248
16	6	0	-1.246798	-0.779800	0.021233
17	6	0	-0.031127	-1.638888	0.433489
18	6	0	-0.391818	-2.872968	0.771710
19	1	0	-2.361251	-3.034070	1.599230
20	1	0	-2.112074	-4.067418	0.207025
21	6	0	-2.182511	-2.428957	-1.764782
22	6	0	-1.680202	0.079843	1.232618
23	1	0	0.280576	-3.641203	1.131781
24	1	0	-2.478141	-1.687999	-2.508048
25	1	0	-1.150465	-2.716332	-1.973809
26	1	0	-2.801040	-3.314239	-1.922372
27	1	0	-0.872780	0.750186	1.523938
28	1	0	-2.554542	0.691040	1.004916
29	1	0	-1.920727	-0.536672	2.101002
30	6	0	-3.820542	-1.542083	-0.024775
31	6	0	-4.367064	-0.445935	-0.966008
32	6	0	-5.613100	0.270950	-0.471955
33	6	0	-6.189471	1.310248	-1.445124
34	6	0	-6.772965	2.386707	-0.521864
35	6	0	-5.948171	2.220949	0.752537
36	8	0	-5.292181	1.030690	0.729257
37	1	0	-6.384437	-0.447545	-0.182074
38	1	0	-6.927106	0.869577	-2.117389
39	1	0	-5.384158	1.725247	-2.056617
40	1	0	-6.600294	3.395016	-0.900574
41	6	0	-8.267849	2.222743	-0.210549
42	1	0	-3.852293	-1.143677	0.991068
43	1	0	-4.612056	-0.883370	-1.940417
44	1	0	-3.611194	0.318252	-1.153670
45	8	0	-5.862488	2.981017	1.675105
46	1	0	-8.583904	2.947188	0.541145
47	1	0	-8.860777	2.381157	-1.113632
48	1	0	-8.491625	1.222603	0.169210
49	1	0	1.367545	-0.974307	-1.650863
50	6	0	3.074488	0.100400	-0.966760
51	6	0	3.471939	0.111444	-2.450571

52	6	0	3.361991	1.485114	-0.329500
53	1	0	4.532906	0.312793	-2.602554
54	1	0	3.254564	-0.844958	-2.927968
55	1	0	2.912837	0.887615	-2.980807
56	6	0	4.829718	1.953116	-0.312195
57	6	0	4.939712	3.293782	0.374048
58	8	0	5.165646	3.458040	1.547795
59	8	0	4.722659	4.313218	-0.487128
60	6	0	4.755745	5.631376	0.088261
61	6	0	4.872458	-1.868715	-0.802878
62	1	0	4.168895	-0.639311	0.763327
63	6	0	4.703180	-3.030772	-1.433986
64	6	0	6.255263	-1.275341	-0.692505
65	1	0	5.545110	-3.543325	-1.884665
66	1	0	3.744182	-3.522172	-1.531116
67	1	0	6.519294	-1.092269	0.354178
68	1	0	7.004651	-1.942307	-1.119843
69	1	0	6.330113	-0.314752	-1.207797
70	1	0	5.226227	2.041353	-1.324447
71	1	0	5.450981	1.262141	0.255003
72	1	0	2.988812	1.480962	0.694009
73	1	0	2.782128	2.233566	-0.876373
74	8	0	2.552038	-3.901985	1.836364
75	1	0	3.735381	-2.329644	2.220972
76	6	0	1.317146	-0.548857	2.853723
77	1	0	1.148473	0.335976	3.467493
78	1	0	2.208638	-1.062252	3.228507
79	1	0	0.458798	-1.217853	2.944239
80	6	0	-4.760258	-2.762475	-0.047097
81	1	0	-5.774261	-2.476521	0.240399
82	1	0	-4.820953	-3.214530	-1.040181
83	1	0	-4.442935	-3.534844	0.653583
84	1	0	5.732896	5.829460	0.528005
85	1	0	4.560340	6.313784	-0.735059
86	1	0	3.991539	5.729202	0.858952

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.940060	0.143914	-1.135579
2	6	0	0.443988	0.811507	-1.030796
3	1	0	-0.953883	-0.416791	-2.070871
4	1	0	-1.703020	0.921272	-1.226341
5	1	0	0.477114	1.524468	-0.206222
6	1	0	0.626663	1.377602	-1.949125
7	6	0	3.705071	-1.134708	-0.187426
8	6	0	2.552791	-1.974128	0.418882
9	6	0	1.317741	-1.023229	0.480520
10	6	0	1.507618	-0.265723	-0.849423
11	6	0	2.959563	-2.708261	1.676130
12	1	0	2.256644	-2.772262	-0.271124
13	8	0	1.442321	-0.039726	1.525411
14	6	0	-1.907497	-3.080432	0.709153
15	6	0	-2.371696	-1.944516	-0.253891
16	6	0	-1.287331	-0.790774	0.056249
17	6	0	-0.065839	-1.635892	0.484307
18	6	0	-0.430935	-2.860504	0.850506
19	1	0	-2.398663	-3.003771	1.687927
20	1	0	-2.150865	-4.073260	0.321610
21	6	0	-2.219483	-2.483455	-1.690673
22	6	0	-1.718831	0.090258	1.252903
23	1	0	0.232126	-3.629109	1.227952
24	1	0	-2.520225	-1.762283	-2.450822
25	1	0	-1.185903	-2.768716	-1.894854
26	1	0	-2.833188	-3.375676	-1.826608
27	1	0	-0.914980	0.772992	1.523725
28	1	0	-2.599808	0.688437	1.017278
29	1	0	-1.948920	-0.509545	2.135749
30	6	0	-3.860507	-1.558428	0.027324
31	6	0	-4.407557	-0.483022	-0.936969
32	6	0	-5.661156	0.234842	-0.463711
33	6	0	-6.230628	1.260697	-1.455068
34	6	0	-6.827267	2.345837	-0.550440
35	6	0	-6.016111	2.197409	0.734737
36	8	0	-5.355128	1.009038	0.731659
37	1	0	-6.433237	-0.482959	-0.174079
38	1	0	-6.959810	0.809734	-2.129702
39	1	0	-5.420435	1.671337	-2.063005
40	1	0	-6.653293	3.350197	-0.938875
41	6	0	-8.325034	2.181027	-0.253769
42	1	0	-3.893514	-1.138628	1.034468
43	1	0	-4.643289	-0.938763	-1.905230
44	1	0	-3.655073	0.282330	-1.132566
45	8	0	-5.943338	2.967178	1.650045
46	1	0	-8.651522	2.913396	0.485660
47	1	0	-8.908214	2.326928	-1.165239
48	1	0	-8.550130	1.184782	0.135359
49	1	0	1.312507	-1.024171	-1.618769
50	6	0	3.024098	0.067648	-0.988419
51	6	0	3.385854	0.113696	-2.481308

52	6	0	3.350441	1.438084	-0.337703
53	1	0	4.453318	0.261762	-2.648697
54	1	0	3.109053	-0.809117	-2.991310
55	1	0	2.859417	0.940307	-2.966942
56	6	0	4.829380	1.872035	-0.368530
57	6	0	4.988665	3.214693	0.303612
58	8	0	5.187073	3.386786	1.480881
59	8	0	4.850049	4.231756	-0.578317
60	6	0	4.936802	5.554193	-0.019717
61	6	0	4.726622	-1.978176	-0.943004
62	1	0	4.237295	-0.698896	0.659276
63	6	0	4.401903	-3.000987	-1.732440
64	6	0	6.170117	-1.598895	-0.741788
65	1	0	5.164160	-3.570666	-2.251072
66	1	0	3.378726	-3.315108	-1.903024
67	1	0	6.839879	-2.271458	-1.278983
68	1	0	6.368261	-0.579846	-1.087252
69	1	0	6.424935	-1.630284	0.321745
70	1	0	5.199007	1.944229	-1.391759
71	1	0	5.448869	1.167699	0.186023
72	1	0	3.016265	1.426922	0.698498
73	1	0	2.765650	2.205297	-0.853476
74	8	0	4.061051	-2.671244	2.167520
75	1	0	2.177791	-3.348361	2.132343
76	6	0	1.299436	-0.463577	2.874998
77	1	0	0.455994	-1.146952	3.003097
78	1	0	2.210993	-0.935677	3.250362
79	1	0	1.115152	0.437469	3.460086
80	6	0	-4.797932	-2.780835	0.030439
81	1	0	-5.811446	-2.490992	0.315146
82	1	0	-4.860688	-3.251901	-0.953632
83	1	0	-4.478436	-3.539427	0.745202
84	1	0	4.807663	6.234021	-0.858211
85	1	0	4.153640	5.706358	0.722770
86	1	0	5.907847	5.704983	0.451286

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960672	0.216039	-1.156765
2	6	0	0.435481	0.859981	-1.054183
3	1	0	-0.982700	-0.352121	-2.087515
4	1	0	-1.708649	1.006875	-1.256626
5	1	0	0.482298	1.578224	-0.234888
6	1	0	0.630336	1.417405	-1.975491
7	6	0	3.653015	-1.092603	-0.110952
8	6	0	2.477561	-1.976599	0.395061
9	6	0	1.270850	-0.984348	0.466330
10	6	0	1.478480	-0.236319	-0.866441
11	6	0	2.863407	-2.736519	1.642851
12	1	0	2.200410	-2.728947	-0.344554
13	8	0	1.440338	-0.006392	1.510472
14	6	0	-1.978925	-2.979845	0.712064
15	6	0	-2.428454	-1.842396	-0.257198
16	6	0	-1.326588	-0.702646	0.042595
17	6	0	-0.121945	-1.566726	0.477656
18	6	0	-0.498876	-2.784621	0.854329
19	1	0	-2.468785	-2.891498	1.690680
20	1	0	-2.237365	-3.971207	0.330533
21	6	0	-2.286947	-2.392411	-1.690815
22	6	0	-1.744476	0.198194	1.229186
23	1	0	0.162829	-3.552778	1.234259
24	1	0	-2.577860	-1.671861	-2.455677
25	1	0	-1.257963	-2.694966	-1.893381
26	1	0	-2.913868	-3.276444	-1.819899
27	1	0	-0.930917	0.872924	1.492482
28	1	0	-2.615805	0.808301	0.988161
29	1	0	-1.984119	-0.388180	2.118365
30	6	0	-3.910351	-1.431905	0.024805
31	6	0	-4.441464	-0.349167	-0.939901
32	6	0	-5.693672	0.376048	-0.474331
33	6	0	-6.240478	1.419864	-1.459524
34	6	0	-6.842335	2.496659	-0.548375
35	6	0	-6.051152	2.323964	0.746323
36	8	0	-5.396958	1.132346	0.735010
37	1	0	-6.476599	-0.337573	-0.204254
38	1	0	-6.963001	0.984031	-2.151097
39	1	0	-5.418210	1.832748	-2.049436
40	1	0	-6.655491	3.505089	-0.919906
41	6	0	-8.345379	2.338675	-0.275584
42	1	0	-3.934914	-1.009597	1.031211
43	1	0	-4.673439	-0.799298	-1.911733
44	1	0	-3.681098	0.410660	-1.126919
45	8	0	-5.988488	3.079580	1.674264
46	1	0	-8.677380	3.063355	0.468974
47	1	0	-8.914393	2.500842	-1.193265
48	1	0	-8.582982	1.338957	0.096892
49	1	0	1.265344	-0.993945	-1.630712
50	6	0	3.001324	0.064527	-1.001108
51	6	0	3.400679	0.026489	-2.486213

52	6	0	3.349669	1.462573	-0.426790
53	1	0	4.482972	0.030684	-2.621582
54	1	0	3.009251	-0.855898	-2.993966
55	1	0	2.997070	0.901280	-3.003745
56	6	0	4.822521	1.867882	-0.503419
57	6	0	5.062843	3.273141	0.002791
58	8	0	4.221805	4.121196	0.167690
59	8	0	6.378607	3.483670	0.236103
60	6	0	6.728354	4.806860	0.678433
61	6	0	4.792262	-1.910725	-0.701520
62	1	0	4.061565	-0.594285	0.771452
63	6	0	6.052424	-1.688016	-0.326812
64	6	0	4.477072	-3.032045	-1.663270
65	1	0	6.875052	-2.266825	-0.731175
66	1	0	6.309223	-0.927272	0.401258
67	1	0	5.388459	-3.409078	-2.128505
68	1	0	4.001766	-3.870183	-1.144409
69	1	0	3.794462	-2.723377	-2.456365
70	1	0	5.195836	1.845697	-1.532203
71	1	0	5.471714	1.194491	0.057667
72	1	0	3.020361	1.514847	0.610434
73	1	0	2.768420	2.213743	-0.965803
74	8	0	2.509484	-3.862708	1.898644
75	1	0	3.554520	-2.206766	2.330194
76	6	0	1.217968	-0.407798	2.855054
77	1	0	0.344712	-1.055664	2.953166
78	1	0	2.088911	-0.921587	3.274711
79	1	0	1.050473	0.505755	3.425855
80	6	0	-4.866745	-2.639519	0.032580
81	1	0	-5.872849	-2.335802	0.328767
82	1	0	-4.946144	-3.106202	-0.952459
83	1	0	-4.550788	-3.405359	0.740993
84	1	0	7.807465	4.794150	0.809295
85	1	0	6.440751	5.547019	-0.068019
86	1	0	6.230106	5.037939	1.619629

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.980094	0.515751	-0.760345
2	6	0	0.357268	1.107629	-0.277321
3	1	0	-0.882543	0.336313	-1.831575
4	1	0	-1.765256	1.267243	-0.640998
5	1	0	0.281939	1.464806	0.750497
6	1	0	0.599470	1.975079	-0.898890
7	6	0	3.595357	-0.976393	0.212074
8	6	0	2.434568	-2.011147	0.236225
9	6	0	1.166191	-1.150038	0.534989
10	6	0	1.446167	0.046369	-0.396816
11	6	0	2.754048	-3.171967	1.150419
12	1	0	2.272169	-2.442146	-0.752556
13	8	0	1.171743	-0.629049	1.879622
14	6	0	-1.960820	-3.170482	-0.330633
15	6	0	-2.392675	-1.763642	-0.849591
16	6	0	-1.394854	-0.793630	-0.033207
17	6	0	-0.182092	-1.728780	0.178059
18	6	0	-0.514840	-3.007364	0.030882
19	1	0	-2.539380	-3.470218	0.552851
20	1	0	-2.121528	-3.951427	-1.078683
21	6	0	-2.089624	-1.731723	-2.361019
22	6	0	-1.974496	-0.416850	1.351102
23	1	0	0.156803	-3.845799	0.165956
24	1	0	-2.353878	-0.783174	-2.828926
25	1	0	-1.030398	-1.913835	-2.551292
26	1	0	-2.648272	-2.515891	-2.874973
27	1	0	-1.233854	0.128473	1.934197
28	1	0	-2.857754	0.216532	1.262006
29	1	0	-2.257465	-1.300712	1.925747
30	6	0	-3.917512	-1.524942	-0.594922
31	6	0	-4.431642	-0.179363	-1.151827
32	6	0	-5.776330	0.278943	-0.592023
33	6	0	-6.252195	1.642227	-1.128182
34	6	0	-5.774982	2.640066	-0.068266
35	6	0	-5.672991	1.779587	1.188025
36	8	0	-5.682289	0.463856	0.850518
37	1	0	-6.534804	-0.489492	-0.735480
38	1	0	-7.343250	1.661312	-1.189050
39	1	0	-5.859440	1.847336	-2.124375
40	1	0	-4.748160	2.956085	-0.287997
41	6	0	-6.637467	3.881871	0.132553
42	1	0	-4.057567	-1.503604	0.487229
43	1	0	-4.545898	-0.249705	-2.238864
44	1	0	-3.704093	0.614636	-0.971757
45	8	0	-5.582754	2.147364	2.325204
46	1	0	-6.266236	4.473415	0.970042
47	1	0	-6.631239	4.506167	-0.763421
48	1	0	-7.672598	3.606497	0.347958
49	1	0	1.350797	-0.375983	-1.404659
50	6	0	2.954300	0.413420	-0.250902
51	6	0	3.483653	0.937942	-1.595043

52	6	0	3.158696	1.497780	0.840554
53	1	0	4.569256	1.043903	-1.597860
54	1	0	3.215466	0.279522	-2.422240
55	1	0	3.050120	1.918146	-1.809128
56	6	0	4.600764	1.974466	1.101293
57	6	0	5.195413	2.973877	0.133241
58	8	0	6.311783	2.918501	-0.321433
59	8	0	4.346121	3.992835	-0.130426
60	6	0	4.857885	5.018945	-0.997702
61	6	0	4.825055	-1.495577	-0.520813
62	1	0	3.901695	-0.831394	1.251045
63	6	0	6.034481	-1.392766	0.029901
64	6	0	4.656768	-2.202126	-1.845600
65	1	0	6.920764	-1.759794	-0.474529
66	1	0	6.187117	-0.937979	1.001599
67	1	0	5.625029	-2.365844	-2.319632
68	1	0	4.187455	-3.181498	-1.710280
69	1	0	4.029470	-1.645233	-2.543548
70	1	0	5.305112	1.147283	1.163711
71	1	0	4.613883	2.474781	2.076171
72	1	0	2.759467	1.111724	1.777803
73	1	0	2.556198	2.371556	0.585433
74	8	0	2.440310	-4.318928	0.939060
75	1	0	3.354629	-2.922028	2.049067
76	6	0	0.869450	-1.518651	2.946256
77	1	0	0.546199	-0.900990	3.784579
78	1	0	0.069299	-2.214997	2.687347
79	1	0	1.750165	-2.089686	3.257513
80	6	0	-4.791530	-2.675844	-1.129043
81	1	0	-5.838468	-2.526825	-0.857515
82	1	0	-4.746009	-2.753148	-2.218331
83	1	0	-4.495832	-3.638853	-0.712799
84	1	0	4.052614	5.742118	-1.100638
85	1	0	5.738940	5.485384	-0.557491
86	1	0	5.125052	4.599776	-1.967545

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.913464	0.606201	-0.805959
2	6	0	0.436034	1.172310	-0.327656
3	1	0	-0.815233	0.401398	-1.872594
4	1	0	-1.678449	1.380747	-0.706495
5	1	0	0.363563	1.550900	0.692551
6	1	0	0.704134	2.021565	-0.963022
7	6	0	3.620343	-0.989828	0.198009
8	6	0	2.430863	-1.985822	0.247388
9	6	0	1.184029	-1.090850	0.530060
10	6	0	1.498492	0.081445	-0.420073
11	6	0	2.722125	-3.147053	1.173520
12	1	0	2.245292	-2.426370	-0.732045
13	8	0	1.197674	-0.550812	1.867170
14	6	0	-1.994313	-3.042551	-0.308980
15	6	0	-2.388453	-1.633964	-0.851752
16	6	0	-1.365032	-0.676330	-0.052560
17	6	0	-0.178753	-1.639911	0.178180
18	6	0	-0.545194	-2.911732	0.052473
19	1	0	-2.581528	-3.313104	0.578361
20	1	0	-2.174672	-3.831472	-1.044306
21	6	0	-2.087077	-1.635717	-2.363709
22	6	0	-1.935859	-0.254730	1.322667
23	1	0	0.103776	-3.764529	0.205716
24	1	0	-2.329022	-0.689119	-2.847406
25	1	0	-1.032663	-1.846198	-2.551108
26	1	0	-2.664720	-2.415353	-2.863488
27	1	0	-1.179434	0.280286	1.895102
28	1	0	-2.800905	0.401383	1.218973
29	1	0	-2.242561	-1.118959	1.915291
30	6	0	-3.905560	-1.350724	-0.600491
31	6	0	-4.381730	0.000474	-1.178752
32	6	0	-5.686558	0.527711	-0.604841
33	6	0	-6.184259	1.838845	-1.231805
34	6	0	-6.878177	2.557811	-0.068558
35	6	0	-6.189148	1.962090	1.156971
36	8	0	-5.507259	0.839759	0.807249
37	1	0	-6.467559	-0.235912	-0.651838
38	1	0	-6.842997	1.655572	-2.081845
39	1	0	-5.331316	2.421899	-1.588537
40	1	0	-6.682198	3.630934	-0.070027
41	6	0	-8.394973	2.331827	0.013169
42	1	0	-4.043606	-1.308142	0.481503
43	1	0	-4.520561	-0.089264	-2.261933
44	1	0	-3.628135	0.775099	-1.028934
45	8	0	-6.219024	2.367444	2.284433
46	1	0	-8.798711	2.773025	0.925373
47	1	0	-8.891592	2.793381	-0.842769
48	1	0	-8.644056	1.267473	0.014235
49	1	0	1.401601	-0.355328	-1.421604
50	6	0	3.014606	0.419430	-0.265037
51	6	0	3.555070	0.892785	-1.622070

52	6	0	3.207786	1.518196	0.813652
53	1	0	4.625827	1.101155	-1.598002
54	1	0	3.395533	0.139310	-2.394892
55	1	0	3.051238	1.812152	-1.928125
56	6	0	4.635499	1.999214	1.109319
57	6	0	5.167812	3.035191	0.143491
58	8	0	4.520843	3.921446	-0.356639
59	8	0	6.496264	2.884799	-0.063944
60	6	0	7.110715	3.875437	-0.908265
61	6	0	4.824860	-1.533137	-0.564728
62	1	0	3.952241	-0.851768	1.233115
63	6	0	4.732980	-2.420262	-1.555706
64	6	0	6.184738	-1.050074	-0.124077
65	1	0	5.622189	-2.782930	-2.058118
66	1	0	3.793299	-2.822525	-1.910202
67	1	0	6.978916	-1.587144	-0.643899
68	1	0	6.325958	0.016430	-0.316073
69	1	0	6.322499	-1.199050	0.952085
70	1	0	5.350536	1.184026	1.202153
71	1	0	4.627523	2.504466	2.082156
72	1	0	2.772932	1.154862	1.743465
73	1	0	2.629351	2.396757	0.520514
74	8	0	2.293645	-4.266695	1.033930
75	1	0	3.411725	-2.923106	2.015089
76	6	0	0.898925	-1.428893	2.943097
77	1	0	0.600966	-0.801408	3.783488
78	1	0	0.083347	-2.113650	2.701338
79	1	0	1.775560	-2.013350	3.242470
80	6	0	-4.811722	-2.484832	-1.115600
81	1	0	-5.854829	-2.297743	-0.852048
82	1	0	-4.764950	-2.584102	-2.202993
83	1	0	-4.547149	-3.448361	-0.679931
84	1	0	6.986321	4.869619	-0.479856
85	1	0	8.162910	3.606331	-0.954367
86	1	0	6.664847	3.857235	-1.902373

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.923726	0.021683	-1.165714
2	6	0	0.440621	0.741015	-1.154558
3	1	0	-0.965306	-0.558944	-2.087742
4	1	0	-1.718437	0.769164	-1.233154
5	1	0	0.485620	1.491679	-0.365008
6	1	0	0.561212	1.271008	-2.103595
7	6	0	3.794522	-0.884866	-0.193858
8	6	0	2.731312	-1.883232	0.332192
9	6	0	1.441356	-0.995236	0.391592
10	6	0	1.540272	-0.301432	-0.981972
11	6	0	3.184597	-2.572376	1.597919
12	1	0	2.525015	-2.674834	-0.391282
13	8	0	1.557061	0.040693	1.386675
14	6	0	-1.650981	-3.203083	0.794212
15	6	0	-2.208788	-2.120102	-0.181108
16	6	0	-1.178890	-0.901335	0.061247
17	6	0	0.096415	-1.673340	0.471781
18	6	0	-0.184130	-2.905486	0.883876
19	1	0	-2.114707	-3.129177	1.786605
20	1	0	-1.851616	-4.217328	0.439209
21	6	0	-2.072912	-2.690418	-1.607224
22	6	0	-1.620513	-0.011882	1.247587
23	1	0	0.540975	-3.618743	1.255237
24	1	0	-2.435770	-2.008643	-2.376660
25	1	0	-1.032120	-2.926346	-1.836311
26	1	0	-2.641355	-3.617601	-1.698343
27	1	0	-0.858406	0.736285	1.461157
28	1	0	-2.549850	0.516401	1.033124
29	1	0	-1.773513	-0.594766	2.157674
30	6	0	-3.707471	-1.808525	0.140971
31	6	0	-4.343693	-0.782028	-0.821581
32	6	0	-5.659168	-0.173295	-0.341204
33	6	0	-6.238668	0.902520	-1.278643
34	6	0	-5.728738	2.219943	-0.685537
35	6	0	-5.488421	1.863628	0.778867
36	8	0	-5.460319	0.513953	0.928463
37	1	0	-6.390461	-0.953756	-0.134936
38	1	0	-7.330819	0.880531	-1.244502
39	1	0	-5.934787	0.747188	-2.314186
40	1	0	-4.738510	2.455153	-1.093514
41	6	0	-6.631470	3.437054	-0.859202
42	1	0	-3.732958	-1.373281	1.141606
43	1	0	-4.546948	-1.257906	-1.787023
44	1	0	-3.647978	0.034682	-1.023883
45	8	0	-5.328146	2.612446	1.700915
46	1	0	-6.226182	4.292962	-0.318629
47	1	0	-6.722012	3.703789	-1.914229
48	1	0	-7.633313	3.237638	-0.471477
49	1	0	1.289603	-1.103502	-1.685535
50	6	0	3.047171	0.014724	-1.266238
51	6	0	3.347218	-0.408888	-2.718465

52	6	0	3.461002	1.505340	-1.185874
53	1	0	4.403966	-0.287954	-2.963859
54	1	0	3.068256	-1.446605	-2.907848
55	1	0	2.773826	0.213375	-3.411269
56	6	0	3.400383	2.235722	0.156501
57	6	0	3.560088	3.731536	0.001447
58	8	0	3.396787	4.363708	-1.013217
59	8	0	3.891037	4.306079	1.180272
60	6	0	4.010376	5.739237	1.162885
61	6	0	5.122133	-1.499252	-0.607589
62	1	0	4.015684	-0.227648	0.648051
63	6	0	6.261558	-0.858549	-0.341956
64	6	0	5.144625	-2.847906	-1.284681
65	1	0	7.222786	-1.263671	-0.637059
66	1	0	6.274981	0.092071	0.179382
67	1	0	6.161241	-3.115743	-1.574743
68	1	0	4.773125	-3.632223	-0.618180
69	1	0	4.520618	-2.875475	-2.180277
70	1	0	4.164688	1.892455	0.856076
71	1	0	2.449308	2.067048	0.665902
72	1	0	2.851898	2.063019	-1.900405
73	1	0	4.485150	1.581549	-1.565580
74	8	0	2.908065	-3.709761	1.897142
75	1	0	3.850523	-1.977922	2.256024
76	6	0	1.433144	-0.322357	2.755698
77	1	0	0.672603	-1.090355	2.909472
78	1	0	2.384542	-0.675243	3.166254
79	1	0	1.140794	0.579837	3.293671
80	6	0	-4.576455	-3.079513	0.196256
81	1	0	-5.585809	-2.843882	0.538884
82	1	0	-4.668389	-3.556761	-0.782688
83	1	0	-4.176863	-3.817200	0.892134
84	1	0	4.788612	6.048312	0.465502
85	1	0	3.066017	6.196881	0.868842
86	1	0	4.272560	6.021721	2.179355

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.894564	0.609838	-0.785323
2	6	0	0.460206	1.163969	-0.306394
3	1	0	-0.800884	0.416730	-1.854525
4	1	0	-1.655251	1.387095	-0.674816
5	1	0	0.395405	1.534528	0.717292
6	1	0	0.731781	2.016337	-0.935990
7	6	0	3.626454	-1.008640	0.240232
8	6	0	2.437555	-2.010863	0.256766
9	6	0	1.194390	-1.106705	0.536634
10	6	0	1.514397	0.066689	-0.410903
11	6	0	2.711563	-3.171296	1.184998
12	1	0	2.273087	-2.444367	-0.730737
13	8	0	1.213064	-0.566032	1.873231
14	6	0	-1.986702	-3.042413	-0.321744
15	6	0	-2.374990	-1.628284	-0.855203
16	6	0	-1.352120	-0.679086	-0.044984
17	6	0	-0.169534	-1.647996	0.182157
18	6	0	-0.538434	-2.917887	0.045514
19	1	0	-2.577964	-3.317926	0.561336
20	1	0	-2.166475	-3.825075	-1.063808
21	6	0	-2.068032	-1.619223	-2.365920
22	6	0	-1.926943	-0.266443	1.331311
23	1	0	0.107635	-3.774454	0.191164
24	1	0	-2.306731	-0.668570	-2.843129
25	1	0	-1.013295	-1.830109	-2.551125
26	1	0	-2.645145	-2.394051	-2.873709
27	1	0	-1.172920	0.267371	1.908045
28	1	0	-2.792335	0.389268	1.228844
29	1	0	-2.234319	-1.133938	1.918746
30	6	0	-3.892204	-1.343540	-0.607008
31	6	0	-4.362606	0.014192	-1.174464
32	6	0	-5.668412	0.539067	-0.600573
33	6	0	-6.160291	1.857632	-1.216506
34	6	0	-6.856486	2.567159	-0.048823
35	6	0	-6.174242	1.957176	1.173436
36	8	0	-5.493947	0.836453	0.815213
37	1	0	-6.451132	-0.222066	-0.658334
38	1	0	-6.816496	1.684325	-2.070586
39	1	0	-5.304533	2.441752	-1.564635
40	1	0	-6.657104	3.639606	-0.038864
41	6	0	-8.374326	2.345291	0.024676
42	1	0	-4.034035	-1.310599	0.474840
43	1	0	-4.497432	-0.065140	-2.258947
44	1	0	-3.607570	0.785361	-1.014325
45	8	0	-6.207660	2.351102	2.304805
46	1	0	-8.780198	2.778320	0.939843
47	1	0	-8.866100	2.817348	-0.828324
48	1	0	-8.626944	1.281815	0.013687
49	1	0	1.405943	-0.365864	-1.413139
50	6	0	3.033052	0.387560	-0.265878
51	6	0	3.582855	0.858862	-1.621918

52	6	0	3.276058	1.492372	0.796161
53	1	0	4.672243	0.932606	-1.621195
54	1	0	3.300554	0.183965	-2.431091
55	1	0	3.185835	1.846768	-1.862959
56	6	0	4.729818	1.953790	0.980074
57	6	0	5.144897	3.109561	0.094358
58	8	0	4.405532	3.926278	-0.397245
59	8	0	6.488126	3.153631	-0.046338
60	6	0	7.000295	4.262506	-0.805996
61	6	0	4.862848	-1.578883	-0.440453
62	1	0	3.905832	-0.847748	1.284348
63	6	0	6.052890	-1.515113	0.158455
64	6	0	4.721196	-2.297951	-1.761177
65	1	0	6.943263	-1.926428	-0.303291
66	1	0	6.180911	-1.057957	1.132963
67	1	0	5.700872	-2.521054	-2.185103
68	1	0	4.194447	-3.248542	-1.633273
69	1	0	4.158081	-1.720977	-2.496097
70	1	0	5.452115	1.147042	0.859735
71	1	0	4.863123	2.322976	2.003538
72	1	0	2.895864	1.134848	1.752018
73	1	0	2.685346	2.371995	0.533230
74	8	0	2.379151	-4.313186	0.973756
75	1	0	3.296271	-2.928213	2.095803
76	6	0	0.875238	-1.427246	2.952096
77	1	0	0.069661	-2.116755	2.691748
78	1	0	1.741035	-2.004471	3.292732
79	1	0	0.544741	-0.787707	3.771089
80	6	0	-4.799271	-2.470488	-1.136034
81	1	0	-5.842567	-2.284218	-0.872758
82	1	0	-4.750300	-2.558185	-2.224334
83	1	0	-4.537532	-3.439118	-0.710052
84	1	0	6.726862	5.206244	-0.334467
85	1	0	8.079969	4.136137	-0.812934
86	1	0	6.604925	4.243487	-1.821241

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.887572	0.070735	-1.074975
2	6	0	0.475866	0.757613	-0.874266
3	1	0	-0.866753	-0.396694	-2.060017
4	1	0	-1.668954	0.834518	-1.109720
5	1	0	0.472968	1.383787	0.019084
6	1	0	0.653765	1.415205	-1.729268
7	6	0	3.764445	-1.165094	-0.089416
8	6	0	2.626135	-2.117174	0.329889
9	6	0	1.366495	-1.201783	0.456157
10	6	0	1.570677	-0.301596	-0.779041
11	6	0	2.991774	-2.987894	1.511725
12	1	0	2.382540	-2.823856	-0.471733
13	8	0	1.452152	-0.324213	1.596534
14	6	0	-1.809051	-3.347527	0.393191
15	6	0	-2.293162	-2.118826	-0.436821
16	6	0	-1.235719	-0.984139	0.009513
17	6	0	-0.001700	-1.842317	0.366712
18	6	0	-0.341604	-3.109081	0.583474
19	1	0	-2.313621	-3.400666	1.366401
20	1	0	-2.019583	-4.293467	-0.112855
21	6	0	-2.121423	-2.488744	-1.924142
22	6	0	-1.704108	-0.240019	1.282392
23	1	0	0.334104	-3.900660	0.882105
24	1	0	-2.426400	-1.689557	-2.599859
25	1	0	-1.082133	-2.734909	-2.150002
26	1	0	-2.720309	-3.368385	-2.166523
27	1	0	-0.921387	0.428281	1.636894
28	1	0	-2.594437	0.361126	1.094314
29	1	0	-1.937279	-0.931361	2.094354
30	6	0	-3.792569	-1.801830	-0.123599
31	6	0	-4.360893	-0.630686	-0.954370
32	6	0	-5.681585	-0.056798	-0.445211
33	6	0	-6.184425	1.167210	-1.233547
34	6	0	-5.671493	2.361949	-0.423208
35	6	0	-5.514429	1.780661	0.978986
36	8	0	-5.527527	0.423214	0.921499
37	1	0	-6.443083	-0.833898	-0.394532
38	1	0	-7.277077	1.176602	-1.254455
39	1	0	-5.831989	1.160272	-2.265335
40	1	0	-4.656093	2.623259	-0.744373
41	6	0	-6.532602	3.620600	-0.449916
42	1	0	-3.840994	-1.505631	0.925726
43	1	0	-4.533432	-0.957903	-1.985383
44	1	0	-3.636812	0.184778	-1.009558
45	8	0	-5.382289	2.375348	2.010962
46	1	0	-6.132367	4.371104	0.232438
47	1	0	-6.563928	4.046320	-1.454999
48	1	0	-7.557180	3.398541	-0.142326
49	1	0	1.411442	-0.977515	-1.629522
50	6	0	3.085164	0.069431	-0.848927
51	6	0	3.490924	0.173410	-2.327190

52	6	0	3.510493	1.355685	-0.088451
53	1	0	4.531585	0.484218	-2.446870
54	1	0	3.375557	-0.781833	-2.839620
55	1	0	2.866128	0.903811	-2.847348
56	6	0	3.145846	2.712159	-0.701951
57	6	0	3.839357	3.857613	0.004658
58	8	0	4.891299	3.793468	0.590740
59	8	0	3.138092	5.006623	-0.126370
60	6	0	3.740396	6.172752	0.462715
61	6	0	4.931076	-1.835141	-0.796296
62	1	0	4.170335	-0.765539	0.841490
63	6	0	4.810072	-2.886710	-1.604793
64	6	0	6.283303	-1.234896	-0.512112
65	1	0	5.677658	-3.324445	-2.084766
66	1	0	3.859373	-3.358594	-1.823437
67	1	0	6.511215	-1.312759	0.555391
68	1	0	7.072859	-1.737311	-1.072363
69	1	0	6.312577	-0.170017	-0.762157
70	1	0	2.075574	2.909576	-0.697569
71	1	0	3.466065	2.773053	-1.747585
72	1	0	4.598225	1.333544	0.008094
73	1	0	3.115364	1.306827	0.926688
74	8	0	4.046878	-2.949796	2.095178
75	1	0	2.223431	-3.724762	1.820446
76	6	0	1.279517	-0.881890	2.894051
77	1	0	2.193864	-1.358935	3.254602
78	1	0	1.041029	-0.049295	3.556217
79	1	0	0.457443	-1.601616	2.923801
80	6	0	-4.700498	-3.037413	-0.273768
81	1	0	-5.712689	-2.818665	0.071183
82	1	0	-4.774468	-3.368505	-1.312690
83	1	0	-4.345106	-3.878957	0.320826
84	1	0	4.710121	6.372247	0.007035
85	1	0	3.049125	6.988261	0.265627
86	1	0	3.872635	6.031696	1.535031

Coordinates of conformers at B3LYP/6-31G+(d,p) in the PCM ($CHCl_3$)

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.086187	0.145393	-1.149989
2	6	0	0.309409	0.798067	-1.051480
3	1	0	-1.111393	-0.415812	-2.088103
4	1	0	-1.842344	0.933797	-1.237700
5	1	0	0.358283	1.505040	-0.218361
6	1	0	0.492094	1.371400	-1.968617
7	6	0	3.556225	-1.168552	-0.193426
8	6	0	2.386393	-2.063946	0.311950
9	6	0	1.174181	-1.076507	0.427968
10	6	0	1.364402	-0.297209	-0.892340
11	6	0	2.802960	-2.862841	1.525638
12	1	0	2.087693	-2.794171	-0.443890
13	8	0	1.357361	-0.122988	1.496900
14	6	0	-2.087806	-3.074407	0.704016
15	6	0	-2.547782	-1.922599	-0.249599
16	6	0	-1.435162	-0.789607	0.045491
17	6	0	-0.221658	-1.661862	0.450149
18	6	0	-0.600885	-2.888766	0.823662
19	1	0	-2.561798	-2.990039	1.694110
20	1	0	-2.359057	-4.063831	0.318116
21	6	0	-2.430701	-2.458828	-1.694853
22	6	0	-1.828546	0.096082	1.256875
23	1	0	0.065178	-3.665001	1.185800
24	1	0	-2.733756	-1.727584	-2.448779
25	1	0	-1.402989	-2.761333	-1.918361
26	1	0	-3.064075	-3.341891	-1.822253
27	1	0	-1.002055	0.757709	1.523916
28	1	0	-2.696673	0.722501	1.033102
29	1	0	-2.067695	-0.505736	2.139125
30	6	0	-4.027679	-1.510271	0.062471
31	6	0	-4.565814	-0.399081	-0.870265
32	6	0	-5.871636	0.260586	-0.422433
33	6	0	-6.324418	1.438661	-1.309191
34	6	0	-5.763787	2.677603	-0.593949
35	6	0	-5.652095	2.206415	0.852131
36	8	0	-5.706823	0.855170	0.910900
37	1	0	-6.663323	-0.481415	-0.305630
38	1	0	-7.418381	1.489791	-1.337371
39	1	0	-5.965598	1.337024	-2.336380
40	1	0	-4.730496	2.862593	-0.920801
41	6	0	-6.566448	3.970114	-0.749547
42	1	0	-4.036838	-1.114400	1.083057
43	1	0	-4.756201	-0.813638	-1.868819
44	1	0	-3.816936	0.387423	-1.004045
45	8	0	-5.517654	2.882621	1.851147
46	1	0	-6.128629	4.771679	-0.148569
47	1	0	-6.574362	4.288796	-1.796317
48	1	0	-7.603453	3.828180	-0.427331
49	1	0	1.151775	-1.040222	-1.674661
50	6	0	2.887543	0.024454	-1.031991

51	6	0	3.260945	0.006983	-2.526430
52	6	0	3.200631	1.420004	-0.423274
53	1	0	4.325355	0.189474	-2.698444
54	1	0	3.019577	-0.954976	-2.987242
55	1	0	2.703000	0.786374	-3.058516
56	6	0	4.667212	1.863156	-0.424111
57	6	0	4.853867	3.270687	0.105201
58	8	0	3.983965	4.116248	0.214315
59	8	0	6.144619	3.500212	0.430413
60	6	0	6.465405	4.828238	0.899143
61	6	0	4.679597	-1.960164	-0.863242
62	1	0	3.995917	-0.705836	0.700428
63	6	0	4.489973	-3.122792	-1.506325
64	6	0	6.074821	-1.386554	-0.749718
65	1	0	5.326050	-3.648151	-1.960073
66	1	0	3.518658	-3.594084	-1.613398
67	1	0	6.169365	-0.434165	-1.282746
68	1	0	6.334889	-1.189235	0.298158
69	1	0	6.818785	-2.073214	-1.162415
70	1	0	5.092460	1.864458	-1.436166
71	1	0	5.301854	1.200772	0.170642
72	1	0	2.827826	1.444254	0.603051
73	1	0	2.625720	2.168621	-0.977964
74	8	0	2.420792	-3.993465	1.777533
75	1	0	3.539349	-2.373290	2.196054
76	6	0	1.168213	-0.564344	2.837633
77	1	0	1.066162	0.337831	3.445561
78	1	0	0.267226	-1.175899	2.948116
79	1	0	2.032309	-1.132220	3.205848
80	6	0	-4.992064	-2.716705	0.054889
81	1	0	-5.982173	-2.425325	0.418807
82	1	0	-5.122676	-3.132499	-0.950491
83	1	0	-4.643103	-3.520802	0.707514
84	1	0	5.908002	5.053937	1.810766
85	1	0	7.535976	4.813257	1.098722
86	1	0	6.227774	5.569024	0.132581

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.821828	0.153939	-1.055909
2	6	0	0.548310	0.821810	-0.807185
3	1	0	-0.789982	-0.266699	-2.064790
4	1	0	-1.598012	0.927546	-1.065614
5	1	0	0.541768	1.412727	0.114046
6	1	0	0.739058	1.512397	-1.636219
7	6	0	3.801985	-1.130115	0.018385
8	6	0	2.658113	-2.149205	0.248513
9	6	0	1.403117	-1.222290	0.430299
10	6	0	1.636037	-0.253285	-0.750566
11	6	0	3.015081	-3.129188	1.343581
12	1	0	2.452557	-2.745859	-0.645554
13	8	0	1.499548	-0.418950	1.626945
14	6	0	-1.795399	-3.328354	0.249760
15	6	0	-2.256657	-2.056377	-0.535609
16	6	0	-1.192587	-0.953078	-0.026544
17	6	0	0.030083	-1.843209	0.298699
18	6	0	-0.321991	-3.122949	0.462920
19	1	0	-2.310278	-3.411379	1.219094
20	1	0	-2.016928	-4.253301	-0.295123
21	6	0	-2.066616	-2.363108	-2.039143
22	6	0	-1.665731	-0.265240	1.281176
23	1	0	0.355088	-3.926713	0.731756
24	1	0	-2.361532	-1.532803	-2.685929
25	1	0	-1.021864	-2.602269	-2.260691
26	1	0	-2.665610	-3.232198	-2.327460
27	1	0	-0.875929	0.376638	1.676471
28	1	0	-2.547941	0.358469	1.111452
29	1	0	-1.916378	-0.995903	2.056437
30	6	0	-3.760864	-1.738038	-0.227516
31	6	0	-4.298418	-0.507805	-0.996855
32	6	0	-5.666842	0.005973	-0.545521
33	6	0	-6.123645	1.299576	-1.250013
34	6	0	-5.676752	2.417518	-0.295544
35	6	0	-5.639907	1.707971	1.054127
36	8	0	-5.628201	0.366110	0.878455
37	1	0	-6.421701	-0.778451	-0.618859
38	1	0	-7.214777	1.309478	-1.347590
39	1	0	-5.695508	1.392355	-2.251177
40	1	0	-4.634103	2.694751	-0.507605
41	6	0	-6.531245	3.685914	-0.291094
42	1	0	-3.822996	-1.507630	0.841184
43	1	0	-4.398003	-0.752201	-2.062383
44	1	0	-3.587070	0.321836	-0.936764
45	8	0	-5.609024	2.206194	2.160634
46	1	0	-6.178098	4.387626	0.469341
47	1	0	-6.481915	4.180151	-1.266088
48	1	0	-7.579752	3.451183	-0.079365
49	1	0	1.482882	-0.878626	-1.642040
50	6	0	3.159976	0.108296	-0.768199
51	6	0	3.624209	0.183426	-2.235573

52	6	0	3.549122	1.403480	0.002951
53	1	0	4.665748	0.508700	-2.327278
54	1	0	3.537892	-0.790749	-2.725479
55	1	0	3.006107	0.891059	-2.799087
56	6	0	3.280739	2.747631	-0.687035
57	6	0	3.826000	3.922375	0.098977
58	8	0	4.652665	3.865384	0.992182
59	8	0	3.293416	5.085906	-0.333223
60	6	0	3.773144	6.290522	0.303190
61	6	0	5.089352	-1.714378	-0.545471
62	1	0	4.056552	-0.742849	1.014168
63	6	0	5.149840	-2.877930	-1.211689
64	6	0	6.349564	-0.922269	-0.274633
65	1	0	6.098396	-3.258661	-1.581031
66	1	0	4.277791	-3.491074	-1.413755
67	1	0	6.307700	0.077050	-0.722688
68	1	0	6.491976	-0.774640	0.803500
69	1	0	7.232207	-1.431249	-0.671400
70	1	0	2.219038	2.931056	-0.864196
71	1	0	3.763324	2.793201	-1.671687
72	1	0	4.622974	1.359022	0.211169
73	1	0	3.050203	1.390046	0.975867
74	8	0	2.647052	-4.291555	1.383299
75	1	0	3.690850	-2.743998	2.134359
76	6	0	1.290677	-1.054848	2.884324
77	1	0	1.073219	-0.259307	3.601117
78	1	0	0.448854	-1.754304	2.857709
79	1	0	2.188775	-1.587107	3.223157
80	6	0	-4.681379	-2.954731	-0.467837
81	1	0	-5.689322	-2.760538	-0.089003
82	1	0	-4.772838	-3.196813	-1.532694
83	1	0	-4.319558	-3.846700	0.049269
84	1	0	4.849787	6.396094	0.153085
85	1	0	3.237023	7.105883	-0.180484
86	1	0	3.553746	6.267828	1.372705

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.052220	0.069589	-1.179980
2	6	0	0.325530	0.764189	-1.130240
3	1	0	-1.073640	-0.531321	-2.093370
4	1	0	-1.831600	0.832149	-1.289800
5	1	0	0.366260	1.504299	-0.325980
6	1	0	0.477360	1.304969	-2.072350
7	6	0	3.638430	-1.073180	-0.238330
8	6	0	2.501380	-1.982620	0.313370
9	6	0	1.263100	-1.026000	0.408730
10	6	0	1.412970	-0.295030	-0.944010
11	6	0	2.954750	-2.727640	1.548450
12	1	0	2.213820	-2.747240	-0.412450
13	8	0	1.434150	-0.024570	1.435440
14	6	0	-1.939810	-3.095091	0.819100
15	6	0	-2.446300	-1.994321	-0.170000
16	6	0	-1.357850	-0.823271	0.058880
17	6	0	-0.115510	-1.647041	0.476700
18	6	0	-0.456380	-2.867751	0.903980
19	1	0	-2.397590	-2.983941	1.814120
20	1	0	-2.192310	-4.105371	0.477100
21	6	0	-2.340510	-2.584431	-1.595060
22	6	0	-1.753360	0.100999	1.240330
23	1	0	0.235450	-3.612221	1.284070
24	1	0	-2.673360	-1.890461	-2.371260
25	1	0	-1.309370	-2.870431	-1.824330
26	1	0	-2.953760	-3.486851	-1.677680
27	1	0	-0.942460	0.797619	1.462920
28	1	0	-2.644800	0.690959	1.010130
29	1	0	-1.955930	-0.470901	2.151140
30	6	0	-3.930770	-1.606371	0.152570
31	6	0	-4.515100	-0.553421	-0.819430
32	6	0	-5.825050	0.098689	-0.373210
33	6	0	-6.335130	1.208719	-1.314840
34	6	0	-5.790010	2.503449	-0.692070
35	6	0	-5.619770	2.123069	0.775090
36	8	0	-5.637920	0.777279	0.916460
37	1	0	-6.592420	-0.654721	-0.187590
38	1	0	-7.430390	1.229309	-1.313760
39	1	0	-6.002470	1.054319	-2.344280
40	1	0	-4.773301	2.698009	-1.062450
41	6	0	-6.636221	3.760819	-0.897770
42	1	0	-3.931850	-1.164571	1.154340
43	1	0	-4.717890	-1.020171	-1.792120
44	1	0	-3.787470	0.241809	-1.008030
45	8	0	-5.469871	2.861589	1.726770
46	1	0	-6.205211	4.609599	-0.359990
47	1	0	-6.685861	4.015189	-1.960840
48	1	0	-7.658111	3.608549	-0.534510
49	1	0	1.211050	-1.073330	-1.694070
50	6	0	2.925410	0.061440	-1.118160
51	6	0	3.281050	-0.007230	-2.614920

52	6	0	3.202750	1.490860	-0.572640
53	1	0	4.334840	0.209790	-2.809670
54	1	0	3.071990	-0.997970	-3.027860
55	1	0	2.686380	0.725260	-3.173010
56	6	0	4.668320	1.980280	-0.608540
57	6	0	4.745749	3.414060	-0.136210
58	8	0	4.548439	4.391530	-0.838760
59	8	0	5.029639	3.500820	1.179750
60	6	0	5.072439	4.830020	1.744420
61	6	0	4.781270	-1.854950	-0.886190
62	1	0	4.069630	-0.560680	0.631890
63	6	0	4.625100	-3.052540	-1.471500
64	6	0	6.156230	-1.228340	-0.816850
65	1	0	5.473750	-3.569480	-1.911310
66	1	0	3.669910	-3.561830	-1.543210
67	1	0	6.918570	-1.904440	-1.212880
68	1	0	6.209080	-0.295500	-1.388670
69	1	0	6.422840	-0.979770	0.218400
70	1	0	5.064500	1.961340	-1.627020
71	1	0	5.301780	1.362000	0.030550
72	1	0	2.840880	1.547000	0.456600
73	1	0	2.605210	2.195590	-1.162180
74	8	0	2.596230	-3.853670	1.850300
75	1	0	3.695290	-2.201450	2.185470
76	6	0	1.289400	-0.419560	2.795960
77	1	0	1.156720	0.500380	3.370440
78	1	0	0.419650	-1.066461	2.947760
79	1	0	2.185740	-0.931730	3.168440
80	6	0	-4.862840	-2.836091	0.218140
81	1	0	-5.855730	-2.552271	0.580540
82	1	0	-4.995290	-3.304561	-0.763530
83	1	0	-4.485570	-3.597521	0.905260
84	1	0	4.104989	5.322800	1.626880
85	1	0	5.305749	4.688660	2.798720
86	1	0	5.847339	5.423970	1.255250

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.894205	0.018072	-1.196963
2	6	0	0.477859	0.728825	-1.183647
3	1	0	-0.931249	-0.575704	-2.114236
4	1	0	-1.685810	0.770990	-1.281787
5	1	0	0.525200	1.487423	-0.397173
6	1	0	0.606319	1.249137	-2.140150
7	6	0	3.824304	-0.928910	-0.203831
8	6	0	2.746033	-1.916691	0.315205
9	6	0	1.461420	-1.013662	0.378597
10	6	0	1.571767	-0.323175	-0.998358
11	6	0	3.202845	-2.626410	1.569961
12	1	0	2.523225	-2.697856	-0.418939
13	8	0	1.594238	0.024003	1.373247
14	6	0	-1.675296	-3.175467	0.810668
15	6	0	-2.210496	-2.097910	-0.189416
16	6	0	-1.163625	-0.889806	0.041609
17	6	0	0.103901	-1.674341	0.464976
18	6	0	-0.200177	-2.901340	0.900973
19	1	0	-2.143640	-3.073357	1.801788
20	1	0	-1.892282	-4.195473	0.473306
21	6	0	-2.071090	-2.694433	-1.609049
22	6	0	-1.593351	0.018390	1.223814
23	1	0	0.514323	-3.620876	1.286958
24	1	0	-2.424436	-2.021107	-2.394127
25	1	0	-1.027946	-2.942032	-1.828276
26	1	0	-2.648662	-3.620331	-1.687504
27	1	0	-0.813260	0.751832	1.438655
28	1	0	-2.510703	0.568353	0.996652
29	1	0	-1.765671	-0.559267	2.137135
30	6	0	-3.711017	-1.762022	0.119107
31	6	0	-4.317758	-0.715469	-0.845449
32	6	0	-5.696624	-0.179395	-0.455932
33	6	0	-6.220691	0.947946	-1.368882
34	6	0	-5.815708	2.237205	-0.637476
35	6	0	-5.713309	1.781206	0.814331
36	8	0	-5.644028	0.431321	0.879040
37	1	0	-6.419152	-0.992186	-0.368072
38	1	0	-7.311971	0.892625	-1.446317
39	1	0	-5.808020	0.879727	-2.378464
40	1	0	-4.794933	2.526644	-0.925309
41	6	0	-6.738933	3.441539	-0.829633
42	1	0	-3.738478	-1.333542	1.126382
43	1	0	-4.430985	-1.154023	-1.845341
44	1	0	-3.641667	0.137569	-0.959785
45	8	0	-5.679484	2.469657	1.813663
46	1	0	-6.406320	4.285188	-0.218927
47	1	0	-6.741108	3.754572	-1.878120
48	1	0	-7.767313	3.196371	-0.543795
49	1	0	1.320720	-1.126388	-1.704788
50	6	0	3.086526	-0.010010	-1.274225
51	6	0	3.390280	-0.460162	-2.721198

52	6	0	3.471867	1.493738	-1.200538
53	1	0	4.430663	-0.271242	-3.003126
54	1	0	3.198617	-1.528685	-2.858021
55	1	0	2.751351	0.088735	-3.423271
56	6	0	3.442496	2.204150	0.156785
57	6	0	3.617390	3.702142	0.036125
58	8	0	3.516940	4.358840	-0.986000
59	8	0	3.884780	4.258021	1.238322
60	6	0	4.023861	5.694916	1.268922
61	6	0	5.138165	-1.564405	-0.633053
62	1	0	4.064664	-0.284753	0.651011
63	6	0	5.270307	-2.862158	-0.948029
64	6	0	6.338435	-0.644183	-0.648780
65	1	0	6.236105	-3.269636	-1.234823
66	1	0	4.440679	-3.561450	-0.936534
67	1	0	7.248193	-1.179208	-0.934050
68	1	0	6.202458	0.187474	-1.349647
69	1	0	6.498996	-0.196635	0.340507
70	1	0	4.220469	1.838223	0.834247
71	1	0	2.498321	2.027352	0.682113
72	1	0	2.812767	2.036517	-1.885968
73	1	0	4.477325	1.610706	-1.621624
74	8	0	2.863032	-3.752716	1.892607
75	1	0	3.922513	-2.070668	2.205006
76	6	0	1.476442	-0.336163	2.746480
77	1	0	1.288752	0.590824	3.293715
78	1	0	0.647866	-1.029879	2.920286
79	1	0	2.403139	-0.780949	3.130598
80	6	0	-4.601003	-3.023829	0.159051
81	1	0	-5.596170	-2.785228	0.546327
82	1	0	-4.733352	-3.465338	-0.835186
83	1	0	-4.187278	-3.793498	0.815145
84	1	0	4.852296	6.010208	0.630852
85	1	0	3.101278	6.173353	0.932968
86	1	0	4.226664	5.943360	2.309808

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022274	0.154094	-1.108582
2	6	0	0.360775	0.825180	-0.967436
3	1	0	-1.030667	-0.361871	-2.072483
4	1	0	-1.791852	0.932241	-1.164120
5	1	0	0.390017	1.490572	-0.099789
6	1	0	0.539931	1.445325	-1.854394
7	6	0	3.635614	-1.126056	-0.178350
8	6	0	2.477340	-2.060657	0.280855
9	6	0	1.247417	-1.099704	0.431220
10	6	0	1.433276	-0.258764	-0.851191
11	6	0	2.899833	-2.905413	1.461288
12	1	0	2.194675	-2.761884	-0.507975
13	8	0	1.406060	-0.190980	1.541659
14	6	0	-1.977581	-3.169782	0.578944
15	6	0	-2.451628	-1.981665	-0.321680
16	6	0	-1.363738	-0.842796	0.038011
17	6	0	-0.137903	-1.710074	0.413994
18	6	0	-0.496165	-2.960642	0.723904
19	1	0	-2.462984	-3.145190	1.566686
20	1	0	-2.224575	-4.144022	0.141410
21	6	0	-2.311460	-2.444703	-1.790167
22	6	0	-1.787952	-0.021901	1.283967
23	1	0	0.182519	-3.739738	1.055272
24	1	0	-2.618315	-1.681988	-2.510572
25	1	0	-1.276934	-2.720431	-2.017009
26	1	0	-2.929270	-3.330073	-1.967250
27	1	0	-0.976567	0.640189	1.592700
28	1	0	-2.664138	0.599325	1.077471
29	1	0	-2.027557	-0.668123	2.134133
30	6	0	-3.942587	-1.613272	-0.006021
31	6	0	-4.495815	-0.476781	-0.899386
32	6	0	-5.801062	0.161748	-0.420642
33	6	0	-6.282755	1.344684	-1.285310
34	6	0	-5.719506	2.580981	-0.567735
35	6	0	-5.577019	2.095623	0.871007
36	8	0	-5.618887	0.743350	0.916290
37	1	0	-6.581950	-0.590666	-0.297723
38	1	0	-7.377480	1.385623	-1.291112
39	1	0	-5.943616	1.257561	-2.320462
40	1	0	-4.693900	2.777840	-0.911609
41	6	0	-6.535338	3.868274	-0.695459
42	1	0	-3.969642	-1.260226	1.029833
43	1	0	-4.692191	-0.863160	-1.908035
44	1	0	-3.753105	0.318311	-1.016205
45	8	0	-5.429437	2.762590	1.874369
46	1	0	-6.093742	4.667275	-0.093797
47	1	0	-6.564334	4.197839	-1.738493
48	1	0	-7.565327	3.714263	-0.356787
49	1	0	1.238839	-0.967938	-1.668709
50	6	0	2.952299	0.092574	-0.964741
51	6	0	3.335164	0.155691	-2.455336

52	6	0	3.237620	1.460350	-0.282950
53	1	0	4.396947	0.364891	-2.612101
54	1	0	3.112751	-0.786670	-2.963720
55	1	0	2.766456	0.950187	-2.952420
56	6	0	4.710597	1.926466	-0.249768
57	6	0	4.819157	3.259973	0.453246
58	8	0	4.938077	3.407899	1.657993
59	8	0	4.737304	4.294630	-0.409259
60	6	0	4.778893	5.619276	0.165798
61	6	0	4.772804	-1.868161	-0.880977
62	1	0	4.066808	-0.697779	0.736331
63	6	0	4.603151	-3.003949	-1.575381
64	6	0	6.157909	-1.276776	-0.739284
65	1	0	5.448312	-3.494813	-2.050355
66	1	0	3.640078	-3.486542	-1.704165
67	1	0	6.913039	-1.928498	-1.186837
68	1	0	6.234722	-0.296855	-1.223160
69	1	0	6.415881	-1.128824	0.317165
70	1	0	5.117782	2.023507	-1.259036
71	1	0	5.324026	1.221765	0.315139
72	1	0	2.861820	1.422283	0.741747
73	1	0	2.656308	2.225674	-0.810586
74	8	0	2.531564	-4.050889	1.661482
75	1	0	3.626412	-2.435518	2.155847
76	6	0	1.215071	-0.693602	2.860652
77	1	0	0.312031	-1.306782	2.942053
78	1	0	2.077090	-1.280138	3.202983
79	1	0	1.116001	0.180228	3.508901
80	6	0	-4.880921	-2.838071	-0.074529
81	1	0	-5.886555	-2.577518	0.269851
82	1	0	-4.975444	-3.226127	-1.094820
83	1	0	-4.532953	-3.653749	0.564150
84	1	0	4.701128	6.303182	-0.678186
85	1	0	3.942633	5.760263	0.853903
86	1	0	5.720141	5.771104	0.698289

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.821658	0.153800	-1.056135
2	6	0	0.548436	0.821711	-0.807273
3	1	0	-0.789652	-0.266949	-2.064965
4	1	0	-1.597848	0.927398	-1.066044
5	1	0	0.541750	1.412726	0.113893
6	1	0	0.739306	1.512210	-1.636354
7	6	0	3.802001	-1.130081	0.019027
8	6	0	2.658109	-2.149171	0.249058
9	6	0	1.403069	-1.222257	0.430545
10	6	0	1.636169	-0.253362	-0.750375
11	6	0	3.014909	-3.129044	1.344279
12	1	0	2.452715	-2.745913	-0.644988
13	8	0	1.499293	-0.418798	1.627129
14	6	0	-1.795398	-3.328371	0.249710
15	6	0	-2.256563	-2.056458	-0.535816
16	6	0	-1.192564	-0.953111	-0.026709
17	6	0	0.030063	-1.843205	0.298788
18	6	0	-0.322022	-3.122936	0.463060
19	1	0	-2.310409	-3.411327	1.218980
20	1	0	-2.016844	-4.253361	-0.295134
21	6	0	-2.066343	-2.363304	-2.039304
22	6	0	-1.665889	-0.265143	1.280877
23	1	0	0.355027	-3.926671	0.732060
24	1	0	-2.361177	-1.533046	-2.686188
25	1	0	-1.021565	-2.602488	-2.260711
26	1	0	-2.665306	-3.232414	-2.327627
27	1	0	-0.876150	0.376789	1.676209
28	1	0	-2.548086	0.358536	1.110973
29	1	0	-1.916624	-0.995730	2.056180
30	6	0	-3.760809	-1.738104	-0.227930
31	6	0	-4.298277	-0.507915	-0.997401
32	6	0	-5.666735	0.005906	-0.546218
33	6	0	-6.123471	1.299468	-1.250832
34	6	0	-5.676671	2.417470	-0.296389
35	6	0	-5.639936	1.708005	1.053327
36	8	0	-5.628210	0.366134	0.877739
37	1	0	-6.421594	-0.778517	-0.619569
38	1	0	-7.214594	1.309362	-1.348515
39	1	0	-5.695236	1.392185	-2.251960
40	1	0	-4.634007	2.694703	-0.508377
41	6	0	-6.531180	3.685856	-0.292085
42	1	0	-3.823075	-1.507634	0.840749
43	1	0	-4.397769	-0.752382	-2.062922
44	1	0	-3.586924	0.321720	-0.937304
45	8	0	-5.609128	2.206296	2.159805
46	1	0	-6.178108	4.387612	0.468343
47	1	0	-6.481767	4.180041	-1.267102
48	1	0	-7.579702	3.451124	-0.080438
49	1	0	1.483174	-0.878789	-1.641817
50	6	0	3.160103	0.108246	-0.767782
51	6	0	3.624592	0.183248	-2.235081

52	6	0	3.549077	1.403516	0.003315
53	1	0	4.666152	0.508499	-2.326631
54	1	0	3.538346	-0.790965	-2.724922
55	1	0	3.006599	0.890844	-2.798759
56	6	0	3.280832	2.747585	-0.686887
57	6	0	3.825830	3.922435	0.099150
58	8	0	4.652301	3.865575	0.992543
59	8	0	3.293264	5.085893	-0.333267
60	6	0	3.772779	6.290595	0.303146
61	6	0	5.089473	-1.714370	-0.544563
62	1	0	4.056394	-0.742719	1.014817
63	6	0	5.150094	-2.877981	-1.210667
64	6	0	6.349622	-0.922205	-0.273594
65	1	0	6.098717	-3.258723	-1.579824
66	1	0	4.278091	-3.491163	-1.412817
67	1	0	6.491875	-0.774507	0.804551
68	1	0	7.232338	-1.431181	-0.670204
69	1	0	6.307786	0.077085	-0.721714
70	1	0	2.219174	2.930947	-0.864372
71	1	0	3.763697	2.793064	-1.671405
72	1	0	4.622882	1.359091	0.211778
73	1	0	3.049940	1.390186	0.976121
74	8	0	2.646884	-4.291410	1.384052
75	1	0	3.690544	-2.743770	2.135131
76	6	0	1.290228	-1.054573	2.884538
77	1	0	0.448443	-1.754072	2.857847
78	1	0	2.188291	-1.586752	3.223589
79	1	0	1.072603	-0.258967	3.601208
80	6	0	-4.681292	-2.954813	-0.468294
81	1	0	-5.689282	-2.760600	-0.089595
82	1	0	-4.772621	-3.196954	-1.533148
83	1	0	-4.319532	-3.846752	0.048906
84	1	0	4.849449	6.396215	0.153274
85	1	0	3.236718	7.105879	-0.180724
86	1	0	3.553141	6.267983	1.372613

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.857085	0.070228	-1.175256
2	6	0	0.501599	0.800828	-1.083403
3	1	0	-0.862246	-0.466932	-2.127364
4	1	0	-1.659745	0.813767	-1.232772
5	1	0	0.516559	1.507947	-0.249416
6	1	0	0.642336	1.383976	-2.001455
7	6	0	3.853824	-0.881537	-0.146654
8	6	0	2.776370	-1.913762	0.280836
9	6	0	1.479947	-1.030987	0.380964
10	6	0	1.610616	-0.242149	-0.940416
11	6	0	3.217764	-2.701611	1.493754
12	1	0	2.575870	-2.646248	-0.508049
13	8	0	1.581626	-0.065054	1.447273
14	6	0	-1.635636	-3.254115	0.603970
15	6	0	-2.169412	-2.116405	-0.327778
16	6	0	-1.138663	-0.916072	-0.001903
17	6	0	0.130029	-1.712669	0.392045
18	6	0	-0.165902	-2.970042	0.737874
19	1	0	-2.120109	-3.225539	1.592067
20	1	0	-1.834797	-4.251094	0.194617
21	6	0	-2.007277	-2.613681	-1.782793
22	6	0	-1.599247	-0.087778	1.226694
23	1	0	0.550772	-3.705853	1.087600
24	1	0	-2.356817	-1.891054	-2.524593
25	1	0	-0.959870	-2.839430	-2.005638
26	1	0	-2.576236	-3.536165	-1.931956
27	1	0	-0.830221	0.636806	1.501640
28	1	0	-2.517077	0.467837	1.015995
29	1	0	-1.783978	-0.721737	2.099392
30	6	0	-3.677359	-1.817107	-0.016681
31	6	0	-4.285325	-0.714121	-0.915700
32	6	0	-5.670118	-0.213306	-0.500629
33	6	0	-6.191301	0.974379	-1.335338
34	6	0	-5.792528	2.209198	-0.512531
35	6	0	-5.702457	1.652608	0.904517
36	8	0	-5.631388	0.301461	0.874863
37	1	0	-6.390024	-1.032818	-0.476903
38	1	0	-7.282016	0.922889	-1.422652
39	1	0	-5.772733	0.977398	-2.344807
40	1	0	-4.768955	2.516475	-0.770561
41	6	0	-6.713571	3.424996	-0.627425
42	1	0	-3.721642	-1.457566	1.016415
43	1	0	-4.389362	-1.088228	-1.942477
44	1	0	-3.614877	0.149381	-0.970737
45	8	0	-5.678436	2.269243	1.949823
46	1	0	-6.387669	4.222071	0.046251
47	1	0	-6.704620	3.812908	-1.650530
48	1	0	-7.744957	3.160638	-0.371049
49	1	0	1.396607	-0.997818	-1.709044
50	6	0	3.123671	0.116363	-1.148670
51	6	0	3.474467	-0.190214	-2.622185

52	6	0	3.493354	1.612189	-0.928975
53	1	0	4.516690	0.047846	-2.854888
54	1	0	3.314179	-1.245931	-2.859943
55	1	0	2.839729	0.405295	-3.288973
56	6	0	3.372828	2.224555	0.484903
57	6	0	3.781893	3.678781	0.448766
58	8	0	4.931815	4.085091	0.491383
59	8	0	2.718770	4.502260	0.331020
60	6	0	3.003622	5.915514	0.241459
61	6	0	5.177655	-1.473559	-0.608072
62	1	0	4.081085	-0.305349	0.758823
63	6	0	5.321126	-2.741406	-1.023754
64	6	0	6.371698	-0.548193	-0.535111
65	1	0	6.292916	-3.120371	-1.328867
66	1	0	4.495293	-3.443102	-1.079560
67	1	0	7.290847	-1.058142	-0.835708
68	1	0	6.245750	0.327802	-1.181692
69	1	0	6.507664	-0.165500	0.484354
70	1	0	4.049113	1.723625	1.182026
71	1	0	2.358564	2.129844	0.868800
72	1	0	2.872117	2.203201	-1.613352
73	1	0	4.526214	1.757878	-1.264823
74	8	0	2.890197	-3.852692	1.729797
75	1	0	3.913613	-2.179758	2.181863
76	6	0	1.434256	-0.519563	2.789215
77	1	0	1.232012	0.367482	3.394433
78	1	0	0.604109	-1.224701	2.897077
79	1	0	2.353112	-0.988763	3.163186
80	6	0	-4.553606	-3.088027	-0.074505
81	1	0	-5.558025	-2.885302	0.309212
82	1	0	-4.663192	-3.465079	-1.097546
83	1	0	-4.142859	-3.894542	0.537816
84	1	0	3.524137	6.254641	1.139597
85	1	0	3.617953	6.123485	-0.637314
86	1	0	2.032728	6.401334	0.154926

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.094073	0.178073	-1.129221
2	6	0	0.299581	0.835828	-1.029732
3	1	0	-1.118471	-0.377157	-2.070886
4	1	0	-1.853970	0.963523	-1.210500
5	1	0	0.348512	1.539391	-0.193569
6	1	0	0.479484	1.413108	-1.944902
7	6	0	3.554852	-1.112722	-0.170800
8	6	0	2.390157	-2.022273	0.332547
9	6	0	1.173245	-1.037046	0.444439
10	6	0	1.357752	-0.256821	-0.876739
11	6	0	2.807949	-2.803437	1.555129
12	1	0	2.107190	-2.760530	-0.423183
13	8	0	1.353937	-0.080910	1.511156
14	6	0	-2.072948	-3.059372	0.710058
15	6	0	-2.539746	-1.908304	-0.241442
16	6	0	-1.438027	-0.766207	0.060941
17	6	0	-0.218593	-1.630012	0.465793
18	6	0	-0.588132	-2.861171	0.834577
19	1	0	-2.550817	-2.982318	1.698852
20	1	0	-2.334359	-4.049792	0.320038
21	6	0	-2.413030	-2.438332	-1.688137
22	6	0	-1.843454	0.111598	1.274004
23	1	0	0.083311	-3.633649	1.195361
24	1	0	-2.720604	-1.707206	-2.440321
25	1	0	-1.381869	-2.730482	-1.909527
26	1	0	-3.037786	-3.326700	-1.820674
27	1	0	-1.025618	0.782975	1.543501
28	1	0	-2.718273	0.728359	1.049949
29	1	0	-2.077284	-0.494574	2.154649
30	6	0	-4.024466	-1.510823	0.066996
31	6	0	-4.570164	-0.402146	-0.864498
32	6	0	-5.879937	0.248484	-0.415012
33	6	0	-6.345327	1.419665	-1.304357
34	6	0	-5.794024	2.665995	-0.594704
35	6	0	-5.672831	2.200402	0.852444
36	8	0	-5.715612	0.848887	0.915728
37	1	0	-6.665146	-0.499560	-0.293029
38	1	0	-7.439755	1.460913	-1.329951
39	1	0	-5.988198	1.317835	-2.332111
40	1	0	-4.763706	2.859963	-0.925674
41	6	0	-6.609741	3.950192	-0.751601
42	1	0	-4.040997	-1.118406	1.088814
43	1	0	-4.758320	-0.817305	-1.863222
44	1	0	-3.826589	0.389452	-0.998161
45	8	0	-5.540381	2.880870	1.848805
46	1	0	-6.177598	4.758001	-0.154905
47	1	0	-6.624494	4.265235	-1.799395
48	1	0	-7.644166	3.799255	-0.425209
49	1	0	1.140608	-1.000682	-1.656991
50	6	0	2.878576	0.061484	-1.025072
51	6	0	3.259869	0.067401	-2.519679

52	6	0	3.223211	1.449793	-0.415662
53	1	0	4.343253	0.072572	-2.668726
54	1	0	2.858139	-0.800287	-3.049754
55	1	0	2.851827	0.961158	-3.006026
56	6	0	4.694364	1.872853	-0.516312
57	6	0	4.948923	3.249385	0.060395
58	8	0	4.114337	4.122845	0.219041
59	8	0	6.254061	3.419511	0.364168
60	6	0	6.634547	4.718058	0.869278
61	6	0	4.692014	-1.911383	-0.800646
62	1	0	3.974709	-0.631645	0.719634
63	6	0	5.963281	-1.697268	-0.426784
64	6	0	4.367364	-3.004483	-1.797421
65	1	0	6.785080	-2.262116	-0.859273
66	1	0	6.225658	-0.959001	0.326337
67	1	0	5.274672	-3.357514	-2.294912
68	1	0	3.909822	-3.867171	-1.297289
69	1	0	3.662332	-2.676624	-2.566227
70	1	0	5.027597	1.916996	-1.561242
71	1	0	5.366031	1.168681	-0.018985
72	1	0	2.917525	1.461910	0.633105
73	1	0	2.618864	2.209066	-0.922865
74	8	0	2.497170	-3.962868	1.775084
75	1	0	3.478669	-2.274200	2.261672
76	6	0	1.137467	-0.506444	2.853579
77	1	0	1.016150	0.402944	3.447103
78	1	0	0.238039	-1.121853	2.952179
79	1	0	1.996079	-1.063797	3.248717
80	6	0	-4.977166	-2.726475	0.052084
81	1	0	-5.972576	-2.444809	0.409114
82	1	0	-5.096676	-3.142806	-0.954430
83	1	0	-4.625321	-3.527605	0.706812
84	1	0	7.707748	4.656734	1.044446
85	1	0	6.409082	5.492796	0.133190
86	1	0	6.105162	4.933291	1.799944

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.071677	0.123894	-1.152169
2	6	0	0.307833	0.816322	-1.107282
3	1	0	-1.099273	-0.471334	-2.069107
4	1	0	-1.851183	0.887540	-1.252551
5	1	0	0.356155	1.553690	-0.300753
6	1	0	0.456691	1.359305	-2.048527
7	6	0	3.622345	-1.028011	-0.237654
8	6	0	2.487228	-1.936398	0.331074
9	6	0	1.251788	-0.972854	0.426371
10	6	0	1.392516	-0.246589	-0.930224
11	6	0	2.946978	-2.655494	1.576714
12	1	0	2.202805	-2.712813	-0.384913
13	8	0	1.431262	0.032765	1.447184
14	6	0	-1.942790	-3.050950	0.843467
15	6	0	-2.452151	-1.954284	-0.149118
16	6	0	-1.371941	-0.776166	0.083366
17	6	0	-0.125676	-1.594127	0.501519
18	6	0	-0.460799	-2.815760	0.930375
19	1	0	-2.403841	-2.940438	1.837011
20	1	0	-2.188875	-4.063077	0.502413
21	6	0	-2.335512	-2.545194	-1.573025
22	6	0	-1.775169	0.142732	1.266386
23	1	0	0.233807	-3.557710	1.310885
24	1	0	-2.670259	-1.854839	-2.351556
25	1	0	-1.301210	-2.823437	-1.797468
26	1	0	-2.941533	-3.452316	-1.657079
27	1	0	-0.970744	0.846914	1.489277
28	1	0	-2.671254	0.725582	1.036225
29	1	0	-1.973325	-0.431416	2.176678
30	6	0	-3.940833	-1.576986	0.166641
31	6	0	-4.527776	-0.526879	-0.806697
32	6	0	-5.855342	0.099698	-0.376196
33	6	0	-6.368754	1.209658	-1.316053
34	6	0	-5.856628	2.507563	-0.672300
35	6	0	-5.704263	2.116196	0.793975
36	8	0	-5.700449	0.768960	0.922370
37	1	0	-6.612968	-0.668029	-0.210454
38	1	0	-7.464073	1.211360	-1.333116
39	1	0	-6.016344	1.070725	-2.341126
40	1	0	-4.837414	2.722763	-1.023647
41	6	0	-6.720729	3.752207	-0.880894
42	1	0	-3.950140	-1.136669	1.169055
43	1	0	-4.708239	-0.989805	-1.785552
44	1	0	-3.810545	0.281679	-0.978395
45	8	0	-5.583739	2.847931	1.754994
46	1	0	-6.313643	4.603021	-0.327922
47	1	0	-6.756480	4.015863	-1.942262
48	1	0	-7.745937	3.579064	-0.536888
49	1	0	1.176291	-1.027086	-1.673977
50	6	0	2.903129	0.094513	-1.124889
51	6	0	3.253390	0.050228	-2.625731

52	6	0	3.231905	1.512535	-0.577412
53	1	0	4.333038	0.073342	-2.797422
54	1	0	2.860271	-0.846369	-3.112098
55	1	0	2.816262	0.915194	-3.137988
56	6	0	4.697305	1.972715	-0.757775
57	6	0	4.882846	3.356948	-0.181557
58	8	0	4.542349	4.392204	-0.729866
59	8	0	5.448832	3.327745	1.043132
60	6	0	5.625378	4.600934	1.702622
61	6	0	4.760636	-1.831543	-0.859362
62	1	0	4.053480	-0.501436	0.620852
63	6	0	6.034603	-1.578672	-0.520405
64	6	0	4.436733	-2.969715	-1.804328
65	1	0	6.858633	-2.145401	-0.946083
66	1	0	6.296536	-0.805085	0.196589
67	1	0	5.340361	-3.326281	-2.305931
68	1	0	4.005548	-3.819657	-1.260799
69	1	0	3.710363	-2.685905	-2.570736
70	1	0	4.954369	2.030161	-1.818630
71	1	0	5.389168	1.283780	-0.270153
72	1	0	2.969573	1.550236	0.482900
73	1	0	2.591561	2.238245	-1.091373
74	8	0	2.663901	-3.809906	1.852808
75	1	0	3.622029	-2.083907	2.244941
76	6	0	1.257788	-0.340978	2.811176
77	1	0	2.145575	-0.846663	3.210991
78	1	0	1.112413	0.587978	3.367904
79	1	0	0.385232	-0.985465	2.955044
80	6	0	-4.863922	-2.813878	0.226045
81	1	0	-5.858433	-2.539416	0.590949
82	1	0	-4.993583	-3.277914	-0.758133
83	1	0	-4.480620	-3.576318	0.908638
84	1	0	6.095725	4.369275	2.657168
85	1	0	6.267660	5.250984	1.104818
86	1	0	4.658458	5.084531	1.857350

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.052227	0.069587	-1.179976
2	6	0	0.325528	0.764195	-1.130232
3	1	0	-1.073648	-0.531315	-2.093365
4	1	0	-1.831601	0.832147	-1.289791
5	1	0	0.366250	1.504297	-0.325975
6	1	0	0.477348	1.304972	-2.072342
7	6	0	3.638430	-1.073176	-0.238333
8	6	0	2.501382	-1.982617	0.313365
9	6	0	1.263103	-1.026000	0.408727
10	6	0	1.412969	-0.295035	-0.944013
11	6	0	2.954749	-2.727648	1.548442
12	1	0	2.213817	-2.747239	-0.412456
13	8	0	1.434145	-0.024574	1.435437
14	6	0	-1.939811	-3.095100	0.819102
15	6	0	-2.446302	-1.994325	-0.169992
16	6	0	-1.357850	-0.823276	0.058883
17	6	0	-0.115516	-1.647041	0.476697
18	6	0	-0.456377	-2.867761	0.903980
19	1	0	-2.397588	-2.983952	1.814120
20	1	0	-2.192312	-4.105378	0.477101
21	6	0	-2.340521	-2.584432	-1.595062
22	6	0	-1.753360	0.100995	1.240334
23	1	0	0.235455	-3.612228	1.284064
24	1	0	-2.673372	-1.890453	-2.371255
25	1	0	-1.309382	-2.870424	-1.824331
26	1	0	-2.953769	-3.486851	-1.677685
27	1	0	-0.942455	0.797609	1.462930
28	1	0	-2.644798	0.690956	1.010136
29	1	0	-1.955930	-0.470909	2.151147
30	6	0	-3.930767	-1.606370	0.152584
31	6	0	-4.515107	-0.553430	-0.819420
32	6	0	-5.825045	0.098690	-0.373195
33	6	0	-6.335135	1.208711	-1.314828
34	6	0	-5.789996	2.503448	-0.692079
35	6	0	-5.619744	2.123079	0.775081
36	8	0	-5.637903	0.777295	0.916466
37	1	0	-6.592422	-0.654712	-0.187553
38	1	0	-7.430391	1.229316	-1.313730
39	1	0	-6.002495	1.054304	-2.344272
40	1	0	-4.773283	2.697992	-1.062473
41	6	0	-6.636193	3.760827	-0.897787
42	1	0	-3.931843	-1.164569	1.154347
43	1	0	-4.717908	-1.020184	-1.792108
44	1	0	-3.787472	0.241798	-1.008036
45	8	0	-5.469828	2.861616	1.726755
46	1	0	-6.205163	4.609611	-0.360021
47	1	0	-6.685837	4.015184	-1.960863
48	1	0	-7.658081	3.608577	-0.534518
49	1	0	1.211045	-1.073327	-1.694068
50	6	0	2.925405	0.061439	-1.118166
51	6	0	3.281039	-0.007225	-2.614926

52	6	0	3.202739	1.490861	-0.572642
53	1	0	4.334826	0.209799	-2.809679
54	1	0	3.071982	-0.997961	-3.027870
55	1	0	2.686365	0.725264	-3.173013
56	6	0	4.668311	1.980283	-0.608537
57	6	0	4.745743	3.414059	-0.136202
58	8	0	4.548437	4.391529	-0.838751
59	8	0	5.029626	3.500819	1.179753
60	6	0	5.072427	4.830016	1.744426
61	6	0	4.781262	-1.854953	-0.886208
62	1	0	4.069633	-0.560678	0.631881
63	6	0	4.625094	-3.052540	-1.471509
64	6	0	6.156221	-1.228333	-0.816868
65	1	0	5.473742	-3.569474	-1.911326
66	1	0	3.669903	-3.561829	-1.543211
67	1	0	6.918569	-1.904433	-1.212907
68	1	0	6.209069	-0.295492	-1.388681
69	1	0	6.422837	-0.979771	0.218386
70	1	0	5.064492	1.961348	-1.627019
71	1	0	5.301774	1.361996	0.030559
72	1	0	2.840869	1.546997	0.456606
73	1	0	2.605204	2.195595	-1.162174
74	8	0	2.596228	-3.853677	1.850294
75	1	0	3.695298	-2.201452	2.185460
76	6	0	1.289401	-0.419571	2.795956
77	1	0	1.156725	0.500370	3.370442
78	1	0	0.419649	-1.066466	2.947764
79	1	0	2.185744	-0.931739	3.168432
80	6	0	-4.862842	-2.836089	0.218151
81	1	0	-5.855733	-2.552274	0.580550
82	1	0	-4.995283	-3.304570	-0.763515
83	1	0	-4.485569	-3.597520	0.905285
84	1	0	4.104971	5.322787	1.626894
85	1	0	5.305745	4.688657	2.798729
86	1	0	5.847317	5.423974	1.255251

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.027486	0.161272	-1.106422
2	6	0	0.352299	0.842672	-0.978677
3	1	0	-1.035573	-0.366707	-2.063826
4	1	0	-1.802343	0.933554	-1.169206
5	1	0	0.381549	1.519496	-0.119777
6	1	0	0.525537	1.451844	-1.874290
7	6	0	3.640992	-1.073925	-0.166865
8	6	0	2.489959	-2.015611	0.308357
9	6	0	1.254661	-1.056623	0.443422
10	6	0	1.431048	-0.233476	-0.852543
11	6	0	2.918688	-2.824899	1.509113
12	1	0	2.221686	-2.736668	-0.468957
13	8	0	1.411724	-0.128835	1.538140
14	6	0	-1.953496	-3.147578	0.628893
15	6	0	-2.438629	-1.976075	-0.287699
16	6	0	-1.359278	-0.823468	0.053782
17	6	0	-0.125999	-1.675950	0.439086
18	6	0	-0.473493	-2.924804	0.767375
19	1	0	-2.436911	-3.112151	1.617266
20	1	0	-2.193826	-4.129871	0.206076
21	6	0	-2.297616	-2.458213	-1.749837
22	6	0	-1.788104	0.011405	1.288865
23	1	0	0.211426	-3.694790	1.107703
24	1	0	-2.613097	-1.708337	-2.479933
25	1	0	-1.261224	-2.727846	-1.975439
26	1	0	-2.907923	-3.351369	-1.913286
27	1	0	-0.983843	0.688362	1.583756
28	1	0	-2.672160	0.619002	1.076230
29	1	0	-2.017154	-0.623859	2.150065
30	6	0	-3.931928	-1.615675	0.026247
31	6	0	-4.496577	-0.495067	-0.880014
32	6	0	-5.806312	0.137671	-0.405795
33	6	0	-6.303256	1.303326	-1.285217
34	6	0	-5.752889	2.555910	-0.586038
35	6	0	-5.598470	2.091555	0.858433
36	8	0	-5.624977	0.739683	0.922161
37	1	0	-6.579229	-0.620616	-0.269289
38	1	0	-7.398371	1.331545	-1.289094
39	1	0	-5.965351	1.205972	-2.319865
40	1	0	-4.731380	2.761635	-0.936730
41	6	0	-6.586044	3.830701	-0.727359
42	1	0	-3.959759	-1.250093	1.057708
43	1	0	-4.691793	-0.895694	-1.883298
44	1	0	-3.761048	0.304966	-1.008436
45	8	0	-5.453679	2.773553	1.852057
46	1	0	-6.152169	4.643607	-0.138864
47	1	0	-6.624132	4.145378	-1.774682
48	1	0	-7.612358	3.667927	-0.381701
49	1	0	1.233880	-0.956598	-1.657216
50	6	0	2.946718	0.117563	-0.980829
51	6	0	3.336897	0.190447	-2.470578

52	6	0	3.260913	1.485569	-0.311622
53	1	0	4.420804	0.225070	-2.611251
54	1	0	2.956932	-0.664967	-3.035253
55	1	0	2.913155	1.093439	-2.925423
56	6	0	4.730690	1.957055	-0.413036
57	6	0	4.924694	3.236749	0.366156
58	8	0	5.215945	3.300219	1.548980
59	8	0	4.703474	4.329999	-0.394161
60	6	0	4.809471	5.609129	0.268351
61	6	0	4.786545	-1.836700	-0.825946
62	1	0	4.058505	-0.616344	0.736866
63	6	0	6.055882	-1.616985	-0.448920
64	6	0	4.473520	-2.903524	-1.854597
65	1	0	6.883643	-2.157469	-0.900768
66	1	0	6.310454	-0.899625	0.326719
67	1	0	5.384704	-3.231540	-2.361998
68	1	0	4.025969	-3.785673	-1.379998
69	1	0	3.764659	-2.562259	-2.614164
70	1	0	5.014411	2.127561	-1.454170
71	1	0	5.406618	1.214610	0.015822
72	1	0	2.973785	1.435909	0.741141
73	1	0	2.630654	2.250134	-0.780645
74	8	0	2.623380	-3.994212	1.695396
75	1	0	3.582346	-2.306923	2.230354
76	6	0	1.200339	-0.598450	2.866817
77	1	0	1.076249	0.291180	3.488839
78	1	0	0.303998	-1.221066	2.947064
79	1	0	2.062459	-1.163363	3.242549
80	6	0	-4.860474	-2.848835	-0.024779
81	1	0	-5.867022	-2.592290	0.319902
82	1	0	-4.955259	-3.249542	-1.040133
83	1	0	-4.504271	-3.654251	0.622325
84	1	0	4.596469	6.351259	-0.499772
85	1	0	4.082846	5.676491	1.080886
86	1	0	5.816923	5.746725	0.666856

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.880920	0.167397	-1.101454
2	6	0	0.501052	0.825054	-0.893915
3	1	0	-0.863979	-0.297486	-2.090990
4	1	0	-1.645131	0.951937	-1.139285
5	1	0	0.512457	1.459000	-0.002052
6	1	0	0.693796	1.473049	-1.756082
7	6	0	3.731114	-1.135014	0.001696
8	6	0	2.575219	-2.128956	0.276465
9	6	0	1.334729	-1.176779	0.425307
10	6	0	1.573159	-0.262700	-0.798304
11	6	0	2.923770	-3.068060	1.409356
12	1	0	2.358162	-2.758788	-0.591811
13	8	0	1.454686	-0.323094	1.584673
14	6	0	-1.893927	-3.242852	0.353575
15	6	0	-2.344188	-1.996220	-0.477805
16	6	0	-1.260030	-0.888112	-0.022902
17	6	0	-0.048159	-1.781844	0.330743
18	6	0	-0.416691	-3.048623	0.549902
19	1	0	-2.404416	-3.283235	1.327988
20	1	0	-2.129967	-4.185105	-0.154440
21	6	0	-2.173601	-2.366239	-1.969451
22	6	0	-1.712892	-0.138728	1.257519
23	1	0	0.251031	-3.850164	0.847299
24	1	0	-2.460795	-1.557689	-2.646626
25	1	0	-1.135357	-2.632526	-2.190750
26	1	0	-2.790477	-3.235489	-2.216097
27	1	0	-0.909543	0.504632	1.621414
28	1	0	-2.584146	0.494095	1.066556
29	1	0	-1.971840	-0.832402	2.063375
30	6	0	-3.841055	-1.644760	-0.169533
31	6	0	-4.366419	-0.433352	-0.976220
32	6	0	-5.727972	0.110354	-0.539030
33	6	0	-6.163815	1.394951	-1.272933
34	6	0	-5.707206	2.526912	-0.339671
35	6	0	-5.684847	1.845497	1.024548
36	8	0	-5.687527	0.500060	0.876938
37	1	0	-6.494021	-0.664471	-0.597694
38	1	0	-7.254130	1.417210	-1.377304
39	1	0	-5.728625	1.460640	-2.273191
40	1	0	-4.660311	2.786846	-0.552216
41	6	0	-6.545666	3.805684	-0.364979
42	1	0	-3.891187	-1.376835	0.890932
43	1	0	-4.471197	-0.709253	-2.033623
44	1	0	-3.645495	0.389423	-0.943457
45	8	0	-5.653713	2.366093	2.120614
46	1	0	-6.186935	4.517914	0.382958
47	1	0	-6.485659	4.279665	-1.349370
48	1	0	-7.598009	3.588537	-0.153475
49	1	0	1.405900	-0.922776	-1.661651
50	6	0	3.102270	0.074506	-0.838386
51	6	0	3.564593	0.078038	-2.307599

52	6	0	3.508232	1.400068	-0.127654
53	1	0	4.615089	0.367831	-2.413591
54	1	0	3.447781	-0.911866	-2.757719
55	1	0	2.966296	0.781480	-2.897021
56	6	0	3.286446	2.716870	-0.908925
57	6	0	3.719070	3.913922	-0.092584
58	8	0	2.967332	4.719633	0.430021
59	8	0	5.062763	3.991261	0.012132
60	6	0	5.588371	5.081974	0.799258
61	6	0	5.011200	-1.756911	-0.537648
62	1	0	3.990146	-0.708876	0.980422
63	6	0	5.056568	-2.944393	-1.161095
64	6	0	6.281298	-0.971296	-0.295500
65	1	0	6.000088	-3.350821	-1.515587
66	1	0	4.176355	-3.552407	-1.342371
67	1	0	6.426872	-0.788342	0.776910
68	1	0	7.157369	-1.504309	-0.674816
69	1	0	6.250884	0.012007	-0.778756
70	1	0	2.237062	2.868581	-1.159379
71	1	0	3.867705	2.708847	-1.836087
72	1	0	4.576977	1.341322	0.103809
73	1	0	2.980952	1.452196	0.829405
74	8	0	2.542669	-4.223486	1.496460
75	1	0	3.606136	-2.659304	2.182586
76	6	0	1.236036	-0.895868	2.870534
77	1	0	0.370915	-1.566484	2.881801
78	1	0	2.118189	-1.443631	3.226363
79	1	0	1.051990	-0.062133	3.552388
80	6	0	-4.781141	-2.855247	-0.360523
81	1	0	-5.782109	-2.634408	0.022225
82	1	0	-4.887005	-3.130519	-1.415967
83	1	0	-4.425914	-3.735027	0.181525
84	1	0	5.218387	5.022696	1.825019
85	1	0	6.670534	4.961815	0.773879
86	1	0	5.297922	6.039245	0.361115

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022266	0.154093	-1.108601
2	6	0	0.360783	0.825179	-0.967449
3	1	0	-1.030654	-0.361873	-2.072501
4	1	0	-1.791843	0.932241	-1.164143
5	1	0	0.390019	1.490573	-0.099802
6	1	0	0.539943	1.445324	-1.854405
7	6	0	3.635617	-1.126056	-0.178345
8	6	0	2.477342	-2.060656	0.280856
9	6	0	1.247419	-1.099704	0.431212
10	6	0	1.433284	-0.258763	-0.851197
11	6	0	2.899829	-2.905413	1.461290
12	1	0	2.194683	-2.761881	-0.507976
13	8	0	1.406058	-0.190981	1.541654
14	6	0	-1.977580	-3.169783	0.578921
15	6	0	-2.451628	-1.981661	-0.321698
16	6	0	-1.363735	-0.842795	0.037994
17	6	0	-0.137902	-1.710075	0.413981
18	6	0	-0.496166	-2.960641	0.723887
19	1	0	-2.462987	-3.145198	1.566662
20	1	0	-2.224571	-4.144019	0.141381
21	6	0	-2.311465	-2.444691	-1.790187
22	6	0	-1.787952	-0.021895	1.283947
23	1	0	0.182518	-3.739739	1.055254
24	1	0	-2.618323	-1.681971	-2.510588
25	1	0	-1.276939	-2.720419	-2.017034
26	1	0	-2.929277	-3.330060	-1.967271
27	1	0	-0.976564	0.640192	1.592683
28	1	0	-2.664134	0.599335	1.077446
29	1	0	-2.027563	-0.668115	2.134111
30	6	0	-3.942585	-1.613268	-0.006028
31	6	0	-4.495822	-0.476780	-0.899391
32	6	0	-5.801067	0.161746	-0.420636
33	6	0	-6.282771	1.344681	-1.285299
34	6	0	-5.719519	2.580980	-0.567727
35	6	0	-5.577034	2.095621	0.871015
36	8	0	-5.618883	0.743347	0.916296
37	1	0	-6.581952	-0.590670	-0.297709
38	1	0	-7.377495	1.385619	-1.291093
39	1	0	-5.943639	1.257560	-2.320454
40	1	0	-4.693911	2.777837	-0.911603
41	6	0	-6.535348	3.868272	-0.695451
42	1	0	-3.969635	-1.260222	1.029825
43	1	0	-4.692204	-0.863159	-1.908039
44	1	0	-3.753114	0.318316	-1.016214
45	8	0	-5.429412	2.762588	1.874371
46	1	0	-6.093750	4.667273	-0.093791
47	1	0	-6.564346	4.197837	-1.738485
48	1	0	-7.565337	3.714262	-0.356777
49	1	0	1.238850	-0.967937	-1.668717
50	6	0	2.952306	0.092574	-0.964741
51	6	0	3.335177	0.155687	-2.455334

52	6	0	3.237625	1.460352	-0.282952
53	1	0	4.396961	0.364888	-2.612097
54	1	0	3.112766	-0.786676	-2.963715
55	1	0	2.766471	0.950179	-2.952423
56	6	0	4.710603	1.926465	-0.249756
57	6	0	4.819158	3.259973	0.453257
58	8	0	4.938065	3.407898	1.658005
59	8	0	4.737309	4.294630	-0.409247
60	6	0	4.778891	5.619276	0.165813
61	6	0	4.772810	-1.868163	-0.880964
62	1	0	4.066808	-0.697776	0.736337
63	6	0	4.603159	-3.003954	-1.575364
64	6	0	6.157917	-1.276784	-0.739263
65	1	0	5.448323	-3.494821	-2.050332
66	1	0	3.640086	-3.486546	-1.704150
67	1	0	6.913049	-1.928509	-1.186809
68	1	0	6.234737	-0.296863	-1.223143
69	1	0	6.415881	-1.128828	0.317185
70	1	0	5.117798	2.023507	-1.259023
71	1	0	5.324025	1.221764	0.315156
72	1	0	2.861818	1.422288	0.741745
73	1	0	2.656319	2.225677	-0.810593
74	8	0	2.531524	-4.050872	1.661503
75	1	0	3.626384	-2.435513	2.155869
76	6	0	1.215076	-0.693613	2.860645
77	1	0	0.312027	-1.306783	2.942049
78	1	0	2.077089	-1.280163	3.202964
79	1	0	1.116022	0.180214	3.508904
80	6	0	-4.880918	-2.838070	-0.074528
81	1	0	-5.886551	-2.577516	0.269858
82	1	0	-4.975447	-3.226127	-1.094818
83	1	0	-4.532944	-3.653746	0.564149
84	1	0	4.701133	6.303182	-0.678172
85	1	0	3.942624	5.760260	0.853909
86	1	0	5.720135	5.771104	0.698312

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.894206	0.018077	-1.196955
2	6	0	0.477859	0.728830	-1.183639
3	1	0	-0.931252	-0.575696	-2.114230
4	1	0	-1.685810	0.770997	-1.281775
5	1	0	0.525202	1.487425	-0.397163
6	1	0	0.606318	1.249143	-2.140141
7	6	0	3.824304	-0.928911	-0.203833
8	6	0	2.746033	-1.916692	0.315204
9	6	0	1.461421	-1.013661	0.378600
10	6	0	1.571765	-0.323172	-0.998354
11	6	0	3.202847	-2.626413	1.569957
12	1	0	2.523222	-2.697855	-0.418941
13	8	0	1.594241	0.024002	1.373252
14	6	0	-1.675295	-3.175469	0.810666
15	6	0	-2.210495	-2.097909	-0.189415
16	6	0	-1.163626	-0.889805	0.041615
17	6	0	0.103901	-1.674340	0.464980
18	6	0	-0.200176	-2.901340	0.900974
19	1	0	-2.143639	-3.073360	1.801787
20	1	0	-1.892280	-4.195474	0.473302
21	6	0	-2.071087	-2.694426	-1.609050
22	6	0	-1.593355	0.018388	1.223820
23	1	0	0.514324	-3.620877	1.286956
24	1	0	-2.424434	-2.021097	-2.394125
25	1	0	-1.027942	-2.942022	-1.828277
26	1	0	-2.648656	-3.620324	-1.687510
27	1	0	-0.813267	0.751831	1.438663
28	1	0	-2.510708	0.568349	0.996657
29	1	0	-1.765675	-0.559270	2.137141
30	6	0	-3.711016	-1.762023	0.119109
31	6	0	-4.317761	-0.715470	-0.845446
32	6	0	-5.696626	-0.179397	-0.455924
33	6	0	-6.220701	0.947938	-1.368876
34	6	0	-5.815713	2.237201	-0.637481
35	6	0	-5.713308	1.781210	0.814329
36	8	0	-5.644024	0.431326	0.879045
37	1	0	-6.419151	-0.992191	-0.368055
38	1	0	-7.311982	0.892615	-1.446301
39	1	0	-5.808040	0.879713	-2.378462
40	1	0	-4.794938	2.526634	-0.925320
41	6	0	-6.738935	3.441536	-0.829641
42	1	0	-3.738477	-1.333542	1.126384
43	1	0	-4.430991	-1.154025	-1.845337
44	1	0	-3.641670	0.137568	-0.959785
45	8	0	-5.679484	2.469667	1.813656
46	1	0	-6.406317	4.285186	-0.218939
47	1	0	-6.741112	3.754565	-1.878129
48	1	0	-7.767315	3.196372	-0.543800
49	1	0	1.320715	-1.126384	-1.704784
50	6	0	3.086524	-0.010010	-1.274225
51	6	0	3.390275	-0.460164	-2.721198

52	6	0	3.471867	1.493738	-1.200540
53	1	0	4.430658	-0.271246	-3.003128
54	1	0	3.198610	-1.528687	-2.858020
55	1	0	2.751345	0.088734	-3.423270
56	6	0	3.442502	2.204150	0.156783
57	6	0	3.617385	3.702143	0.036124
58	8	0	3.516898	4.358844	-0.985996
59	8	0	3.884812	4.258019	1.238313
60	6	0	4.023884	5.694914	1.268915
61	6	0	5.138164	-1.564405	-0.633058
62	1	0	4.064665	-0.284754	0.651009
63	6	0	5.270304	-2.862158	-0.948037
64	6	0	6.338434	-0.644185	-0.648784
65	1	0	6.236102	-3.269636	-1.234833
66	1	0	4.440676	-3.561449	-0.936541
67	1	0	7.248190	-1.179209	-0.934062
68	1	0	6.202456	0.187477	-1.349645
69	1	0	6.499001	-0.196644	0.340504
70	1	0	4.220482	1.838226	0.834239
71	1	0	2.498331	2.027346	0.682116
72	1	0	2.812764	2.036517	-1.885968
73	1	0	4.477324	1.610706	-1.621630
74	8	0	2.863040	-3.752722	1.892598
75	1	0	3.922512	-2.070670	2.205006
76	6	0	1.476442	-0.336164	2.746485
77	1	0	1.288768	0.590827	3.293720
78	1	0	0.647856	-1.029868	2.920291
79	1	0	2.403133	-0.780965	3.130602
80	6	0	-4.601002	-3.023830	0.159055
81	1	0	-5.596172	-2.785227	0.546325
82	1	0	-4.733347	-3.465343	-0.835181
83	1	0	-4.187280	-3.793496	0.815154
84	1	0	4.852297	6.010215	0.630820
85	1	0	3.101288	6.173347	0.932992
86	1	0	4.226719	5.943356	2.309796

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.955114	0.178442	-1.177880
2	6	0	0.443171	0.825990	-1.082930
3	1	0	-0.974686	-0.405760	-2.102141
4	1	0	-1.706047	0.968351	-1.291436
5	1	0	0.489150	1.552465	-0.266636
6	1	0	0.636842	1.376166	-2.011903
7	6	0	3.671251	-1.138244	-0.151432
8	6	0	2.491840	-2.013867	0.366085
9	6	0	1.285036	-1.016543	0.449112
10	6	0	1.490553	-0.270856	-0.888281
11	6	0	2.894008	-2.785374	1.602033
12	1	0	2.194231	-2.760388	-0.374076
13	8	0	1.465586	-0.039021	1.496503
14	6	0	-1.989929	-2.988958	0.747866
15	6	0	-2.435859	-1.858709	-0.237198
16	6	0	-1.319529	-0.724237	0.038068
17	6	0	-0.114385	-1.592992	0.474287
18	6	0	-0.503016	-2.808537	0.874483
19	1	0	-2.470605	-2.877315	1.732012
20	1	0	-2.264628	-3.985877	0.384281
21	6	0	-2.310223	-2.429810	-1.668442
22	6	0	-1.718925	0.195115	1.222219
23	1	0	0.155710	-3.579261	1.260910
24	1	0	-2.607784	-1.716306	-2.441387
25	1	0	-1.281115	-2.737508	-1.877811
26	1	0	-2.942700	-3.315698	-1.779669
27	1	0	-0.891384	0.860073	1.478112
28	1	0	-2.583385	0.817750	0.975094
29	1	0	-1.965792	-0.383142	2.118239
30	6	0	-3.915823	-1.431350	0.052353
31	6	0	-4.441974	-0.346634	-0.918151
32	6	0	-5.712548	0.368960	-0.478619
33	6	0	-6.247742	1.412499	-1.474161
34	6	0	-6.875961	2.489551	-0.573822
35	6	0	-6.103857	2.321422	0.731844
36	8	0	-5.443975	1.139990	0.742703
37	1	0	-6.497066	-0.346870	-0.212457
38	1	0	-6.958215	0.970493	-2.177925
39	1	0	-5.416092	1.832502	-2.050542
40	1	0	-6.691209	3.500943	-0.947196
41	6	0	-8.388078	2.319525	-0.330591
42	1	0	-3.929740	-1.005117	1.060983
43	1	0	-4.658509	-0.797320	-1.895956
44	1	0	-3.683587	0.421410	-1.094352
45	8	0	-6.056560	3.087404	1.672829
46	1	0	-8.747471	3.051586	0.398059
47	1	0	-8.932643	2.469482	-1.267644
48	1	0	-8.626469	1.318328	0.044370
49	1	0	1.279693	-1.031765	-1.653736
50	6	0	3.016688	0.038376	-1.023505
51	6	0	3.403069	-0.017037	-2.513608

52	6	0	3.334175	1.446183	-0.445863
53	1	0	4.471083	0.149824	-2.678768
54	1	0	3.155735	-0.986727	-2.954486
55	1	0	2.858902	0.756002	-3.068808
56	6	0	4.802550	1.882826	-0.453223
57	6	0	4.994940	3.300340	0.046790
58	8	0	4.122446	4.140788	0.172594
59	8	0	6.293960	3.544403	0.325791
60	6	0	6.618766	4.880547	0.767864
61	6	0	4.794552	-1.953311	-0.792535
62	1	0	4.106550	-0.656758	0.734613
63	6	0	4.602234	-3.129016	-1.410539
64	6	0	6.192564	-1.386447	-0.680074
65	1	0	5.438421	-3.670344	-1.844914
66	1	0	3.628512	-3.595796	-1.515598
67	1	0	6.935424	-2.086524	-1.071667
68	1	0	6.297378	-0.446517	-1.232955
69	1	0	6.445333	-1.167855	0.365375
70	1	0	5.231608	1.858737	-1.463297
71	1	0	5.432997	1.231362	0.158339
72	1	0	2.958402	1.496719	0.578350
73	1	0	2.763936	2.184011	-1.019534
74	8	0	2.506651	-3.909109	1.876059
75	1	0	3.624490	-2.282037	2.268638
76	6	0	1.261944	-0.446950	2.845579
77	1	0	1.151861	0.469802	3.429857
78	1	0	0.360679	-1.057126	2.961123
79	1	0	2.122749	-1.003944	3.237341
80	6	0	-4.884437	-2.634045	0.072567
81	1	0	-5.883752	-2.323437	0.393159
82	1	0	-4.988360	-3.094250	-0.916328
83	1	0	-4.558060	-3.408729	0.770957
84	1	0	6.347489	5.610381	0.001977
85	1	0	6.091834	5.111874	1.696090
86	1	0	7.695790	4.877311	0.929730

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.135653	0.111763	-1.125949
2	6	0	0.256548	0.773901	-1.052572
3	1	0	-1.165745	-0.466084	-2.053807
4	1	0	-1.898392	0.892896	-1.219886
5	1	0	0.309800	1.497994	-0.234583
6	1	0	0.428237	1.328639	-1.982957
7	6	0	3.527412	-1.191615	-0.253083
8	6	0	2.379068	-2.021494	0.384267
9	6	0	1.148247	-1.056950	0.465115
10	6	0	1.317271	-0.312707	-0.878310
11	6	0	2.795974	-2.756820	1.636438
12	1	0	2.056537	-2.822436	-0.294989
13	8	0	1.312844	-0.067080	1.504768
14	6	0	-2.104865	-3.076267	0.799975
15	6	0	-2.573563	-1.950783	-0.179296
16	6	0	-1.468679	-0.803767	0.089077
17	6	0	-0.243998	-1.656474	0.507400
18	6	0	-0.619222	-2.875870	0.908588
19	1	0	-2.575810	-2.970823	1.789314
20	1	0	-2.369920	-4.076351	0.438347
21	6	0	-2.453358	-2.519142	-1.612038
22	6	0	-1.864361	0.101042	1.285460
23	1	0	0.040652	-3.649092	1.289643
24	1	0	-2.765237	-1.808358	-2.381554
25	1	0	-1.422914	-2.815406	-1.831281
26	1	0	-3.077851	-3.411275	-1.718405
27	1	0	-1.044439	0.778084	1.532914
28	1	0	-2.741744	0.711430	1.054334
29	1	0	-2.090545	-0.485649	2.181225
30	6	0	-4.056419	-1.543003	0.124983
31	6	0	-4.604866	-0.459644	-0.834072
32	6	0	-5.915512	0.199668	-0.400293
33	6	0	-6.384145	1.346138	-1.319688
34	6	0	-5.837146	2.612335	-0.642530
35	6	0	-5.711755	2.184293	0.815890
36	8	0	-5.750649	0.834671	0.914005
37	1	0	-6.699107	-0.546485	-0.258044
38	1	0	-7.478656	1.383244	-1.346652
39	1	0	-6.026373	1.218811	-2.344381
40	1	0	-4.808227	2.802662	-0.979840
41	6	0	-6.659154	3.888310	-0.830839
42	1	0	-4.067520	-1.122556	1.135715
43	1	0	-4.792755	-0.900182	-1.821868
44	1	0	-3.863056	0.329795	-0.987939
45	8	0	-5.579263	2.890311	1.794234
46	1	0	-6.230419	4.712977	-0.255136
47	1	0	-6.676278	4.176614	-1.886255
48	1	0	-7.692591	3.740636	-0.499780
49	1	0	1.097420	-1.079991	-1.635941
50	6	0	2.834732	0.008519	-1.056087
51	6	0	3.160743	0.028881	-2.562431

52	6	0	3.185168	1.389406	-0.433232
53	1	0	4.226813	0.171102	-2.760917
54	1	0	2.865755	-0.903202	-3.051228
55	1	0	2.622325	0.851292	-3.047786
56	6	0	4.657359	1.811001	-0.509434
57	6	0	4.900785	3.199292	0.045328
58	8	0	4.059844	4.067978	0.195046
59	8	0	6.205907	3.384658	0.339931
60	6	0	6.577321	4.692074	0.828243
61	6	0	4.535595	-2.046498	-1.021497
62	1	0	4.077550	-0.745883	0.581268
63	6	0	4.196942	-3.102666	-1.775731
64	6	0	5.984895	-1.641067	-0.887736
65	1	0	4.952902	-3.675907	-2.305748
66	1	0	3.170968	-3.435140	-1.905614
67	1	0	6.645330	-2.329425	-1.422254
68	1	0	6.158763	-0.633465	-1.283668
69	1	0	6.283993	-1.621828	0.167550
70	1	0	5.019142	1.834902	-1.545741
71	1	0	5.315059	1.120409	0.025825
72	1	0	2.870946	1.393926	0.612475
73	1	0	2.588663	2.156005	-0.938830
74	8	0	3.915725	-2.729413	2.118581
75	1	0	2.018665	-3.390908	2.105877
76	6	0	1.156331	-0.474564	2.861030
77	1	0	0.263997	-1.092911	3.004943
78	1	0	2.035509	-1.015867	3.229281
79	1	0	1.050227	0.443429	3.444077
80	6	0	-5.010663	-2.757335	0.147851
81	1	0	-6.003028	-2.464850	0.504470
82	1	0	-5.138113	-3.199061	-0.846798
83	1	0	-4.655929	-3.542152	0.820577
84	1	0	7.651933	4.642315	0.998357
85	1	0	6.340915	5.456505	0.084797
86	1	0	6.051080	4.912875	1.759387

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704470	0.214670	-1.067228
2	6	0	0.674688	0.863089	-0.816097
3	1	0	-0.674406	-0.210940	-2.074089
4	1	0	-1.467980	1.000571	-1.083430
5	1	0	0.672486	1.460970	0.100604
6	1	0	0.880035	1.544395	-1.649336
7	6	0	3.893939	-1.128826	0.046178
8	6	0	2.734402	-2.130351	0.274997
9	6	0	1.491252	-1.184438	0.440096
10	6	0	1.745982	-0.227422	-0.746123
11	6	0	3.068805	-3.105972	1.380835
12	1	0	2.527627	-2.731245	-0.615968
13	8	0	1.590752	-0.373594	1.631371
14	6	0	-1.733695	-3.248435	0.247152
15	6	0	-2.173926	-1.973034	-0.544259
16	6	0	-1.097428	-0.881486	-0.034111
17	6	0	0.110590	-1.786877	0.302668
18	6	0	-0.258987	-3.061544	0.468294
19	1	0	-2.254715	-3.321490	1.214056
20	1	0	-1.965346	-4.172007	-0.296006
21	6	0	-1.983069	-2.285426	-2.046418
22	6	0	-1.571218	-0.178547	1.265298
23	1	0	0.405765	-3.873161	0.744275
24	1	0	-2.269527	-1.453638	-2.695236
25	1	0	-0.939911	-2.534129	-2.264953
26	1	0	-2.588550	-3.150005	-2.334686
27	1	0	-0.776911	0.458746	1.659137
28	1	0	-2.447869	0.450201	1.086067
29	1	0	-1.830559	-0.901516	2.045185
30	6	0	-3.674180	-1.632669	-0.243693
31	6	0	-4.194664	-0.403972	-1.028874
32	6	0	-5.500973	0.192840	-0.522167
33	6	0	-6.031653	1.387133	-1.333286
34	6	0	-6.732827	2.260998	-0.279653
35	6	0	-6.000343	1.880897	1.004132
36	8	0	-5.300529	0.736066	0.828103
37	1	0	-6.272677	-0.577278	-0.422375
38	1	0	-6.697410	1.064523	-2.138362
39	1	0	-5.192643	1.929182	-1.783432
40	1	0	-6.574690	3.329013	-0.455096
41	6	0	-8.244989	2.001156	-0.135490
42	1	0	-3.734973	-1.389985	0.822479
43	1	0	-4.362205	-0.678969	-2.078814
44	1	0	-3.451798	0.398822	-1.034140
45	8	0	-6.010711	2.465424	2.068450
46	1	0	-8.658680	2.575014	0.698493
47	1	0	-8.760706	2.303708	-1.051783
48	1	0	-8.457991	0.941125	0.039807
49	1	0	1.588940	-0.856513	-1.634254
50	6	0	3.275284	0.111271	-0.756381
51	6	0	3.751139	0.164806	-2.220974

52	6	0	3.677664	1.408449	0.004717
53	1	0	4.799044	0.470367	-2.307769
54	1	0	3.650878	-0.811981	-2.702969
55	1	0	3.149819	0.878241	-2.795211
56	6	0	3.435742	2.748347	-0.702788
57	6	0	3.988091	3.924975	0.075303
58	8	0	4.792400	3.866956	0.988641
59	8	0	3.490083	5.091261	-0.389515
60	6	0	3.978688	6.297156	0.237471
61	6	0	5.178124	-1.734847	-0.501731
62	1	0	4.145102	-0.736413	1.040793
63	6	0	5.228789	-2.904765	-1.157506
64	6	0	6.446376	-0.956813	-0.227529
65	1	0	6.175237	-3.301092	-1.515692
66	1	0	4.350376	-3.508044	-1.361719
67	1	0	6.582190	-0.801611	0.850389
68	1	0	7.325466	-1.480504	-0.612891
69	1	0	6.420757	0.038976	-0.684558
70	1	0	2.378512	2.944315	-0.893302
71	1	0	3.928707	2.775871	-1.682874
72	1	0	4.748786	1.349881	0.223289
73	1	0	3.170111	1.413179	0.973230
74	8	0	2.685578	-4.263232	1.426591
75	1	0	3.742277	-2.723017	2.174646
76	6	0	1.360926	-0.995815	2.891865
77	1	0	0.509113	-1.682941	2.863239
78	1	0	2.247805	-1.538460	3.243642
79	1	0	1.148666	-0.191183	3.600040
80	6	0	-4.610056	-2.839175	-0.473792
81	1	0	-5.626929	-2.612416	-0.138360
82	1	0	-4.670301	-3.115273	-1.532397
83	1	0	-4.284190	-3.719595	0.085554
84	1	0	5.060031	6.380806	0.108475
85	1	0	3.468050	7.114059	-0.270571
86	1	0	3.736598	6.296171	1.302298

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.790091	0.037265	-1.226760
2	6	0	0.589313	0.733682	-1.220406
3	1	0	-0.826748	-0.579017	-2.129090
4	1	0	-1.571721	0.797325	-1.336228
5	1	0	0.638269	1.511438	-0.453181
6	1	0	0.730567	1.228250	-2.188708
7	6	0	3.909798	-0.928188	-0.166555
8	6	0	2.818115	-1.895339	0.362978
9	6	0	1.541192	-0.979561	0.392802
10	6	0	1.671075	-0.323690	-0.999374
11	6	0	3.256306	-2.580703	1.637706
12	1	0	2.596334	-2.690580	-0.356225
13	8	0	1.675768	0.080302	1.363546
14	6	0	-1.620688	-3.098427	0.851820
15	6	0	-2.139881	-2.037071	-0.172910
16	6	0	-1.079270	-0.835213	0.033101
17	6	0	0.176099	-1.623970	0.483342
18	6	0	-0.143143	-2.838258	0.943510
19	1	0	-2.091052	-2.969648	1.838812
20	1	0	-1.849186	-4.122778	0.535541
21	6	0	-2.005143	-2.663740	-1.580025
22	6	0	-1.508404	0.110371	1.185653
23	1	0	0.561578	-3.556000	1.350182
24	1	0	-2.353013	-2.002424	-2.377852
25	1	0	-0.963691	-2.923272	-1.793619
26	1	0	-2.588943	-3.587054	-1.641523
27	1	0	-0.722481	0.841840	1.386102
28	1	0	-2.419614	0.660240	0.935081
29	1	0	-1.691648	-0.440404	2.113667
30	6	0	-3.636184	-1.674889	0.122881
31	6	0	-4.232640	-0.663843	-0.885918
32	6	0	-5.527545	0.011232	-0.453712
33	6	0	-6.134038	0.974920	-1.487951
34	6	0	-6.794620	2.066136	-0.628811
35	6	0	-5.986689	2.003864	0.664309
36	8	0	-5.271070	0.856778	0.720444
37	1	0	-6.270325	-0.726339	-0.132952
38	1	0	-6.837262	0.463879	-2.150966
39	1	0	-5.336658	1.403668	-2.104826
40	1	0	-6.668109	3.064339	-1.057928
41	6	0	-8.290843	1.837124	-0.339866
42	1	0	-3.658594	-1.204971	1.111862
43	1	0	-4.444626	-1.170562	-1.836861
44	1	0	-3.515250	0.129856	-1.112707
45	8	0	-5.955032	2.820416	1.562557
46	1	0	-8.668446	2.586976	0.360922
47	1	0	-8.862942	1.914337	-1.269268
48	1	0	-8.472349	0.845923	0.089483
49	1	0	1.419285	-1.141364	-1.688682
50	6	0	3.191325	-0.030325	-1.267245
51	6	0	3.506173	-0.518572	-2.699386

52	6	0	3.588642	1.471598	-1.227425
53	1	0	4.550847	-0.344467	-2.975078
54	1	0	3.307423	-1.588592	-2.812523
55	1	0	2.878869	0.017855	-3.421297
56	6	0	3.553384	2.215758	0.111479
57	6	0	3.740794	3.708979	-0.044583
58	8	0	3.670859	4.338917	-1.085884
59	8	0	3.982259	4.294962	1.148840
60	6	0	4.131085	5.731155	1.144567
61	6	0	5.224026	-1.582511	-0.564562
62	1	0	4.143976	-0.265636	0.675849
63	6	0	5.351046	-2.888125	-0.847648
64	6	0	6.430579	-0.670663	-0.587484
65	1	0	6.317442	-3.308506	-1.113024
66	1	0	4.516615	-3.581527	-0.830009
67	1	0	7.339915	-1.217948	-0.849980
68	1	0	6.308139	0.145686	-1.308621
69	1	0	6.582860	-0.201611	0.393126
70	1	0	4.323777	1.861400	0.803797
71	1	0	2.604295	2.057792	0.633777
72	1	0	2.939721	2.002249	-1.931769
73	1	0	4.598442	1.569747	-1.642712
74	8	0	2.901670	-3.695629	1.983304
75	1	0	3.976684	-2.018131	2.265934
76	6	0	1.542190	-0.246162	2.743667
77	1	0	0.702581	-0.924075	2.926766
78	1	0	2.459323	-0.695094	3.145706
79	1	0	1.363438	0.695934	3.267561
80	6	0	-4.539433	-2.924148	0.212913
81	1	0	-5.551227	-2.650376	0.528188
82	1	0	-4.627290	-3.437904	-0.750853
83	1	0	-4.167725	-3.644926	0.945622
84	1	0	4.975921	6.023936	0.517359
85	1	0	3.219736	6.206509	0.775199
86	1	0	4.312034	6.005934	2.182861

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.914254	0.110503	-1.219663
2	6	0	0.472097	0.788391	-1.173774
3	1	0	-0.931905	-0.517515	-2.114652
4	1	0	-1.682079	0.879181	-1.362269
5	1	0	0.513106	1.552739	-0.392702
6	1	0	0.643183	1.296826	-2.130428
7	6	0	3.748676	-1.061540	-0.179713
8	6	0	2.592786	-1.934027	0.391656
9	6	0	1.365957	-0.959505	0.436405
10	6	0	1.542578	-0.278435	-0.939001
11	6	0	3.021138	-2.637718	1.659539
12	1	0	2.303250	-2.721876	-0.308147
13	8	0	1.534666	0.074550	1.430552
14	6	0	-1.862490	-2.984401	0.860838
15	6	0	-2.344079	-1.908166	-0.166646
16	6	0	-1.247628	-0.740243	0.042157
17	6	0	-0.020432	-1.562708	0.504737
18	6	0	-0.378819	-2.767297	0.962369
19	1	0	-2.334492	-2.841532	1.845052
20	1	0	-2.119122	-4.001677	0.543346
21	6	0	-2.224583	-2.539379	-1.573065
22	6	0	-1.653465	0.225687	1.186409
23	1	0	0.300312	-3.505965	1.375209
24	1	0	-2.544831	-1.865564	-2.372101
25	1	0	-1.192043	-2.835864	-1.781893
26	1	0	-2.840418	-3.441463	-1.638245
27	1	0	-0.839845	0.922628	1.398763
28	1	0	-2.536796	0.813931	0.922799
29	1	0	-1.873383	-0.315292	2.112208
30	6	0	-3.828974	-1.498409	0.123896
31	6	0	-4.390129	-0.469925	-0.887261
32	6	0	-5.673885	0.233023	-0.466477
33	6	0	-6.244129	1.218835	-1.500442
34	6	0	-6.892868	2.316315	-0.640318
35	6	0	-6.102883	2.226046	0.662285
36	8	0	-5.413217	1.063009	0.717663
37	1	0	-6.438112	-0.489287	-0.161881
38	1	0	-6.948737	0.729081	-2.177942
39	1	0	-5.428736	1.635420	-2.101983
40	1	0	-6.740571	3.315317	-1.059023
41	6	0	-8.396876	2.115178	-0.372034
42	1	0	-3.838903	-1.026346	1.112061
43	1	0	-4.603640	-0.967370	-1.842741
44	1	0	-3.651783	0.307670	-1.102544
45	8	0	-6.064856	3.034259	1.567752
46	1	0	-8.768268	2.866642	0.330330
47	1	0	-8.955542	2.211385	-1.307811
48	1	0	-8.603313	1.124262	0.046548
49	1	0	1.337937	-1.079545	-1.663839
50	6	0	3.061914	0.050429	-1.107765
51	6	0	3.434981	-0.077010	-2.596505

52	6	0	3.355033	1.494212	-0.610657
53	1	0	4.495441	0.113024	-2.783157
54	1	0	3.212900	-1.077472	-2.977987
55	1	0	2.862266	0.646604	-3.188222
56	6	0	4.827288	1.962714	-0.656914
57	6	0	4.922148	3.411717	-0.236941
58	8	0	4.721447	4.365235	-0.970704
59	8	0	5.227115	3.542609	1.070680
60	6	0	5.289740	4.890382	1.587353
61	6	0	4.886602	-1.883602	-0.784743
62	1	0	4.177963	-0.523815	0.676098
63	6	0	4.719273	-3.098594	-1.329624
64	6	0	6.269825	-1.275141	-0.720754
65	1	0	5.565201	-3.643343	-1.740115
66	1	0	3.757372	-3.595891	-1.395649
67	1	0	7.026361	-1.974146	-1.087022
68	1	0	6.341495	-0.361955	-1.321435
69	1	0	6.529448	-0.997082	0.308756
70	1	0	5.226885	1.900574	-1.672537
71	1	0	5.450452	1.360221	0.006831
72	1	0	2.989029	1.591252	0.414215
73	1	0	2.769742	2.185563	-1.227516
74	8	0	2.645691	-3.747695	1.998107
75	1	0	3.759019	-2.096318	2.286854
76	6	0	1.366156	-0.272843	2.801283
77	1	0	1.229394	0.666696	3.342128
78	1	0	0.490714	-0.910099	2.961105
79	1	0	2.253722	-0.776376	3.205198
80	6	0	-4.771263	-2.718780	0.212594
81	1	0	-5.772408	-2.414905	0.533953
82	1	0	-4.879328	-3.225245	-0.753002
83	1	0	-4.419139	-3.454384	0.940132
84	1	0	5.535607	4.783953	2.642916
85	1	0	6.063727	5.459181	1.067685
86	1	0	4.325503	5.388192	1.464886

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891373	0.191303	-1.141590
2	6	0	0.496097	0.854597	-1.006084
3	1	0	-0.895608	-0.349669	-2.091770
4	1	0	-1.653335	0.974460	-1.224111
5	1	0	0.523628	1.543627	-0.156986
6	1	0	0.688392	1.448755	-1.907985
7	6	0	3.747383	-1.103051	-0.138541
8	6	0	2.577296	-2.015023	0.335854
9	6	0	1.354742	-1.039755	0.450958
10	6	0	1.558476	-0.234211	-0.851388
11	6	0	2.983124	-2.830692	1.542227
12	1	0	2.295033	-2.734949	-0.435982
13	8	0	1.512483	-0.103999	1.538807
14	6	0	-1.888810	-3.077527	0.628768
15	6	0	-2.344010	-1.912455	-0.310487
16	6	0	-1.251086	-0.772001	0.028121
17	6	0	-0.035603	-1.638550	0.438477
18	6	0	-0.406789	-2.877023	0.780377
19	1	0	-2.382187	-3.018459	1.611198
20	1	0	-2.141616	-4.062059	0.218472
21	6	0	-2.192677	-2.416790	-1.764224
22	6	0	-1.680604	0.086164	1.247081
23	1	0	0.262157	-3.652271	1.139331
24	1	0	-2.491811	-1.673634	-2.508053
25	1	0	-1.156879	-2.700550	-1.974505
26	1	0	-2.810640	-3.305608	-1.922530
27	1	0	-0.866247	0.749913	1.544767
28	1	0	-2.550635	0.707197	1.015609
29	1	0	-1.930875	-0.535497	2.112592
30	6	0	-3.834794	-1.524186	-0.021190
31	6	0	-4.371631	-0.413160	-0.956048
32	6	0	-5.641596	0.284088	-0.486197
33	6	0	-6.201862	1.337406	-1.457357
34	6	0	-6.822625	2.397041	-0.531592
35	6	0	-6.027405	2.216406	0.758407
36	8	0	-5.359540	1.039592	0.741853
37	1	0	-6.415015	-0.442742	-0.217332
38	1	0	-6.920820	0.899799	-2.155235
39	1	0	-5.383323	1.771834	-2.041840
40	1	0	-6.651202	3.414861	-0.893739
41	6	0	-8.329347	2.213381	-0.265623
42	1	0	-3.868649	-1.138523	1.003080
43	1	0	-4.592925	-0.836942	-1.944769
44	1	0	-3.618173	0.363365	-1.115804
45	8	0	-5.968806	2.970011	1.708740
46	1	0	-8.681026	2.932919	0.479092
47	1	0	-8.890504	2.373018	-1.191222
48	1	0	-8.555408	1.205585	0.099196
49	1	0	1.365454	-0.963144	-1.651733
50	6	0	3.081136	0.101619	-0.960488
51	6	0	3.478204	0.124862	-2.448402

52	6	0	3.372634	1.483553	-0.310253
53	1	0	4.543773	0.318367	-2.599144
54	1	0	3.249956	-0.826895	-2.936276
55	1	0	2.923405	0.913585	-2.969857
56	6	0	4.849527	1.936874	-0.273743
57	6	0	4.963102	3.286671	0.396662
58	8	0	5.060495	3.464350	1.599341
59	8	0	4.912805	4.299508	-0.493643
60	6	0	4.962292	5.637938	0.047879
61	6	0	4.882327	-1.873149	-0.814282
62	1	0	4.175936	-0.655910	0.768304
63	6	0	4.706723	-3.024042	-1.481848
64	6	0	6.271974	-1.291227	-0.677279
65	1	0	5.550470	-3.534134	-1.938753
66	1	0	3.739974	-3.500463	-1.606130
67	1	0	7.024068	-1.961135	-1.102557
68	1	0	6.361729	-0.324670	-1.185299
69	1	0	6.523777	-1.118814	0.376944
70	1	0	5.268218	2.004923	-1.280630
71	1	0	5.450557	1.241044	0.315163
72	1	0	2.986636	1.475374	0.711242
73	1	0	2.803804	2.240482	-0.863042
74	8	0	2.606644	-3.968601	1.768739
75	1	0	3.705187	-2.346491	2.231623
76	6	0	1.303714	-0.569487	2.868590
77	1	0	1.201344	0.322112	3.491670
78	1	0	0.396832	-1.176076	2.955847
79	1	0	2.158835	-1.150388	3.236922
80	6	0	-4.780793	-2.744238	-0.060588
81	1	0	-5.794331	-2.460406	0.239925
82	1	0	-4.848847	-3.177926	-1.064363
83	1	0	-4.459117	-3.532103	0.625188
84	1	0	5.897326	5.791894	0.590670
85	1	0	4.905861	6.300779	-0.814397
86	1	0	4.117708	5.806667	0.719317

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.101849	0.052790	-1.150619
2	6	0	0.278232	0.742912	-1.129028
3	1	0	-1.134469	-0.565610	-2.051800
4	1	0	-1.880922	0.814530	-1.266888
5	1	0	0.330065	1.501972	-0.343452
6	1	0	0.425155	1.259159	-2.085349
7	6	0	3.598337	-1.123323	-0.291670
8	6	0	2.475945	-1.940588	0.404799
9	6	0	1.227128	-0.998052	0.456965
10	6	0	1.361199	-0.316169	-0.922776
11	6	0	2.924954	-2.603969	1.685759
12	1	0	2.159694	-2.780761	-0.228285
13	8	0	1.384424	0.045095	1.445114
14	6	0	-1.978529	-3.066339	0.925933
15	6	0	-2.483532	-1.994435	-0.094295
16	6	0	-1.399313	-0.814660	0.108396
17	6	0	-0.151728	-1.622646	0.547338
18	6	0	-0.496297	-2.830989	1.005729
19	1	0	-2.438833	-2.929387	1.916322
20	1	0	-2.226322	-4.086270	0.610462
21	6	0	-2.368372	-2.622690	-1.502446
22	6	0	-1.798573	0.133120	1.269853
23	1	0	0.183922	-3.574147	1.410500
24	1	0	-2.702012	-1.952070	-2.298344
25	1	0	-1.334526	-2.907860	-1.720531
26	1	0	-2.975805	-3.530787	-1.563040
27	1	0	-0.992663	0.840882	1.474358
28	1	0	-2.694554	0.710785	1.026977
29	1	0	-1.995920	-0.419217	2.193788
30	6	0	-3.971035	-1.604236	0.211721
31	6	0	-4.554850	-0.578231	-0.788597
32	6	0	-5.883992	0.058294	-0.377741
33	6	0	-6.388190	1.152959	-1.340323
34	6	0	-5.877128	2.460739	-0.715728
35	6	0	-5.734199	2.094402	0.757910
36	8	0	-5.736095	0.749431	0.909868
37	1	0	-6.644430	-0.704911	-0.204126
38	1	0	-7.483329	1.157026	-1.364936
39	1	0	-6.029213	0.995338	-2.360430
40	1	0	-4.855497	2.668187	-1.064730
41	6	0	-6.737676	3.703307	-0.950284
42	1	0	-3.978161	-1.137142	1.201960
43	1	0	-4.731919	-1.064150	-1.756801
44	1	0	-3.837163	0.226066	-0.976703
45	8	0	-5.616386	2.842151	1.706737
46	1	0	-6.332593	4.562444	-0.408800
47	1	0	-6.766216	3.949477	-2.016057
48	1	0	-7.765356	3.537539	-0.609993
49	1	0	1.143745	-1.121423	-1.640443
50	6	0	2.869813	0.021534	-1.141130
51	6	0	3.173252	-0.022967	-2.650828

52	6	0	3.203465	1.436505	-0.588335
53	1	0	4.233442	0.128332	-2.871305
54	1	0	2.887799	-0.982656	-3.089071
55	1	0	2.613716	0.766078	-3.166559
56	6	0	4.674100	1.891981	-0.730516
57	6	0	4.831842	3.305939	-0.220642
58	8	0	4.526299	4.309261	-0.844067
59	8	0	5.328184	3.344031	1.032920
60	6	0	5.470821	4.651143	1.631173
61	6	0	4.610051	-1.995294	-1.035954
62	1	0	4.154407	-0.625311	0.508650
63	6	0	4.283376	-3.105385	-1.714067
64	6	0	6.049361	-1.540215	-0.971306
65	1	0	5.042010	-3.687898	-2.229867
66	1	0	3.265134	-3.475226	-1.793891
67	1	0	6.715224	-2.242278	-1.480615
68	1	0	6.180619	-0.555785	-1.436026
69	1	0	6.377780	-1.444048	0.070997
70	1	0	4.979713	1.897787	-1.780211
71	1	0	5.343305	1.234528	-0.171635
72	1	0	2.921572	1.476264	0.466227
73	1	0	2.578252	2.165988	-1.115700
74	8	0	4.051020	-2.532405	2.147750
75	1	0	2.165942	-3.226277	2.198855
76	6	0	1.260958	-0.300921	2.821931
77	1	0	0.398488	-0.949853	3.007233
78	1	0	2.167717	-0.783762	3.203869
79	1	0	1.120217	0.638852	3.361400
80	6	0	-4.897851	-2.836244	0.304257
81	1	0	-5.890560	-2.549076	0.664065
82	1	0	-5.031184	-3.324623	-0.667591
83	1	0	-4.515903	-3.582505	1.005315
84	1	0	5.878873	4.471020	2.624670
85	1	0	6.153692	5.265371	1.040371
86	1	0	4.499174	5.145270	1.697723

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704536	0.214745	-1.067131
2	6	0	0.674642	0.863142	-0.816054
3	1	0	-0.674541	-0.210806	-2.074020
4	1	0	-1.468043	1.000652	-1.083238
5	1	0	0.672502	1.460974	0.100679
6	1	0	0.879939	1.544491	-1.649270
7	6	0	3.893939	-1.128838	0.045900
8	6	0	2.734410	-2.130366	0.274749
9	6	0	1.491277	-1.184454	0.439979
10	6	0	1.745933	-0.227381	-0.746209
11	6	0	3.068883	-3.106047	1.380513
12	1	0	2.527570	-2.731214	-0.616233
13	8	0	1.590864	-0.373671	1.631289
14	6	0	-1.733690	-3.248427	0.247137
15	6	0	-2.173959	-1.972991	-0.544197
16	6	0	-1.097433	-0.881467	-0.034052
17	6	0	0.110603	-1.786878	0.302613
18	6	0	-0.258970	-3.061551	0.468205
19	1	0	-2.254657	-3.321519	1.214067
20	1	0	-1.965375	-4.171975	-0.296046
21	6	0	-1.983170	-2.285317	-2.046378
22	6	0	-1.571152	-0.178598	1.265422
23	1	0	0.405795	-3.873183	0.744110
24	1	0	-2.269652	-1.453499	-2.695146
25	1	0	-0.940022	-2.534015	-2.264968
26	1	0	-2.588667	-3.149881	-2.334658
27	1	0	-0.776821	0.458668	1.659255
28	1	0	-2.447809	0.450164	1.086271
29	1	0	-1.830458	-0.901609	2.045283
30	6	0	-3.674197	-1.632638	-0.243546
31	6	0	-4.194719	-0.403911	-1.028655
32	6	0	-5.501013	0.192872	-0.521877
33	6	0	-6.031731	1.387193	-1.332928
34	6	0	-6.732882	2.261005	-0.279236
35	6	0	-6.000351	1.880860	1.004509
36	8	0	-5.300526	0.736046	0.828409
37	1	0	-6.272708	-0.577255	-0.422088
38	1	0	-6.697510	1.064611	-2.137998
39	1	0	-5.192740	1.929272	-1.783076
40	1	0	-6.574765	3.329030	-0.454640
41	6	0	-8.245036	2.001138	-0.135034
42	1	0	-3.734940	-1.389995	0.822639
43	1	0	-4.362297	-0.678865	-2.078600
44	1	0	-3.451857	0.398887	-1.033916
45	8	0	-6.010689	2.465343	2.068852
46	1	0	-8.658706	2.574957	0.698987
47	1	0	-8.760787	2.303722	-1.051298
48	1	0	-8.458020	0.941097	0.040226
49	1	0	1.588823	-0.856426	-1.634360
50	6	0	3.275237	0.111301	-0.756558
51	6	0	3.750988	0.164903	-2.221182

52	6	0	3.677683	1.408438	0.004574
53	1	0	4.798884	0.470476	-2.308037
54	1	0	3.650699	-0.811864	-2.703211
55	1	0	3.149621	0.878359	-2.795346
56	6	0	3.435715	2.748375	-0.702841
57	6	0	3.988157	3.924955	0.075256
58	8	0	4.792564	3.866881	0.988503
59	8	0	3.490107	5.091271	-0.389445
60	6	0	3.978793	6.297129	0.237549
61	6	0	5.178081	-1.734843	-0.502127
62	1	0	4.145173	-0.736475	1.040515
63	6	0	5.228693	-2.904727	-1.157965
64	6	0	6.446359	-0.956836	-0.227965
65	1	0	6.175114	-3.301045	-1.516233
66	1	0	4.350262	-3.507987	-1.362154
67	1	0	6.582244	-0.801691	0.849952
68	1	0	7.325419	-1.480516	-0.613411
69	1	0	6.420722	0.038977	-0.684940
70	1	0	2.378471	2.944369	-0.893247
71	1	0	3.928589	2.775942	-1.682972
72	1	0	4.748822	1.349852	0.223058
73	1	0	3.170206	1.413122	0.973128
74	8	0	2.685640	-4.263303	1.426243
75	1	0	3.742423	-2.723141	2.174290
76	6	0	1.361130	-0.995959	2.891766
77	1	0	0.509301	-1.683068	2.863171
78	1	0	2.248027	-1.538642	3.243440
79	1	0	1.148944	-0.191363	3.600004
80	6	0	-4.610083	-2.839136	-0.473646
81	1	0	-5.626940	-2.612394	-0.138155
82	1	0	-4.670380	-3.115194	-1.532259
83	1	0	-4.284187	-3.719577	0.085650
84	1	0	3.736804	6.296101	1.302399
85	1	0	5.060125	6.380764	0.108455
86	1	0	3.468122	7.114063	-0.270408

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.239352	-0.303746	-1.162915
2	6	0	-0.101452	-1.066445	-1.104470
3	1	0	1.244644	0.261301	-2.099188
4	1	0	2.059449	-1.027383	-1.230584
5	1	0	-0.117242	-1.772917	-0.269660
6	1	0	-0.207837	-1.653159	-2.025221
7	6	0	-3.519026	0.654348	-0.367202
8	6	0	-2.434719	1.623500	0.192026
9	6	0	-1.157164	0.727607	0.348291
10	6	0	-1.245629	-0.058500	-0.977553
11	6	0	-2.954970	2.377632	1.394112
12	1	0	-2.157897	2.382486	-0.543827
13	8	0	-1.294874	-0.243831	1.405603
14	6	0	1.927448	2.975690	0.727068
15	6	0	2.503956	1.870608	-0.217874
16	6	0	1.477862	0.651508	0.043294
17	6	0	0.187219	1.421104	0.414736
18	6	0	0.457243	2.672284	0.802614
19	1	0	2.378763	2.923792	1.729875
20	1	0	2.129273	3.985850	0.352545
21	6	0	2.380535	2.405526	-1.663172
22	6	0	1.907295	-0.203900	1.264442
23	1	0	-0.278603	3.391953	1.146269
24	1	0	2.754842	1.704179	-2.413232
25	1	0	1.338275	2.630669	-1.909114
26	1	0	2.947954	3.334732	-1.771457
27	1	0	1.132647	-0.935381	1.503518
28	1	0	2.832648	-0.752325	1.067211
29	1	0	2.065572	0.411506	2.155428
30	6	0	4.005287	1.577715	0.130123
31	6	0	4.653295	0.517323	-0.792057
32	6	0	6.018762	-0.004922	-0.341393
33	6	0	6.597053	-1.122268	-1.233541
34	6	0	6.166479	-2.418629	-0.530154
35	6	0	5.995000	-1.972107	0.918205
36	8	0	5.910769	-0.623098	0.986902
37	1	0	6.727857	0.814762	-0.215918
38	1	0	7.690382	-1.057822	-1.255929
39	1	0	6.234718	-1.051253	-2.262090
40	1	0	5.161514	-2.711129	-0.866716
41	6	0	7.103894	-3.616890	-0.687981
42	1	0	4.022817	1.180242	1.150142
43	1	0	4.801046	0.940507	-1.794073
44	1	0	3.986015	-0.341227	-0.916560
45	8	0	5.922776	-2.666516	1.911255
46	1	0	6.747210	-4.467205	-0.100548
47	1	0	7.157155	-3.921150	-1.737722
48	1	0	8.116370	-3.369331	-0.351912
49	1	0	-1.067589	0.701925	-1.751757
50	6	0	-2.736460	-0.495156	-1.168012
51	6	0	-3.044724	-0.513800	-2.677573

52	6	0	-2.959591	-1.914195	-0.565781
53	1	0	-4.082607	-0.779158	-2.897223
54	1	0	-2.858480	0.462034	-3.134293
55	1	0	-2.405366	-1.249731	-3.179357
56	6	0	-4.343325	-2.576256	-0.693894
57	6	0	-5.308147	-2.332620	0.449489
58	8	0	-5.033422	-1.857338	1.536843
59	8	0	-6.546646	-2.767540	0.132533
60	6	0	-7.550393	-2.672716	1.166685
61	6	0	-4.649634	1.371383	-1.103716
62	1	0	-3.974837	0.164786	0.500412
63	6	0	-4.501622	2.533440	-1.758153
64	6	0	-6.008873	0.712911	-1.038323
65	1	0	-5.345414	2.998785	-2.260716
66	1	0	-3.557379	3.063643	-1.825073
67	1	0	-6.763809	1.302181	-1.565825
68	1	0	-5.998474	-0.288663	-1.482064
69	1	0	-6.331086	0.594185	0.003592
70	1	0	-4.210075	-3.666709	-0.712633
71	1	0	-4.852540	-2.345271	-1.633933
72	1	0	-2.674256	-1.901317	0.487626
73	1	0	-2.252883	-2.580809	-1.071490
74	8	0	-2.671093	3.533547	1.663196
75	1	0	-3.673390	1.828344	2.036070
76	6	0	-1.200527	0.203785	2.753838
77	1	0	-1.034994	-0.688515	3.362315
78	1	0	-0.367675	0.899070	2.900743
79	1	0	-2.129952	0.680220	3.089974
80	6	0	4.867109	2.859479	0.146771
81	1	0	5.865475	2.651801	0.543658
82	1	0	4.994969	3.281243	-0.856522
83	1	0	4.433446	3.634139	0.783966
84	1	0	-7.691462	-1.631991	1.465851
85	1	0	-8.461718	-3.069833	0.721812
86	1	0	-7.256760	-3.266003	2.035377

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.857083	0.070231	-1.175260
2	6	0	0.501601	0.800829	-1.083405
3	1	0	-0.862242	-0.466929	-2.127369
4	1	0	-1.659742	0.813770	-1.232777
5	1	0	0.516560	1.507948	-0.249416
6	1	0	0.642340	1.383978	-2.001455
7	6	0	3.853823	-0.881540	-0.146653
8	6	0	2.776368	-1.913763	0.280835
9	6	0	1.479945	-1.030986	0.380963
10	6	0	1.610617	-0.242148	-0.940416
11	6	0	3.217758	-2.701616	1.493751
12	1	0	2.575866	-2.646248	-0.508052
13	8	0	1.581625	-0.065055	1.447274
14	6	0	-1.635639	-3.254113	0.603961
15	6	0	-2.169414	-2.116401	-0.327785
16	6	0	-1.138664	-0.916070	-0.001908
17	6	0	0.130026	-1.712668	0.392042
18	6	0	-0.165905	-2.970041	0.737871
19	1	0	-2.120115	-3.225540	1.592056
20	1	0	-1.834798	-4.251091	0.194604
21	6	0	-2.007281	-2.613675	-1.782800
22	6	0	-1.599249	-0.087775	1.226688
23	1	0	0.550767	-3.705851	1.087599
24	1	0	-2.356822	-1.891047	-2.524598
25	1	0	-0.959874	-2.839422	-2.005648
26	1	0	-2.576240	-3.536159	-1.931964
27	1	0	-0.830222	0.636806	1.501637
28	1	0	-2.517076	0.467844	1.015986
29	1	0	-1.783987	-0.721734	2.099385
30	6	0	-3.677361	-1.817104	-0.016685
31	6	0	-4.285328	-0.714114	-0.915700
32	6	0	-5.670121	-0.213301	-0.500625
33	6	0	-6.191305	0.974387	-1.335328
34	6	0	-5.792530	2.209202	-0.512518
35	6	0	-5.702460	1.652607	0.904529
36	8	0	-5.631390	0.301460	0.874869
37	1	0	-6.390026	-1.032814	-0.476903
38	1	0	-7.282019	0.922897	-1.422642
39	1	0	-5.772738	0.977409	-2.344799
40	1	0	-4.768956	2.516478	-0.770546
41	6	0	-6.713571	3.425003	-0.627408
42	1	0	-3.721643	-1.457567	1.016412
43	1	0	-4.389366	-1.088217	-1.942478
44	1	0	-3.614881	0.149387	-0.970733
45	8	0	-5.678437	2.269237	1.949838
46	1	0	-6.387667	4.222075	0.046272
47	1	0	-6.704618	3.812918	-1.650511
48	1	0	-7.744957	3.160645	-0.371034
49	1	0	1.396609	-0.997817	-1.709045
50	6	0	3.123673	0.116363	-1.148668
51	6	0	3.474469	-0.190213	-2.622183

52	6	0	3.493357	1.612188	-0.928971
53	1	0	4.516692	0.047849	-2.854886
54	1	0	3.314184	-1.245930	-2.859942
55	1	0	2.839731	0.405295	-3.288971
56	6	0	3.372832	2.224553	0.484907
57	6	0	3.781902	3.678778	0.448772
58	8	0	4.931825	4.085085	0.491413
59	8	0	2.718785	4.502259	0.330994
60	6	0	3.003642	5.915511	0.241430
61	6	0	5.177653	-1.473564	-0.608071
62	1	0	4.081085	-0.305353	0.758825
63	6	0	5.321122	-2.741410	-1.023755
64	6	0	6.371698	-0.548201	-0.535106
65	1	0	6.292911	-3.120377	-1.328868
66	1	0	4.495287	-3.443105	-1.079564
67	1	0	7.290846	-1.058152	-0.835702
68	1	0	6.245755	0.327795	-1.181687
69	1	0	6.507663	-0.165510	0.484359
70	1	0	4.049115	1.723620	1.182031
71	1	0	2.358567	2.129845	0.868802
72	1	0	2.872122	2.203201	-1.613348
73	1	0	4.526219	1.757874	-1.264819
74	8	0	2.890189	-3.852697	1.729790
75	1	0	3.913607	-2.179766	2.181864
76	6	0	1.434247	-0.519567	2.789214
77	1	0	1.232011	0.367479	3.394434
78	1	0	0.604091	-1.224697	2.897072
79	1	0	2.353097	-0.988778	3.163187
80	6	0	-4.553607	-3.088023	-0.074513
81	1	0	-5.558025	-2.885301	0.309206
82	1	0	-4.663194	-3.465073	-1.097554
83	1	0	-4.142859	-3.894541	0.537806
84	1	0	3.524140	6.254643	1.139576
85	1	0	3.617991	6.123474	-0.637332
86	1	0	2.032751	6.401333	0.154874

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.966058	0.219807	-1.149856
2	6	0	0.431337	0.869941	-1.053363
3	1	0	-0.986690	-0.355566	-2.079596
4	1	0	-1.719524	1.008601	-1.253721
5	1	0	0.479208	1.590916	-0.232106
6	1	0	0.622562	1.426269	-1.979226
7	6	0	3.666009	-1.084400	-0.132090
8	6	0	2.490962	-1.972951	0.385123
9	6	0	1.281145	-0.975837	0.468404
10	6	0	1.479967	-0.226837	-0.868513
11	6	0	2.895775	-2.729500	1.627301
12	1	0	2.205818	-2.725946	-0.355082
13	8	0	1.462689	0.001633	1.515203
14	6	0	-1.981227	-2.968213	0.756957
15	6	0	-2.431417	-1.838049	-0.226551
16	6	0	-1.325727	-0.695405	0.058597
17	6	0	-0.115337	-1.557692	0.493555
18	6	0	-0.496057	-2.777305	0.888612
19	1	0	-2.466289	-2.862706	1.739604
20	1	0	-2.247378	-3.965961	0.389423
21	6	0	-2.293247	-2.402672	-1.659214
22	6	0	-1.737149	0.213406	1.246706
23	1	0	0.167002	-3.545530	1.273090
24	1	0	-2.593601	-1.689099	-2.430976
25	1	0	-1.260342	-2.700115	-1.864604
26	1	0	-2.917036	-3.293829	-1.776790
27	1	0	-0.917640	0.886634	1.507099
28	1	0	-2.607454	0.828026	1.000198
29	1	0	-1.979952	-0.371283	2.139592
30	6	0	-3.916486	-1.424460	0.056377
31	6	0	-4.446914	-0.342021	-0.914415
32	6	0	-5.723108	0.364987	-0.477452
33	6	0	-6.266801	1.400191	-1.477005
34	6	0	-6.903504	2.475645	-0.580782
35	6	0	-6.129474	2.319206	0.725198
36	8	0	-5.460361	1.142950	0.740743
37	1	0	-6.501839	-0.355988	-0.208253
38	1	0	-6.973807	0.949596	-2.178813
39	1	0	-5.438678	1.824584	-2.055264
40	1	0	-6.727369	3.487013	-0.958365
41	6	0	-8.414033	2.294053	-0.336038
42	1	0	-3.939962	-1.001418	1.066170
43	1	0	-4.657848	-0.793380	-1.893120
44	1	0	-3.693189	0.431211	-1.088047
45	8	0	-6.087724	3.089483	1.662894
46	1	0	-8.779094	3.026292	0.389597
47	1	0	-8.960249	2.435423	-1.273463
48	1	0	-8.643993	1.292580	0.043440
49	1	0	1.261795	-0.986537	-1.633079
50	6	0	3.003846	0.076273	-1.015066
51	6	0	3.391948	0.047761	-2.507684

52	6	0	3.357938	1.474132	-0.433215
53	1	0	4.475959	0.042065	-2.652009
54	1	0	2.985877	-0.827678	-3.021490
55	1	0	2.992330	0.934134	-3.014150
56	6	0	4.831505	1.883516	-0.543957
57	6	0	5.104043	3.260321	0.023921
58	8	0	4.267436	4.109317	0.276068
59	8	0	6.427965	3.459857	0.205022
60	6	0	6.822591	4.758655	0.697981
61	6	0	4.800324	-1.905897	-0.737114
62	1	0	4.084796	-0.587443	0.750053
63	6	0	6.070344	-1.696051	-0.356531
64	6	0	4.474062	-3.014507	-1.715979
65	1	0	6.890752	-2.276111	-0.771141
66	1	0	6.332784	-0.945858	0.384748
67	1	0	5.382357	-3.385326	-2.198531
68	1	0	4.003958	-3.863358	-1.204009
69	1	0	3.779216	-2.694320	-2.497154
70	1	0	5.163976	1.913226	-1.589290
71	1	0	5.499047	1.177232	-0.042626
72	1	0	3.052312	1.510477	0.614808
73	1	0	2.758220	2.227156	-0.955249
74	8	0	2.577096	-3.882266	1.870095
75	1	0	3.564173	-2.188695	2.327229
76	6	0	1.232895	-0.392686	2.864817
77	1	0	1.110793	0.530209	3.436941
78	1	0	0.329934	-1.001924	2.969303
79	1	0	2.085647	-0.944802	3.279575
80	6	0	-4.874464	-2.635798	0.067683
81	1	0	-5.879440	-2.334129	0.378984
82	1	0	-4.965154	-3.096665	-0.922183
83	1	0	-4.547744	-3.407652	0.769063
84	1	0	7.908670	4.722255	0.771026
85	1	0	6.510358	5.540105	0.001724
86	1	0	6.377797	4.943866	1.678034

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.897902	0.202554	-1.136628
2	6	0	0.487495	0.873648	-1.014341
3	1	0	-0.903076	-0.349032	-2.080755
4	1	0	-1.664019	0.980957	-1.224972
5	1	0	0.516592	1.572572	-0.173267
6	1	0	0.674305	1.457801	-1.923872
7	6	0	3.750322	-1.053489	-0.127155
8	6	0	2.586264	-1.972103	0.361563
9	6	0	1.359813	-0.997435	0.463193
10	6	0	1.554373	-0.209162	-0.851683
11	6	0	2.997246	-2.754698	1.585926
12	1	0	2.317059	-2.710030	-0.399495
13	8	0	1.518767	-0.044192	1.535520
14	6	0	-1.870263	-3.050621	0.679151
15	6	0	-2.334615	-1.901731	-0.275657
16	6	0	-1.248942	-0.749311	0.045459
17	6	0	-0.026987	-1.602685	0.464254
18	6	0	-0.389205	-2.838664	0.824136
19	1	0	-2.361766	-2.980169	1.661745
20	1	0	-2.117851	-4.042382	0.283504
21	6	0	-2.181533	-2.424736	-1.722521
22	6	0	-1.682360	0.121718	1.253868
23	1	0	0.285023	-3.605572	1.191520
24	1	0	-2.488174	-1.694338	-2.475857
25	1	0	-1.143738	-2.702580	-1.930736
26	1	0	-2.792286	-3.320740	-1.867724
27	1	0	-0.874382	0.799013	1.538297
28	1	0	-2.559678	0.730018	1.016721
29	1	0	-1.922932	-0.489525	2.129406
30	6	0	-3.827670	-1.520101	0.010676
31	6	0	-4.373422	-0.424699	-0.937320
32	6	0	-5.648781	0.268022	-0.475548
33	6	0	-6.219808	1.301950	-1.461080
34	6	0	-6.849095	2.368992	-0.549717
35	6	0	-6.049674	2.215000	0.741112
36	8	0	-5.371602	1.043849	0.740949
37	1	0	-6.415459	-0.461454	-0.194971
38	1	0	-6.935559	0.847523	-2.151462
39	1	0	-5.406100	1.735454	-2.052945
40	1	0	-6.688384	3.383019	-0.927105
41	6	0	-8.353361	2.174508	-0.277660
42	1	0	-3.862996	-1.122059	1.030180
43	1	0	-4.591422	-0.862211	-1.920751
44	1	0	-3.626304	0.355951	-1.106627
45	8	0	-5.995691	2.983406	1.679763
46	1	0	-8.710362	2.901318	0.457388
47	1	0	-8.918038	2.315251	-1.204176
48	1	0	-8.568785	1.169982	0.102267
49	1	0	1.356196	-0.950636	-1.639230
50	6	0	3.074342	0.123455	-0.976722
51	6	0	3.476906	0.155556	-2.464628

52	6	0	3.397988	1.505037	-0.340270
53	1	0	4.562242	0.175975	-2.596553
54	1	0	3.093056	-0.709459	-3.011812
55	1	0	3.065802	1.051300	-2.944647
56	6	0	4.873580	1.958029	-0.443105
57	6	0	5.076362	3.253994	0.306361
58	8	0	5.353387	3.342975	1.490989
59	8	0	4.880888	4.330914	-0.483666
60	6	0	4.996754	5.624460	0.148489
61	6	0	4.894469	-1.842972	-0.756372
62	1	0	4.163684	-0.577328	0.768777
63	6	0	6.161887	-1.628608	-0.369901
64	6	0	4.580764	-2.928091	-1.765378
65	1	0	6.988717	-2.187430	-0.800667
66	1	0	6.415553	-0.897219	0.392855
67	1	0	5.493001	-3.273767	-2.258998
68	1	0	4.122401	-3.796738	-1.276425
69	1	0	3.880548	-2.596072	-2.536860
70	1	0	5.166214	2.100225	-1.486004
71	1	0	5.538384	1.218720	0.008108
72	1	0	3.103107	1.485879	0.711321
73	1	0	2.779359	2.263796	-0.833611
74	8	0	2.690529	-3.916575	1.798648
75	1	0	3.658406	-2.224158	2.300245
76	6	0	1.290814	-0.477287	2.873718
77	1	0	0.388738	-1.090546	2.961117
78	1	0	2.144686	-1.039002	3.272475
79	1	0	1.167989	0.429145	3.471276
80	6	0	-4.765196	-2.747163	-0.012200
81	1	0	-5.779927	-2.466943	0.287636
82	1	0	-4.832768	-3.192831	-1.010742
83	1	0	-4.436649	-3.524882	0.681850
84	1	0	4.801723	6.350161	-0.639837
85	1	0	4.262554	5.721046	0.951174
86	1	0	6.001671	5.758778	0.554494

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758710	0.107201	-1.185526
2	6	0	0.609796	0.820327	-1.102994
3	1	0	-0.769357	-0.445796	-2.128550
4	1	0	-1.549538	0.862034	-1.256763
5	1	0	0.632272	1.542904	-0.282529
6	1	0	0.761134	1.384154	-2.031411
7	6	0	3.936014	-0.888992	-0.125709
8	6	0	2.843462	-1.898242	0.318328
9	6	0	1.558894	-0.995993	0.398243
10	6	0	1.703774	-0.234607	-0.937503
11	6	0	3.270883	-2.668879	1.547042
12	1	0	2.635046	-2.642451	-0.457342
13	8	0	1.671624	-0.011435	1.446037
14	6	0	-1.584791	-3.175293	0.651966
15	6	0	-2.101201	-2.049029	-0.302367
16	6	0	-1.057478	-0.854126	0.004886
17	6	0	0.199772	-1.659149	0.418275
18	6	0	-0.112036	-2.906708	0.785247
19	1	0	-2.071278	-3.121187	1.638110
20	1	0	-1.796646	-4.177165	0.261096
21	6	0	-1.940939	-2.571600	-1.748651
22	6	0	-1.515142	0.004653	1.213321
23	1	0	0.594707	-3.644563	1.150473
24	1	0	-2.286879	-1.858644	-2.501585
25	1	0	-0.894441	-2.805549	-1.967026
26	1	0	-2.513812	-3.493762	-1.883992
27	1	0	-0.738714	0.725755	1.477078
28	1	0	-2.426528	0.564352	0.985980
29	1	0	-1.709210	-0.609865	2.098124
30	6	0	-3.605853	-1.725475	-0.003736
31	6	0	-4.201391	-0.648653	-0.943304
32	6	0	-5.503520	-0.014081	-0.472929
33	6	0	-6.120805	1.003512	-1.447429
34	6	0	-6.791889	2.034776	-0.524692
35	6	0	-5.984477	1.902121	0.763469
36	8	0	-5.256482	0.761653	0.750404
37	1	0	-6.238332	-0.777435	-0.197610
38	1	0	-6.819128	0.525362	-2.139574
39	1	0	-5.328384	1.476186	-2.038204
40	1	0	-6.673686	3.058151	-0.892553
41	6	0	-8.286487	1.776473	-0.252313
42	1	0	-3.648335	-1.332455	1.017468
43	1	0	-4.404405	-1.089360	-1.928510
44	1	0	-3.488721	0.164031	-1.110241
45	8	0	-5.962283	2.662689	1.709856
46	1	0	-8.671191	2.480910	0.490480
47	1	0	-8.858189	1.903221	-1.176528
48	1	0	-8.460484	0.760477	0.118199
49	1	0	1.481218	-1.001720	-1.692238
50	6	0	3.222085	0.099709	-1.148318
51	6	0	3.571182	-0.239474	-2.615197

52	6	0	3.610036	1.594589	-0.956228
53	1	0	4.616886	-0.020459	-2.850960
54	1	0	3.396270	-1.297171	-2.833105
55	1	0	2.945699	0.352244	-3.294044
56	6	0	3.500886	2.233984	0.446489
57	6	0	3.927985	3.682213	0.383318
58	8	0	5.083616	4.074049	0.402582
59	8	0	2.873762	4.517633	0.271219
60	6	0	3.174537	5.925925	0.159335
61	6	0	5.252519	-1.508070	-0.572215
62	1	0	4.169014	-0.299437	0.769664
63	6	0	5.380337	-2.786487	-0.959736
64	6	0	6.458484	-0.596989	-0.517382
65	1	0	6.347698	-3.184242	-1.254820
66	1	0	4.545867	-3.478904	-1.001073
67	1	0	7.371040	-1.124768	-0.807104
68	1	0	6.344028	0.267397	-1.181400
69	1	0	6.599045	-0.195696	0.494278
70	1	0	4.173599	1.737629	1.150480
71	1	0	2.486953	2.159534	0.835759
72	1	0	2.994008	2.180351	-1.649750
73	1	0	4.643661	1.722230	-1.296980
74	8	0	2.928087	-3.811219	1.803393
75	1	0	3.971027	-2.143123	2.227795
76	6	0	1.510938	-0.437204	2.795664
77	1	0	0.667375	-1.124553	2.913635
78	1	0	2.419509	-0.916009	3.182481
79	1	0	1.322878	0.464961	3.382856
80	6	0	-4.495681	-2.987718	-0.024106
81	1	0	-5.516409	-2.749056	0.290997
82	1	0	-4.558872	-3.427773	-1.025397
83	1	0	-4.129160	-3.757595	0.659592
84	1	0	2.208501	6.422503	0.079891
85	1	0	3.711496	6.270065	1.045830
86	1	0	3.779083	6.115057	-0.730389

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.027483	0.161270	-1.106431
2	6	0	0.352304	0.842668	-0.978691
3	1	0	-1.035573	-0.366711	-2.063834
4	1	0	-1.802338	0.933553	-1.169216
5	1	0	0.381554	1.519496	-0.119793
6	1	0	0.525541	1.451836	-1.874306
7	6	0	3.640996	-1.073921	-0.166862
8	6	0	2.489964	-2.015606	0.308361
9	6	0	1.254663	-1.056622	0.443415
10	6	0	1.431052	-0.233479	-0.852552
11	6	0	2.918689	-2.824888	1.509123
12	1	0	2.221696	-2.736669	-0.468950
13	8	0	1.411720	-0.128829	1.538130
14	6	0	-1.953492	-3.147579	0.628885
15	6	0	-2.438629	-1.976073	-0.287702
16	6	0	-1.359275	-0.823468	0.053775
17	6	0	-0.125996	-1.675951	0.439077
18	6	0	-0.473490	-2.924805	0.767364
19	1	0	-2.436905	-3.112156	1.617259
20	1	0	-2.193824	-4.129871	0.206065
21	6	0	-2.297624	-2.458208	-1.749841
22	6	0	-1.788093	0.011408	1.288858
23	1	0	0.211430	-3.694791	1.107691
24	1	0	-2.613114	-1.708333	-2.479934
25	1	0	-1.261233	-2.727837	-1.975451
26	1	0	-2.907930	-3.351367	-1.913288
27	1	0	-0.983826	0.688357	1.583750
28	1	0	-2.672143	0.619014	1.076224
29	1	0	-2.017150	-0.623854	2.150058
30	6	0	-3.931926	-1.615675	0.026252
31	6	0	-4.496584	-0.495071	-0.880010
32	6	0	-5.806317	0.137665	-0.405785
33	6	0	-6.303271	1.303314	-1.285210
34	6	0	-5.752904	2.555904	-0.586042
35	6	0	-5.598472	2.091557	0.858431
36	8	0	-5.624977	0.739685	0.922166
37	1	0	-6.579231	-0.620624	-0.269271
38	1	0	-7.398386	1.331529	-1.289081
39	1	0	-5.965372	1.205956	-2.319860
40	1	0	-4.731399	2.761630	-0.936741
41	6	0	-6.586065	3.830691	-0.727363
42	1	0	-3.959753	-1.250090	1.057713
43	1	0	-4.691805	-0.895702	-1.883291
44	1	0	-3.761058	0.304963	-1.008440
45	8	0	-5.453685	2.773560	1.852052
46	1	0	-6.152189	4.643601	-0.138874
47	1	0	-6.624161	4.145363	-1.774687
48	1	0	-7.612376	3.667915	-0.381697
49	1	0	1.233887	-0.956604	-1.657223
50	6	0	2.946723	0.117561	-0.980833
51	6	0	3.336905	0.190440	-2.470582

52	6	0	3.260915	1.485570	-0.311631
53	1	0	4.420812	0.225068	-2.611254
54	1	0	2.956946	-0.664979	-3.035254
55	1	0	2.913161	1.093428	-2.925432
56	6	0	4.730691	1.957057	-0.413044
57	6	0	4.924696	3.236747	0.366154
58	8	0	5.215963	3.300211	1.548975
59	8	0	4.703463	4.330000	-0.394153
60	6	0	4.809461	5.609127	0.268365
61	6	0	4.786552	-1.836697	-0.825936
62	1	0	4.058505	-0.616335	0.736868
63	6	0	6.055887	-1.616980	-0.448905
64	6	0	4.473533	-2.903525	-1.854584
65	1	0	6.883650	-2.157465	-0.900749
66	1	0	6.310456	-0.899617	0.326733
67	1	0	5.384718	-3.231542	-2.361980
68	1	0	4.025979	-3.785672	-1.379983
69	1	0	3.764674	-2.562264	-2.614156
70	1	0	5.014411	2.127568	-1.454178
71	1	0	5.406620	1.214610	0.015809
72	1	0	2.973783	1.435913	0.741131
73	1	0	2.630657	2.250134	-0.780658
74	8	0	2.623365	-3.994195	1.695421
75	1	0	3.582361	-2.306914	2.230354
76	6	0	1.200348	-0.598445	2.866808
77	1	0	0.304019	-1.221078	2.947059
78	1	0	2.062480	-1.163343	3.242537
79	1	0	1.076244	0.291183	3.488830
80	6	0	-4.860470	-2.848837	-0.024764
81	1	0	-5.867019	-2.592291	0.319916
82	1	0	-4.955256	-3.249551	-1.040115
83	1	0	-4.504265	-3.654247	0.622345
84	1	0	4.596450	6.351260	-0.499752
85	1	0	4.082843	5.676482	1.080907
86	1	0	5.816917	5.746724	0.666862

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.941090	0.163596	-1.182302
2	6	0	0.446077	0.840901	-1.145425
3	1	0	-0.967593	-0.457934	-2.081639
4	1	0	-1.710302	0.933133	-1.311750
5	1	0	0.496138	1.601684	-0.361224
6	1	0	0.610347	1.352954	-2.101383
7	6	0	3.730798	-1.014672	-0.191099
8	6	0	2.580225	-1.887070	0.402495
9	6	0	1.355343	-0.906633	0.454791
10	6	0	1.515677	-0.228852	-0.924401
11	6	0	3.022326	-2.567394	1.676073
12	1	0	2.290147	-2.685149	-0.286855
13	8	0	1.536493	0.130355	1.443224
14	6	0	-1.862603	-2.941639	0.900906
15	6	0	-2.350213	-1.872435	-0.131253
16	6	0	-1.263223	-0.695644	0.077145
17	6	0	-0.029442	-1.510799	0.536246
18	6	0	-0.380000	-2.715624	0.999051
19	1	0	-2.334906	-2.797059	1.884676
20	1	0	-2.113511	-3.961662	0.587845
21	6	0	-2.220604	-2.506919	-1.535378
22	6	0	-1.675007	0.264228	1.224284
23	1	0	0.303705	-3.450743	1.411125
24	1	0	-2.544654	-1.838737	-2.337499
25	1	0	-1.184682	-2.794195	-1.740183
26	1	0	-2.827826	-3.414872	-1.599457
27	1	0	-0.867975	0.969522	1.434993
28	1	0	-2.564431	0.844186	0.962704
29	1	0	-1.887787	-0.279523	2.150065
30	6	0	-3.839301	-1.473951	0.153002
31	6	0	-4.405666	-0.456236	-0.866087
32	6	0	-5.697360	0.237644	-0.455038
33	6	0	-6.272763	1.210230	-1.498599
34	6	0	-6.934821	2.308065	-0.649221
35	6	0	-6.149066	2.234858	0.657044
36	8	0	-5.448585	1.078809	0.723709
37	1	0	-6.456074	-0.489359	-0.147861
38	1	0	-6.970421	0.708965	-2.174851
39	1	0	-5.459055	1.629722	-2.100397
40	1	0	-6.790062	3.305273	-1.074818
41	6	0	-8.437985	2.094972	-0.385471
42	1	0	-3.856613	-0.996485	1.138480
43	1	0	-4.610613	-0.961093	-1.819522
44	1	0	-3.673413	0.326746	-1.082666
45	8	0	-6.122249	3.050056	1.556577
46	1	0	-8.819271	2.848009	0.309867
47	1	0	-8.993587	2.179166	-1.324225
48	1	0	-8.637021	1.105233	0.039448
49	1	0	1.294660	-1.031362	-1.642814
50	6	0	3.031644	0.086274	-1.120008
51	6	0	3.389086	-0.012796	-2.616512

52	6	0	3.375574	1.517375	-0.617952
53	1	0	4.469685	-0.009627	-2.783677
54	1	0	2.986157	-0.919946	-3.074433
55	1	0	2.965438	0.840102	-3.159408
56	6	0	4.848323	1.951438	-0.803275
57	6	0	5.047783	3.353730	-0.277659
58	8	0	4.748182	4.373014	-0.877314
59	8	0	5.574162	3.362003	0.964975
60	6	0	5.756776	4.656614	1.579481
61	6	0	4.861217	-1.854742	-0.778071
62	1	0	4.165566	-0.464578	0.650703
63	6	0	6.136355	-1.608126	-0.438756
64	6	0	4.528852	-3.019054	-1.687613
65	1	0	6.955283	-2.199617	-0.839879
66	1	0	6.404246	-0.814804	0.254039
67	1	0	5.431702	-3.404385	-2.168970
68	1	0	4.081457	-3.844733	-1.120404
69	1	0	3.813341	-2.751241	-2.469847
70	1	0	5.114595	1.965146	-1.863166
71	1	0	5.526436	1.272334	-0.283444
72	1	0	3.106228	1.594062	0.438545
73	1	0	2.748291	2.233311	-1.160881
74	8	0	2.723991	-3.708389	1.989568
75	1	0	3.698473	-1.980717	2.329997
76	6	0	1.346959	-0.197092	2.816884
77	1	0	1.203115	0.750541	3.341609
78	1	0	0.468353	-0.830485	2.972987
79	1	0	2.227143	-0.695727	3.241632
80	6	0	-4.771058	-2.702058	0.245746
81	1	0	-5.776738	-2.404754	0.558957
82	1	0	-4.869038	-3.216970	-0.716467
83	1	0	-4.416663	-3.428766	0.981097
84	1	0	6.193121	4.453893	2.556500
85	1	0	6.430056	5.270119	0.977169
86	1	0	4.795707	5.164498	1.685196

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908224	0.522189	-0.759024
2	6	0	0.435120	1.081082	-0.242622
3	1	0	-0.796259	0.380403	-1.837285
4	1	0	-1.683907	1.284743	-0.625136
5	1	0	0.355740	1.417563	0.795768
6	1	0	0.683748	1.957517	-0.850805
7	6	0	3.620892	-1.064099	0.310848
8	6	0	2.469202	-2.091960	0.179686
9	6	0	1.198356	-1.224776	0.491889
10	6	0	1.519110	0.010193	-0.381814
11	6	0	2.746702	-3.325239	1.009957
12	1	0	2.340897	-2.436038	-0.851224
13	8	0	1.194784	-0.753585	1.858160
14	6	0	-1.962909	-3.165263	-0.478799
15	6	0	-2.363150	-1.728259	-0.949589
16	6	0	-1.354856	-0.808418	-0.086499
17	6	0	-0.156370	-1.770628	0.098524
18	6	0	-0.513514	-3.044346	-0.099327
19	1	0	-2.556654	-3.485067	0.391336
20	1	0	-2.132497	-3.917540	-1.257826
21	6	0	-2.042860	-1.643055	-2.459594
22	6	0	-1.940406	-0.476475	1.311316
23	1	0	0.142958	-3.901235	0.008652
24	1	0	-2.288147	-0.670729	-2.894197
25	1	0	-0.981341	-1.833539	-2.645299
26	1	0	-2.609196	-2.400527	-3.009619
27	1	0	-1.191837	0.031504	1.922737
28	1	0	-2.811215	0.180597	1.236418
29	1	0	-2.246865	-1.379935	1.847534
30	6	0	-3.890065	-1.473779	-0.698260
31	6	0	-4.367892	-0.081159	-1.174127
32	6	0	-5.756748	0.338824	-0.689323
33	6	0	-6.165953	1.768983	-1.097831
34	6	0	-5.785706	2.626623	0.119070
35	6	0	-5.822354	1.619190	1.263696
36	8	0	-5.797030	0.355976	0.778840
37	1	0	-6.510368	-0.392854	-0.984914
38	1	0	-7.247732	1.818106	-1.263007
39	1	0	-5.670061	2.086443	-2.018396
40	1	0	-4.735304	2.941771	0.041601
41	6	0	-6.651356	3.862029	0.371653
42	1	0	-4.043352	-1.521554	0.384755
43	1	0	-4.405271	-0.057323	-2.270907
44	1	0	-3.654886	0.693503	-0.875141
45	8	0	-5.854734	1.843146	2.456375
46	1	0	-6.347601	4.365931	1.293154
47	1	0	-6.553314	4.570036	-0.456876
48	1	0	-7.707547	3.587488	0.463428
49	1	0	1.437466	-0.364617	-1.412054
50	6	0	3.039944	0.339379	-0.189984
51	6	0	3.620522	0.768375	-1.550327

52	6	0	3.342738	1.397909	0.913192
53	1	0	4.679561	1.034703	-1.486601
54	1	0	3.528988	-0.035176	-2.286968
55	1	0	3.080018	1.636518	-1.942302
56	6	0	3.148645	2.893745	0.580682
57	6	0	4.225690	3.575118	-0.238875
58	8	0	4.013499	4.384548	-1.126620
59	8	0	5.469807	3.240032	0.160010
60	6	0	6.563755	3.892084	-0.520941
61	6	0	4.955829	-1.505407	-0.272420
62	1	0	3.787468	-0.944967	1.390271
63	6	0	5.079674	-2.455516	-1.212022
64	6	0	6.181611	-0.831952	0.304217
65	1	0	6.058315	-2.742773	-1.587359
66	1	0	4.230878	-2.977951	-1.640841
67	1	0	6.240536	-0.997804	1.387841
68	1	0	7.098433	-1.215879	-0.151505
69	1	0	6.157953	0.253539	0.155972
70	1	0	3.124166	3.441962	1.532623
71	1	0	2.200906	3.099062	0.083738
72	1	0	4.378865	1.269302	1.240458
73	1	0	2.717236	1.162163	1.777924
74	8	0	2.383784	-4.453722	0.722532
75	1	0	3.358510	-3.164981	1.921320
76	6	0	0.884320	-1.683542	2.891480
77	1	0	0.037258	-2.325284	2.628615
78	1	0	1.746710	-2.314243	3.143035
79	1	0	0.624857	-1.091025	3.772201
80	6	0	-4.779525	-2.575310	-1.315406
81	1	0	-5.823435	-2.448232	-1.012630
82	1	0	-4.752183	-2.558707	-2.410757
83	1	0	-4.477851	-3.573036	-0.986914
84	1	0	7.467949	3.498357	-0.058717
85	1	0	6.542002	3.655277	-1.586867
86	1	0	6.503192	4.974127	-0.386153

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022266	0.154088	-1.108607
2	6	0	0.360782	0.825176	-0.967454
3	1	0	-1.030652	-0.361880	-2.072506
4	1	0	-1.791844	0.932236	-1.164153
5	1	0	0.390016	1.490570	-0.099808
6	1	0	0.539943	1.445319	-1.854411
7	6	0	3.635616	-1.126057	-0.178343
8	6	0	2.477341	-2.060656	0.280862
9	6	0	1.247416	-1.099704	0.431213
10	6	0	1.433283	-0.258766	-0.851198
11	6	0	2.899827	-2.905406	1.461301
12	1	0	2.194682	-2.761885	-0.507967
13	8	0	1.406053	-0.190978	1.541653
14	6	0	-1.977582	-3.169784	0.578922
15	6	0	-2.451630	-1.981664	-0.321700
16	6	0	-1.363737	-0.842797	0.037989
17	6	0	-0.137905	-1.710076	0.413980
18	6	0	-0.496168	-2.960642	0.723888
19	1	0	-2.462989	-3.145196	1.566663
20	1	0	-2.224574	-4.144021	0.141385
21	6	0	-2.311470	-2.444699	-1.790187
22	6	0	-1.787956	-0.021894	1.283940
23	1	0	0.182516	-3.739739	1.055257
24	1	0	-2.618335	-1.681984	-2.510590
25	1	0	-1.276944	-2.720422	-2.017036
26	1	0	-2.929277	-3.330072	-1.967265
27	1	0	-0.976568	0.640194	1.592674
28	1	0	-2.664137	0.599334	1.077436
29	1	0	-2.027567	-0.668112	2.134106
30	6	0	-3.942587	-1.613269	-0.006029
31	6	0	-4.495821	-0.476780	-0.899391
32	6	0	-5.801063	0.161750	-0.420635
33	6	0	-6.282761	1.344690	-1.285294
34	6	0	-5.719501	2.580983	-0.567719
35	6	0	-5.577021	2.095620	0.871022
36	8	0	-5.618878	0.743347	0.916299
37	1	0	-6.581952	-0.590663	-0.297711
38	1	0	-7.377485	1.385635	-1.291086
39	1	0	-5.943633	1.257569	-2.320450
40	1	0	-4.693892	2.777833	-0.911594
41	6	0	-6.535322	3.868281	-0.695443
42	1	0	-3.969636	-1.260224	1.029824
43	1	0	-4.692207	-0.863158	-1.908038
44	1	0	-3.753111	0.318313	-1.016216
45	8	0	-5.429395	2.762584	1.874379
46	1	0	-6.093717	4.667280	-0.093783
47	1	0	-6.564317	4.197846	-1.738477
48	1	0	-7.565311	3.714278	-0.356769
49	1	0	1.238850	-0.967943	-1.668717
50	6	0	2.952305	0.092571	-0.964742
51	6	0	3.335177	0.155681	-2.455334

52	6	0	3.237624	1.460351	-0.282956
53	1	0	4.396961	0.364882	-2.612097
54	1	0	3.112767	-0.786683	-2.963713
55	1	0	2.766471	0.950172	-2.952426
56	6	0	4.710601	1.926466	-0.249766
57	6	0	4.819157	3.259975	0.453246
58	8	0	4.938079	3.407901	1.657992
59	8	0	4.737287	4.294632	-0.409257
60	6	0	4.778867	5.619277	0.165801
61	6	0	4.772808	-1.868167	-0.880960
62	1	0	4.066808	-0.697776	0.736338
63	6	0	4.603155	-3.003960	-1.575357
64	6	0	6.157914	-1.276787	-0.739263
65	1	0	5.448319	-3.494829	-2.050324
66	1	0	3.640082	-3.486552	-1.704140
67	1	0	6.913046	-1.928514	-1.186808
68	1	0	6.234734	-0.296868	-1.223147
69	1	0	6.415880	-1.128829	0.317184
70	1	0	5.117791	2.023508	-1.259035
71	1	0	5.324027	1.221767	0.315144
72	1	0	2.861820	1.422289	0.741743
73	1	0	2.656315	2.225674	-0.810597
74	8	0	2.531524	-4.050866	1.661519
75	1	0	3.626379	-2.435500	2.155879
76	6	0	1.215072	-0.693608	2.860645
77	1	0	2.077095	-1.280142	3.202970
78	1	0	1.116002	0.180219	3.508901
79	1	0	0.312034	-1.306793	2.942049
80	6	0	-4.880921	-2.838070	-0.074528
81	1	0	-5.886554	-2.577515	0.269858
82	1	0	-4.975452	-3.226127	-1.094818
83	1	0	-4.532948	-3.653747	0.564148
84	1	0	4.701112	6.303183	-0.678184
85	1	0	3.942597	5.760263	0.853894
86	1	0	5.720109	5.771107	0.698304

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.003255	0.555487	-0.839329
2	6	0	0.341193	1.137406	-0.354764
3	1	0	-0.889754	0.330068	-1.903161
4	1	0	-1.775884	1.329156	-0.766090
5	1	0	0.257984	1.530424	0.662698
6	1	0	0.612152	1.980089	-1.002311
7	6	0	3.541402	-1.011776	0.203053
8	6	0	2.350670	-2.015798	0.263914
9	6	0	1.096432	-1.117468	0.539657
10	6	0	1.411640	0.047285	-0.425208
11	6	0	2.657385	-3.160344	1.202726
12	1	0	2.164875	-2.468916	-0.712768
13	8	0	1.111238	-0.565334	1.874184
14	6	0	-2.086466	-3.094184	-0.280089
15	6	0	-2.475436	-1.692326	-0.855767
16	6	0	-1.457090	-0.718403	-0.066157
17	6	0	-0.267200	-1.675933	0.191121
18	6	0	-0.636279	-2.957292	0.089925
19	1	0	-2.683506	-3.345577	0.610010
20	1	0	-2.261382	-3.900167	-1.002196
21	6	0	-2.158485	-1.723780	-2.368497
22	6	0	-2.037192	-0.276254	1.303143
23	1	0	0.013069	-3.809437	0.262483
24	1	0	-2.400083	-0.786522	-2.876348
25	1	0	-1.098251	-1.932785	-2.541027
26	1	0	-2.729720	-2.518318	-2.857762
27	1	0	-1.280836	0.262363	1.877575
28	1	0	-2.896456	0.388779	1.179449
29	1	0	-2.360031	-1.132378	1.903481
30	6	0	-3.999853	-1.408496	-0.621011
31	6	0	-4.464544	-0.042616	-1.180026
32	6	0	-5.865539	0.401562	-0.755092
33	6	0	-6.245910	1.823937	-1.214713
34	6	0	-5.890814	2.709816	-0.010437
35	6	0	-5.983271	1.735477	1.159288
36	8	0	-5.957622	0.459095	0.709829
37	1	0	-6.615212	-0.331169	-1.057910
38	1	0	-7.321945	1.880557	-1.412176
39	1	0	-5.720448	2.110934	-2.128953
40	1	0	-4.832676	3.003965	-0.061604
41	6	0	-6.741186	3.966952	0.178253
42	1	0	-4.153867	-1.388299	0.462756
43	1	0	-4.472897	-0.074096	-2.277222
44	1	0	-3.758637	0.745893	-0.901670
45	8	0	-6.056402	1.992404	2.343438
46	1	0	-6.459802	4.491215	1.095563
47	1	0	-6.601492	4.649687	-0.665388
48	1	0	-7.804929	3.714232	0.240941
49	1	0	1.320648	-0.403217	-1.424254
50	6	0	2.927584	0.394224	-0.268278
51	6	0	3.470060	0.868935	-1.628434

52	6	0	3.116273	1.498456	0.810744
53	1	0	4.542519	1.083119	-1.601689
54	1	0	3.314851	0.112150	-2.402526
55	1	0	2.957663	1.785897	-1.938190
56	6	0	4.547062	1.981332	1.111923
57	6	0	5.087675	3.019518	0.150669
58	8	0	4.446066	3.943174	-0.318677
59	8	0	6.403217	2.840030	-0.095917
60	6	0	7.041940	3.822301	-0.941525
61	6	0	4.745562	-1.558340	-0.566479
62	1	0	3.879339	-0.865827	1.237787
63	6	0	4.645602	-2.427784	-1.583874
64	6	0	6.111313	-1.094721	-0.110285
65	1	0	5.534481	-2.791449	-2.092303
66	1	0	3.698605	-2.805805	-1.954419
67	1	0	6.905918	-1.636554	-0.630460
68	1	0	6.263870	-0.025605	-0.295585
69	1	0	6.239747	-1.251099	0.968473
70	1	0	5.260742	1.161409	1.204520
71	1	0	4.535507	2.484471	2.088441
72	1	0	2.680660	1.133636	1.742535
73	1	0	2.532622	2.376485	0.515228
74	8	0	2.296027	-4.312951	1.033287
75	1	0	3.291283	-2.910265	2.078684
76	6	0	0.772885	-1.420096	2.961874
77	1	0	0.596754	-0.767197	3.820098
78	1	0	-0.130734	-2.004593	2.762760
79	1	0	1.591737	-2.106221	3.213008
80	6	0	-4.900392	-2.537245	-1.169424
81	1	0	-5.937979	-2.396455	-0.851569
82	1	0	-4.894642	-2.570835	-2.264830
83	1	0	-4.591306	-3.518962	-0.802006
84	1	0	6.963149	4.815601	-0.494520
85	1	0	8.084002	3.512634	-1.007268
86	1	0	6.579492	3.828644	-1.930837

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.768233	0.227861	-1.107686
2	6	0	0.620877	0.868144	-0.893871
3	1	0	-0.750593	-0.241286	-2.095187
4	1	0	-1.521058	1.022789	-1.153563
5	1	0	0.634576	1.506096	-0.004949
6	1	0	0.828243	1.509318	-1.757843
7	6	0	3.818962	-1.130989	0.031232
8	6	0	2.647562	-2.106922	0.305559
9	6	0	1.419207	-1.136909	0.441477
10	6	0	1.677626	-0.233069	-0.785706
11	6	0	2.976752	-3.043305	1.446286
12	1	0	2.426858	-2.739100	-0.560079
13	8	0	1.544296	-0.278054	1.596179
14	6	0	-1.833623	-3.164000	0.353608
15	6	0	-2.263367	-1.915150	-0.484701
16	6	0	-1.169127	-0.817440	-0.026712
17	6	0	0.028986	-1.724306	0.340252
18	6	0	-0.355759	-2.986137	0.560360
19	1	0	-2.351346	-3.195291	1.324600
20	1	0	-2.077742	-4.105008	-0.153054
21	6	0	-2.089127	-2.290210	-1.974584
22	6	0	-1.624543	-0.054233	1.244560
23	1	0	0.300122	-3.794452	0.865671
24	1	0	-2.367202	-1.480323	-2.654101
25	1	0	-1.052034	-2.565028	-2.190805
26	1	0	-2.711348	-3.155197	-2.222742
27	1	0	-0.816772	0.582799	1.610080
28	1	0	-2.488676	0.584821	1.042317
29	1	0	-1.895249	-0.740306	2.053313
30	6	0	-3.757138	-1.544230	-0.187160
31	6	0	-4.265622	-0.336415	-1.011305
32	6	0	-5.566430	0.289572	-0.525732
33	6	0	-6.072914	1.475434	-1.364436
34	6	0	-6.766286	2.381963	-0.333529
35	6	0	-6.050674	2.014764	0.963460
36	8	0	-5.367689	0.855843	0.815037
37	1	0	-6.350358	-0.466926	-0.416907
38	1	0	-6.739049	1.147127	-2.166921
39	1	0	-5.222557	1.994372	-1.820455
40	1	0	-6.587945	3.443354	-0.528663
41	6	0	-8.283793	2.151420	-0.196103
42	1	0	-3.807914	-1.264062	0.870240
43	1	0	-4.435341	-0.642339	-2.052359
44	1	0	-3.514631	0.458165	-1.040954
45	8	0	-6.061258	2.618924	2.016676
46	1	0	-8.693644	2.748924	0.623053
47	1	0	-8.787358	2.444382	-1.122227
48	1	0	-8.516396	1.098900	-0.001437
49	1	0	1.506618	-0.895781	-1.646311
50	6	0	3.211331	0.082468	-0.818996
51	6	0	3.681638	0.071521	-2.285575

52	6	0	3.634599	1.405246	-0.113275
53	1	0	4.736149	0.348070	-2.386974
54	1	0	3.555233	-0.919533	-2.730507
55	1	0	3.095223	0.778560	-2.882522
56	6	0	3.420877	2.724630	-0.893759
57	6	0	3.910839	3.905543	-0.086995
58	8	0	3.203658	4.660728	0.558628
59	8	0	5.254799	4.025544	-0.139353
60	6	0	5.838545	5.097150	0.632900
61	6	0	5.092972	-1.774323	-0.497557
62	1	0	4.079102	-0.702919	1.008803
63	6	0	5.124762	-2.965700	-1.114343
64	6	0	6.372952	-1.005608	-0.252930
65	1	0	6.064331	-3.387495	-1.461291
66	1	0	4.236914	-3.561929	-1.297554
67	1	0	7.243454	-1.553747	-0.623400
68	1	0	6.359466	-0.025404	-0.743138
69	1	0	6.514839	-0.817423	0.819068
70	1	0	2.366627	2.899934	-1.106260
71	1	0	3.970411	2.700441	-1.838949
72	1	0	4.704971	1.334435	0.109119
73	1	0	3.115475	1.464903	0.847626
74	8	0	2.582146	-4.193953	1.537132
75	1	0	3.657802	-2.637760	2.222360
76	6	0	1.303154	-0.837145	2.883870
77	1	0	0.416850	-1.479397	2.895597
78	1	0	2.165639	-1.411355	3.246230
79	1	0	1.143740	0.005983	3.560334
80	6	0	-4.709823	-2.745871	-0.369301
81	1	0	-5.720468	-2.496212	-0.031530
82	1	0	-4.783452	-3.055313	-1.417808
83	1	0	-4.388709	-3.611767	0.215008
84	1	0	6.911800	5.025741	0.461959
85	1	0	5.458206	6.061717	0.289987
86	1	0	5.608476	4.969744	1.692887

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.986992	0.563204	-0.819840
2	6	0	0.360547	1.134180	-0.330063
3	1	0	-0.875509	0.351990	-1.886773
4	1	0	-1.756917	1.338412	-0.735337
5	1	0	0.281734	1.516445	0.691882
6	1	0	0.634624	1.982317	-0.969131
7	6	0	3.546541	-1.017599	0.253454
8	6	0	2.360195	-2.032120	0.271448
9	6	0	1.105268	-1.130115	0.543930
10	6	0	1.425413	0.040013	-0.413268
11	6	0	2.650565	-3.182740	1.205363
12	1	0	2.199644	-2.471334	-0.717430
13	8	0	1.120993	-0.581976	1.879884
14	6	0	-2.077354	-3.092718	-0.305287
15	6	0	-2.461656	-1.684032	-0.867957
16	6	0	-1.445606	-0.719775	-0.063545
17	6	0	-0.258226	-1.682191	0.188523
18	6	0	-0.628629	-2.961850	0.072581
19	1	0	-2.678745	-3.352411	0.579443
20	1	0	-2.250119	-3.890788	-1.036613
21	6	0	-2.138062	-1.699533	-2.379409
22	6	0	-2.031638	-0.291468	1.307652
23	1	0	0.018108	-3.817510	0.238033
24	1	0	-2.377704	-0.756851	-2.878042
25	1	0	-1.077088	-1.906715	-2.549611
26	1	0	-2.707117	-2.488743	-2.879686
27	1	0	-1.278680	0.243689	1.889738
28	1	0	-2.891200	0.373446	1.186321
29	1	0	-2.356008	-1.153186	1.899060
30	6	0	-3.986735	-1.401216	-0.636568
31	6	0	-4.448126	-0.028545	-1.181476
32	6	0	-5.849139	0.412762	-0.753526
33	6	0	-6.227872	1.840082	-1.199052
34	6	0	-5.875456	2.713405	0.015164
35	6	0	-5.968580	1.726766	1.174472
36	8	0	-5.942731	0.455114	0.711746
37	1	0	-6.599143	-0.316132	-1.064691
38	1	0	-7.303391	1.899084	-1.398552
39	1	0	-5.700071	2.136332	-2.108964
40	1	0	-4.817671	3.009539	-0.031187
41	6	0	-6.727816	3.967324	0.216070
42	1	0	-4.145174	-1.393573	0.446729
43	1	0	-4.454965	-0.048074	-2.278962
44	1	0	-3.741521	0.755864	-0.893490
45	8	0	-6.042387	1.971273	2.361196
46	1	0	-6.448619	4.481870	1.139509
47	1	0	-6.587663	4.659425	-0.619821
48	1	0	-7.791313	3.712480	0.274191
49	1	0	1.327524	-0.402789	-1.415084
50	6	0	2.942639	0.374517	-0.259310
51	6	0	3.497783	0.851904	-1.615215

52	6	0	3.169914	1.485241	0.805520
53	1	0	4.588467	0.943428	-1.605380
54	1	0	3.232580	0.170600	-2.428023
55	1	0	3.082088	1.833934	-1.862798
56	6	0	4.624670	1.949739	1.010442
57	6	0	5.068194	3.085251	0.110256
58	8	0	4.349730	3.966838	-0.327918
59	8	0	6.398743	3.046097	-0.114458
60	6	0	6.954290	4.128222	-0.893193
61	6	0	4.789114	-1.583468	-0.428868
62	1	0	3.825619	-0.851858	1.299992
63	6	0	5.985950	-1.512275	0.175327
64	6	0	4.651193	-2.304881	-1.753310
65	1	0	6.881228	-1.918151	-0.288474
66	1	0	6.110712	-1.054330	1.153031
67	1	0	5.634048	-2.510259	-2.185956
68	1	0	4.142152	-3.267910	-1.623066
69	1	0	4.068868	-1.738397	-2.485087
70	1	0	5.345041	1.133643	0.926698
71	1	0	4.731032	2.344494	2.030312
72	1	0	2.779570	1.126933	1.759946
73	1	0	2.575681	2.363818	0.534163
74	8	0	2.354960	-4.345665	0.982891
75	1	0	3.211616	-2.929341	2.127521
76	6	0	0.755828	-1.428811	2.965781
77	1	0	1.566253	-2.116182	3.238723
78	1	0	0.563547	-0.769908	3.815949
79	1	0	-0.145552	-2.010838	2.751039
80	6	0	-4.885818	-2.522668	-1.202083
81	1	0	-5.924962	-2.383757	-0.888514
82	1	0	-4.874032	-2.544366	-2.297735
83	1	0	-4.580226	-3.508773	-0.843611
84	1	0	8.022995	3.925536	-0.947748
85	1	0	6.514518	4.140622	-1.892802
86	1	0	6.768886	5.085203	-0.400541

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.790087	0.037268	-1.226766
2	6	0	0.589318	0.733683	-1.220411
3	1	0	-0.826744	-0.579015	-2.129094
4	1	0	-1.571715	0.797330	-1.336235
5	1	0	0.638274	1.511440	-0.453188
6	1	0	0.730573	1.228250	-2.188714
7	6	0	3.909800	-0.928192	-0.166557
8	6	0	2.818115	-1.895340	0.362977
9	6	0	1.541194	-0.979560	0.392798
10	6	0	1.671079	-0.323689	-0.999377
11	6	0	3.256304	-2.580701	1.637707
12	1	0	2.596333	-2.690582	-0.356225
13	8	0	1.675770	0.080303	1.363543
14	6	0	-1.620690	-3.098420	0.851817
15	6	0	-2.139883	-2.037062	-0.172912
16	6	0	-1.079268	-0.835207	0.033097
17	6	0	0.176099	-1.623966	0.483339
18	6	0	-0.143145	-2.838253	0.943507
19	1	0	-2.091054	-2.969641	1.838809
20	1	0	-1.849189	-4.122771	0.535538
21	6	0	-2.005149	-2.663732	-1.580027
22	6	0	-1.508400	0.110379	1.185648
23	1	0	0.561574	-3.555997	1.350178
24	1	0	-2.353022	-2.002416	-2.377853
25	1	0	-0.963698	-2.923263	-1.793625
26	1	0	-2.588950	-3.587046	-1.641524
27	1	0	-0.722474	0.841845	1.386097
28	1	0	-2.419608	0.660251	0.935075
29	1	0	-1.691647	-0.440395	2.113662
30	6	0	-3.636184	-1.674878	0.122883
31	6	0	-4.232641	-0.663833	-0.885916
32	6	0	-5.527553	0.011233	-0.453717
33	6	0	-6.134041	0.974926	-1.487954
34	6	0	-6.794633	2.066135	-0.628813
35	6	0	-5.986713	2.003857	0.664314
36	8	0	-5.271092	0.856772	0.720448
37	1	0	-6.270332	-0.726343	-0.132969
38	1	0	-6.837258	0.463887	-2.150978
39	1	0	-5.336657	1.403681	-2.104820
40	1	0	-6.668123	3.064341	-1.057923
41	6	0	-8.290858	1.837115	-0.339881
42	1	0	-3.658589	-1.204957	1.111863
43	1	0	-4.444620	-1.170551	-1.836861
44	1	0	-3.515254	0.129871	-1.112700
45	8	0	-5.955063	2.820405	1.562566
46	1	0	-8.668470	2.586961	0.360908
47	1	0	-8.862949	1.914332	-1.269287
48	1	0	-8.472364	0.845911	0.089460
49	1	0	1.419288	-1.141364	-1.688685
50	6	0	3.191329	-0.030326	-1.267246
51	6	0	3.506178	-0.518570	-2.699388

52	6	0	3.588648	1.471596	-1.227423
53	1	0	4.550852	-0.344466	-2.975079
54	1	0	3.307427	-1.588591	-2.812528
55	1	0	2.878875	0.017859	-3.421298
56	6	0	3.553391	2.215752	0.111483
57	6	0	3.740811	3.708973	-0.044575
58	8	0	3.670882	4.338914	-1.085875
59	8	0	3.982278	4.294951	1.148850
60	6	0	4.131113	5.731143	1.144582
61	6	0	5.224027	-1.582517	-0.564564
62	1	0	4.143980	-0.265640	0.675847
63	6	0	5.351044	-2.888131	-0.847650
64	6	0	6.430581	-0.670671	-0.587486
65	1	0	6.317439	-3.308514	-1.113029
66	1	0	4.516611	-3.581532	-0.830012
67	1	0	7.339914	-1.217956	-0.849991
68	1	0	6.308139	0.145682	-1.308617
69	1	0	6.582868	-0.201627	0.393127
70	1	0	4.323779	1.861388	0.803803
71	1	0	2.604299	2.057791	0.633778
72	1	0	2.939729	2.002249	-1.931766
73	1	0	4.598449	1.569744	-1.642709
74	8	0	2.901667	-3.695626	1.983307
75	1	0	3.976682	-2.018128	2.265935
76	6	0	1.542188	-0.246160	2.743663
77	1	0	0.702578	-0.924072	2.926759
78	1	0	2.459319	-0.695093	3.145705
79	1	0	1.363434	0.695936	3.267557
80	6	0	-4.539435	-2.924135	0.212921
81	1	0	-5.551226	-2.650360	0.528203
82	1	0	-4.627299	-3.437891	-0.750843
83	1	0	-4.167724	-3.644913	0.945629
84	1	0	4.975954	6.023920	0.517379
85	1	0	3.219770	6.206504	0.775210
86	1	0	4.312058	6.005918	2.182878

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.002686	0.152722	-1.151326
2	6	0	0.394477	0.804347	-1.078844
3	1	0	-1.028099	-0.446290	-2.065899
4	1	0	-1.757410	0.937942	-1.270907
5	1	0	0.446213	1.546465	-0.277195
6	1	0	0.580639	1.335888	-2.019895
7	6	0	3.639686	-1.169203	-0.199172
8	6	0	2.477757	-1.972232	0.447554
9	6	0	1.254822	-0.995265	0.492580
10	6	0	1.443396	-0.287149	-0.867739
11	6	0	2.876450	-2.680526	1.721066
12	1	0	2.153720	-2.786536	-0.214849
13	8	0	1.417837	0.018860	1.508689
14	6	0	-2.016718	-2.981977	0.839520
15	6	0	-2.465940	-1.876944	-0.171206
16	6	0	-1.356198	-0.730923	0.081852
17	6	0	-0.142799	-1.582166	0.535025
18	6	0	-0.531127	-2.789153	0.960615
19	1	0	-2.498109	-2.850177	1.820598
20	1	0	-2.285202	-3.988285	0.498119
21	6	0	-2.333020	-2.479075	-1.589120
22	6	0	-1.760491	0.206428	1.250084
23	1	0	0.118773	-3.557535	1.367666
24	1	0	-2.635246	-1.785272	-2.377812
25	1	0	-1.300938	-2.781988	-1.790767
26	1	0	-2.957883	-3.372483	-1.681772
27	1	0	-0.939205	0.884897	1.489760
28	1	0	-2.632321	0.814468	0.993223
29	1	0	-1.998788	-0.357025	2.157767
30	6	0	-3.949251	-1.452282	0.105276
31	6	0	-4.479072	-0.392805	-0.890642
32	6	0	-5.759279	0.319371	-0.474431
33	6	0	-6.295603	1.338621	-1.494233
34	6	0	-6.939733	2.427458	-0.619740
35	6	0	-6.176338	2.291500	0.694761
36	8	0	-5.506712	1.115862	0.733707
37	1	0	-6.539751	-0.398099	-0.200955
38	1	0	-6.997078	0.876807	-2.194276
39	1	0	-5.463336	1.754472	-2.072713
40	1	0	-6.760781	3.432937	-1.011449
41	6	0	-8.452077	2.248914	-0.384504
42	1	0	-3.968442	-1.003442	1.103978
43	1	0	-4.684278	-0.864998	-1.860654
44	1	0	-3.726852	0.378859	-1.076626
45	8	0	-6.142735	3.075756	1.621031
46	1	0	-8.823373	2.992060	0.326718
47	1	0	-8.990625	2.375381	-1.328458
48	1	0	-8.684511	1.253260	0.008502
49	1	0	1.223032	-1.071391	-1.607652
50	6	0	2.965324	0.015516	-1.039797
51	6	0	3.305921	-0.007574	-2.542715

52	6	0	3.323977	1.408844	-0.449934
53	1	0	4.375695	0.115934	-2.733166
54	1	0	3.004255	-0.948752	-3.009527
55	1	0	2.783071	0.808279	-3.055479
56	6	0	4.798811	1.817399	-0.534125
57	6	0	5.054937	3.215738	-0.011045
58	8	0	4.210660	4.066806	0.205096
59	8	0	6.375918	3.430615	0.173714
60	6	0	6.757463	4.746592	0.629740
61	6	0	4.647995	-2.052923	-0.934101
62	1	0	4.185167	-0.706390	0.629031
63	6	0	4.308333	-3.127788	-1.660961
64	6	0	6.098983	-1.653931	-0.799478
65	1	0	5.064793	-3.721224	-2.167510
66	1	0	3.281130	-3.456412	-1.790758
67	1	0	6.759068	-2.362107	-1.307901
68	1	0	6.283112	-0.659617	-1.223298
69	1	0	6.389346	-1.605601	0.257337
70	1	0	5.165805	1.809412	-1.568424
71	1	0	5.450027	1.135715	0.021334
72	1	0	3.007025	1.442421	0.594279
73	1	0	2.733621	2.166603	-0.975842
74	8	0	3.991070	-2.648631	2.214728
75	1	0	2.090297	-3.298990	2.196659
76	6	0	1.242892	-0.353307	2.872656
77	1	0	0.341345	-0.956654	3.022478
78	1	0	2.111317	-0.896528	3.262987
79	1	0	1.143030	0.579970	3.432022
80	6	0	-4.910250	-2.660445	0.150067
81	1	0	-5.911727	-2.349164	0.462918
82	1	0	-5.010248	-3.142195	-0.828922
83	1	0	-4.580579	-3.418164	0.865389
84	1	0	7.842970	4.719594	0.714444
85	1	0	6.447272	5.503978	-0.093550
86	1	0	6.301909	4.959152	1.599218

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.094100	0.178121	-1.129191
2	6	0	0.299561	0.835866	-1.029719
3	1	0	-1.118530	-0.377072	-2.070876
4	1	0	-1.853996	0.963579	-1.210417
5	1	0	0.348517	1.539399	-0.193533
6	1	0	0.479439	1.413177	-1.944874
7	6	0	3.554849	-1.112721	-0.170938
8	6	0	2.390164	-2.022287	0.332407
9	6	0	1.173257	-1.037061	0.444362
10	6	0	1.357732	-0.256792	-0.876794
11	6	0	2.807987	-2.803491	1.554954
12	1	0	2.107177	-2.760519	-0.423339
13	8	0	1.353979	-0.080960	1.511106
14	6	0	-2.072931	-3.059393	0.709989
15	6	0	-2.539752	-1.908286	-0.241454
16	6	0	-1.438024	-0.766203	0.060945
17	6	0	-0.218580	-1.630026	0.465732
18	6	0	-0.588111	-2.861198	0.834477
19	1	0	-2.550774	-2.982379	1.698798
20	1	0	-2.334351	-4.049798	0.319936
21	6	0	-2.413077	-2.438259	-1.688172
22	6	0	-1.843418	0.111556	1.274052
23	1	0	0.083341	-3.633692	1.195212
24	1	0	-2.720664	-1.707100	-2.440321
25	1	0	-1.381925	-2.730409	-1.909601
26	1	0	-3.037845	-3.326616	-1.820728
27	1	0	-1.025577	0.782926	1.543549
28	1	0	-2.718247	0.728323	1.050044
29	1	0	-2.077221	-0.494648	2.154681
30	6	0	-4.024463	-1.510816	0.067042
31	6	0	-4.570184	-0.402095	-0.864388
32	6	0	-5.879955	0.248503	-0.414853
33	6	0	-6.345344	1.419746	-1.304116
34	6	0	-5.794025	2.666023	-0.594383
35	6	0	-5.672841	2.200332	0.852735
36	8	0	-5.715632	0.848813	0.915928
37	1	0	-6.665164	-0.499550	-0.292923
38	1	0	-7.439773	1.461005	-1.329697
39	1	0	-5.988226	1.317983	-2.331880
40	1	0	-4.763702	2.859994	-0.925338
41	6	0	-6.609720	3.950244	-0.751196
42	1	0	-4.040965	-1.118442	1.088876
43	1	0	-4.758351	-0.817204	-1.863131
44	1	0	-3.826615	0.389514	-0.998021
45	8	0	-5.540391	2.880733	1.849142
46	1	0	-6.177559	4.758008	-0.154453
47	1	0	-6.624472	4.265351	-1.798972
48	1	0	-7.644145	3.799305	-0.424808
49	1	0	1.140565	-1.000625	-1.657066
50	6	0	2.878554	0.061514	-1.025156
51	6	0	3.259810	0.067475	-2.519772

52	6	0	3.223206	1.449802	-0.415711
53	1	0	4.343191	0.072648	-2.668846
54	1	0	2.858066	-0.800197	-3.049863
55	1	0	2.851758	0.961247	-3.006082
56	6	0	4.694355	1.872864	-0.516378
57	6	0	4.948927	3.249383	0.060356
58	8	0	4.114341	4.122833	0.219055
59	8	0	6.254074	3.419507	0.364086
60	6	0	6.634574	4.718043	0.869216
61	6	0	4.691994	-1.911361	-0.800841
62	1	0	3.974729	-0.631673	0.719501
63	6	0	5.963272	-1.697252	-0.427012
64	6	0	4.367318	-3.004436	-1.797634
65	1	0	6.785060	-2.262086	-0.859543
66	1	0	6.225671	-0.959006	0.326122
67	1	0	5.274610	-3.357441	-2.295171
68	1	0	3.909806	-3.867143	-1.297507
69	1	0	3.662250	-2.676565	-2.566403
70	1	0	5.027573	1.917032	-1.561313
71	1	0	5.366033	1.168682	-0.019079
72	1	0	2.917542	1.461888	0.633063
73	1	0	2.618849	2.209091	-0.922877
74	8	0	2.497221	-3.962932	1.774873
75	1	0	3.478717	-2.274275	2.261502
76	6	0	1.137540	-0.506537	2.853521
77	1	0	1.016239	0.402832	3.447077
78	1	0	0.238113	-1.121947	2.952124
79	1	0	1.996160	-1.063905	3.248619
80	6	0	-4.977167	-2.726464	0.052104
81	1	0	-5.972563	-2.444813	0.409183
82	1	0	-5.096713	-3.142745	-0.954426
83	1	0	-4.625300	-3.527627	0.706780
84	1	0	7.707784	4.656727	1.044321
85	1	0	6.409055	5.492802	0.133165
86	1	0	6.105238	4.933239	1.799919

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.962705	0.069946	-1.205386
2	6	0	0.424646	0.746052	-1.198119
3	1	0	-0.991068	-0.586760	-2.078919
4	1	0	-1.731815	0.833946	-1.364324
5	1	0	0.474235	1.541428	-0.449349
6	1	0	0.589315	1.213709	-2.176212
7	6	0	3.714922	-1.103520	-0.216479
8	6	0	2.574706	-1.870883	0.507234
9	6	0	1.332378	-0.920486	0.485857
10	6	0	1.493867	-0.312220	-0.924928
11	6	0	2.996765	-2.463336	1.831499
12	1	0	2.263016	-2.743837	-0.082423
13	8	0	1.477259	0.172920	1.420265
14	6	0	-1.889481	-2.955182	0.985744
15	6	0	-2.374796	-1.921160	-0.081679
16	6	0	-1.286352	-0.738726	0.086763
17	6	0	-0.051428	-1.533049	0.581676
18	6	0	-0.408089	-2.721801	1.080432
19	1	0	-2.364509	-2.779690	1.962936
20	1	0	-2.136667	-3.985449	0.705020
21	6	0	-2.247327	-2.603500	-1.463403
22	6	0	-1.701361	0.263737	1.195950
23	1	0	0.262407	-3.451445	1.524280
24	1	0	-2.573478	-1.963029	-2.286906
25	1	0	-1.211724	-2.897173	-1.661329
26	1	0	-2.854046	-3.513502	-1.495468
27	1	0	-0.897025	0.979468	1.378363
28	1	0	-2.593494	0.828678	0.912338
29	1	0	-1.911731	-0.244445	2.142392
30	6	0	-3.863271	-1.512063	0.190701
31	6	0	-4.429374	-0.522564	-0.855950
32	6	0	-5.719460	0.183566	-0.460339
33	6	0	-6.288228	1.142355	-1.520330
34	6	0	-6.947742	2.255961	-0.689505
35	6	0	-6.165489	2.199744	0.619568
36	8	0	-5.470056	1.041800	0.705710
37	1	0	-6.481962	-0.535590	-0.144033
38	1	0	-6.986493	0.633948	-2.190567
39	1	0	-5.471374	1.549273	-2.126483
40	1	0	-6.797860	3.245820	-1.130185
41	6	0	-8.452312	2.053165	-0.425841
42	1	0	-3.878637	-1.006124	1.161797
43	1	0	-4.636496	-1.052920	-1.794924
44	1	0	-3.696178	0.252959	-1.094398
45	8	0	-6.137325	3.028295	1.506670
46	1	0	-8.831817	2.818152	0.257320
47	1	0	-9.005600	2.125580	-1.366912
48	1	0	-8.656251	1.070753	0.013457
49	1	0	1.277782	-1.150516	-1.603979
50	6	0	3.009182	-0.000690	-1.137782
51	6	0	3.335891	-0.131283	-2.637638

52	6	0	3.348826	1.438589	-0.656400
53	1	0	4.401637	-0.006550	-2.847452
54	1	0	3.044466	-1.110058	-3.027188
55	1	0	2.796277	0.635561	-3.205583
56	6	0	4.827521	1.869263	-0.796098
57	6	0	4.996151	3.303885	-0.352453
58	8	0	4.842925	4.279574	-1.068890
59	8	0	5.307342	3.396491	0.956771
60	6	0	5.433547	4.729488	1.498305
61	6	0	4.728349	-2.024800	-0.896315
62	1	0	4.265140	-0.566748	0.562611
63	6	0	4.401807	-3.172132	-1.509259
64	6	0	6.169649	-1.574072	-0.846152
65	1	0	5.162060	-3.788323	-1.981703
66	1	0	3.382404	-3.541076	-1.576627
67	1	0	6.836246	-2.310646	-1.303102
68	1	0	6.311343	-0.622199	-1.371625
69	1	0	6.488501	-1.413778	0.191218
70	1	0	5.153338	1.817690	-1.837614
71	1	0	5.475434	1.232133	-0.189657
72	1	0	3.048714	1.538676	0.388962
73	1	0	2.740550	2.143779	-1.234643
74	8	0	4.119138	-2.385298	2.301341
75	1	0	2.220051	-3.037862	2.373117
76	6	0	1.336671	-0.101428	2.811512
77	1	0	0.481597	-0.754040	3.017613
78	1	0	2.245075	-0.548022	3.232013
79	1	0	1.171993	0.862790	3.298590
80	6	0	-4.796975	-2.735476	0.319635
81	1	0	-5.800792	-2.427539	0.628357
82	1	0	-4.899613	-3.275789	-0.628060
83	1	0	-4.441681	-3.443107	1.073059
84	1	0	5.672530	4.591836	2.551865
85	1	0	6.234592	5.270315	0.989872
86	1	0	4.494413	5.275176	1.384623

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022269	0.154088	-1.108603
2	6	0	0.360779	0.825176	-0.967448
3	1	0	-1.030654	-0.361877	-2.072503
4	1	0	-1.791847	0.932236	-1.164147
5	1	0	0.390015	1.490568	-0.099801
6	1	0	0.539940	1.445321	-1.854405
7	6	0	3.635613	-1.126058	-0.178341
8	6	0	2.477338	-2.060660	0.280856
9	6	0	1.247414	-1.099707	0.431213
10	6	0	1.433280	-0.258767	-0.851196
11	6	0	2.899823	-2.905414	1.461293
12	1	0	2.194679	-2.761886	-0.507975
13	8	0	1.406055	-0.190984	1.541655
14	6	0	-1.977585	-3.169786	0.578921
15	6	0	-2.451633	-1.981666	-0.321699
16	6	0	-1.363739	-0.842799	0.037991
17	6	0	-0.137907	-1.710078	0.413980
18	6	0	-0.496170	-2.960644	0.723886
19	1	0	-2.462991	-3.145200	1.566662
20	1	0	-2.224576	-4.144023	0.141383
21	6	0	-2.311471	-2.444700	-1.790187
22	6	0	-1.787957	-0.021898	1.283943
23	1	0	0.182514	-3.739743	1.055255
24	1	0	-2.618338	-1.681985	-2.510590
25	1	0	-1.276943	-2.720419	-2.017037
26	1	0	-2.929275	-3.330075	-1.967266
27	1	0	-0.976569	0.640189	1.592680
28	1	0	-2.664138	0.599332	1.077441
29	1	0	-2.027569	-0.668117	2.134108
30	6	0	-3.942590	-1.613271	-0.006029
31	6	0	-4.495823	-0.476781	-0.899392
32	6	0	-5.801061	0.161754	-0.420632
33	6	0	-6.282759	1.344694	-1.285292
34	6	0	-5.719495	2.580987	-0.567720
35	6	0	-5.577010	2.095625	0.871021
36	8	0	-5.618870	0.743352	0.916300
37	1	0	-6.581953	-0.590656	-0.297704
38	1	0	-7.377482	1.385640	-1.291084
39	1	0	-5.943631	1.257571	-2.320449
40	1	0	-4.693887	2.777837	-0.911598
41	6	0	-6.535315	3.868286	-0.695441
42	1	0	-3.969639	-1.260226	1.029824
43	1	0	-4.692211	-0.863160	-1.908038
44	1	0	-3.753111	0.318310	-1.016219
45	8	0	-5.429379	2.762590	1.874377
46	1	0	-6.093710	4.667282	-0.093780
47	1	0	-6.564312	4.197853	-1.738473
48	1	0	-7.565305	3.714282	-0.356766
49	1	0	1.238847	-0.967941	-1.668716
50	6	0	2.952303	0.092571	-0.964739
51	6	0	3.335175	0.155681	-2.455332

52	6	0	3.237620	1.460350	-0.282953
53	1	0	4.396958	0.364889	-2.612093
54	1	0	3.112772	-0.786684	-2.963710
55	1	0	2.766464	0.950169	-2.952424
56	6	0	4.710597	1.926467	-0.249763
57	6	0	4.819153	3.259978	0.453245
58	8	0	4.938073	3.407906	1.657991
59	8	0	4.737285	4.294632	-0.409260
60	6	0	4.778867	5.619279	0.165796
61	6	0	4.772809	-1.868163	-0.880957
62	1	0	4.066799	-0.697778	0.736343
63	6	0	4.603161	-3.003952	-1.575360
64	6	0	6.157915	-1.276782	-0.739252
65	1	0	5.448327	-3.494819	-2.050325
66	1	0	3.640088	-3.486543	-1.704150
67	1	0	6.913050	-1.928513	-1.186786
68	1	0	6.234739	-0.296867	-1.223142
69	1	0	6.415873	-1.128817	0.317197
70	1	0	5.117788	2.023507	-1.259032
71	1	0	5.324024	1.221770	0.315148
72	1	0	2.861817	1.422288	0.741746
73	1	0	2.656310	2.225673	-0.810593
74	8	0	2.531529	-4.050878	1.661500
75	1	0	3.626367	-2.435508	2.155879
76	6	0	1.215069	-0.693614	2.860646
77	1	0	0.312027	-1.306793	2.942047
78	1	0	2.077087	-1.280153	3.202973
79	1	0	1.116002	0.180214	3.508902
80	6	0	-4.880924	-2.838072	-0.074531
81	1	0	-5.886558	-2.577517	0.269852
82	1	0	-4.975452	-3.226130	-1.094821
83	1	0	-4.532953	-3.653748	0.564148
84	1	0	4.701102	6.303184	-0.678190
85	1	0	3.942604	5.760263	0.853897
86	1	0	5.720114	5.771112	0.698289

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.812630	0.147664	-1.064948
2	6	0	0.550428	0.834714	-0.828155
3	1	0	-0.774809	-0.294389	-2.064415
4	1	0	-1.597094	0.912398	-1.092279
5	1	0	0.537548	1.442207	0.082111
6	1	0	0.735517	1.511525	-1.669801
7	6	0	3.823837	-1.076150	0.031229
8	6	0	2.684351	-2.098180	0.296492
9	6	0	1.424492	-1.171697	0.454379
10	6	0	1.648514	-0.228587	-0.750075
11	6	0	3.046853	-3.032029	1.426289
12	1	0	2.487861	-2.728015	-0.576624
13	8	0	1.513569	-0.338205	1.630644
14	6	0	-1.748347	-3.317858	0.314057
15	6	0	-2.223570	-2.067967	-0.498429
16	6	0	-1.173524	-0.940731	-0.012338
17	6	0	0.058264	-1.809009	0.335686
18	6	0	-0.278337	-3.089100	0.526747
19	1	0	-2.265165	-3.387991	1.283319
20	1	0	-1.956096	-4.256287	-0.212853
21	6	0	-2.028767	-2.403600	-1.995173
22	6	0	-1.658409	-0.228925	1.278047
23	1	0	0.407126	-3.879565	0.814133
24	1	0	-2.333290	-1.590307	-2.658968
25	1	0	-0.981126	-2.634836	-2.211589
26	1	0	-2.617052	-3.285631	-2.265589
27	1	0	-0.878648	0.433066	1.659741
28	1	0	-2.547907	0.379208	1.091419
29	1	0	-1.901608	-0.944245	2.069759
30	6	0	-3.731809	-1.761663	-0.197702
31	6	0	-4.283906	-0.552426	-0.989735
32	6	0	-5.659029	-0.048230	-0.547863
33	6	0	-6.131977	1.227221	-1.274602
34	6	0	-5.705700	2.367405	-0.337050
35	6	0	-5.657055	1.680148	1.023719
36	8	0	-5.625718	0.335943	0.869860
37	1	0	-6.403898	-0.843250	-0.608538
38	1	0	-7.222670	1.219246	-1.376750
39	1	0	-5.700967	1.309874	-2.275408
40	1	0	-4.668276	2.660802	-0.552819
41	6	0	-6.583667	3.619694	-0.352327
42	1	0	-3.797648	-1.512370	0.866490
43	1	0	-4.379731	-0.817259	-2.050740
44	1	0	-3.583343	0.287311	-0.944371
45	8	0	-5.632484	2.196598	2.121977
46	1	0	-6.244450	4.339152	0.397792
47	1	0	-6.542526	4.099997	-1.334618
48	1	0	-7.627852	3.368534	-0.137999
49	1	0	1.497122	-0.875911	-1.626347
50	6	0	3.168538	0.138791	-0.781907
51	6	0	3.634979	0.220774	-2.247507

52	6	0	3.577929	1.436869	-0.026043
53	1	0	4.703935	0.446699	-2.320370
54	1	0	3.448797	-0.713514	-2.783377
55	1	0	3.088014	1.004651	-2.781943
56	6	0	3.284906	2.782871	-0.701089
57	6	0	3.796990	3.959234	0.104589
58	8	0	4.561813	3.903050	1.051097
59	8	0	3.308437	5.124153	-0.374650
60	6	0	3.756785	6.330122	0.281363
61	6	0	5.109607	-1.679365	-0.519958
62	1	0	4.080877	-0.659197	1.010511
63	6	0	6.297810	-1.251377	-0.063478
64	6	0	5.037712	-2.792413	-1.543164
65	1	0	7.232075	-1.653315	-0.447184
66	1	0	6.373681	-0.488359	0.706815
67	1	0	6.034157	-3.033959	-1.922962
68	1	0	4.621713	-3.706528	-1.101574
69	1	0	4.401168	-2.541362	-2.397289
70	1	0	2.219360	2.945744	-0.879228
71	1	0	3.768299	2.854811	-1.683231
72	1	0	4.660722	1.386884	0.137863
73	1	0	3.115202	1.423080	0.964220
74	8	0	2.779806	-4.222718	1.451784
75	1	0	3.635449	-2.588276	2.253943
76	6	0	1.273563	-0.928523	2.905584
77	1	0	1.013928	-0.110435	3.581956
78	1	0	0.447933	-1.646633	2.879038
79	1	0	2.169825	-1.426110	3.296447
80	6	0	-4.637459	-2.993632	-0.416048
81	1	0	-5.647639	-2.804964	-0.040478
82	1	0	-4.726001	-3.255686	-1.476393
83	1	0	-4.265064	-3.871928	0.116783
84	1	0	4.841696	6.426076	0.199337
85	1	0	3.259647	7.145657	-0.242081
86	1	0	3.469605	6.318556	1.334902

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.128249	-0.292116	-1.220647
2	6	0	-0.220951	-1.041688	-1.196950
3	1	0	1.134610	0.325612	-2.123044
4	1	0	1.938467	-1.021108	-1.334737
5	1	0	-0.239629	-1.794621	-0.404061
6	1	0	-0.340038	-1.573260	-2.149199
7	6	0	-3.614687	0.660598	-0.324808
8	6	0	-2.516914	1.591224	0.270718
9	6	0	-1.246166	0.677125	0.363591
10	6	0	-1.352922	-0.030564	-1.004524
11	6	0	-3.017087	2.287391	1.515595
12	1	0	-2.242331	2.384925	-0.428561
13	8	0	-1.386193	-0.351772	1.364641
14	6	0	1.865145	2.867595	0.847611
15	6	0	2.425280	1.809622	-0.158518
16	6	0	1.385440	0.588871	0.037539
17	6	0	0.106214	1.351477	0.459428
18	6	0	0.391809	2.576797	0.913235
19	1	0	2.318623	2.755641	1.844502
20	1	0	2.078708	3.894211	0.527914
21	6	0	2.305156	2.422876	-1.572757
22	6	0	1.813654	-0.341972	1.202269
23	1	0	-0.334462	3.284049	1.300274
24	1	0	2.671264	1.758106	-2.359455
25	1	0	1.264328	2.669602	-1.803679
26	1	0	2.880361	3.351728	-1.633447
27	1	0	1.032902	-1.078499	1.403950
28	1	0	2.733092	-0.884432	0.965330
29	1	0	1.982169	0.219725	2.126512
30	6	0	3.922923	1.478378	0.166630
31	6	0	4.561456	0.486861	-0.836132
32	6	0	5.851000	-0.178659	-0.374225
33	6	0	6.511086	-1.104121	-1.410381
34	6	0	7.160424	-2.205865	-0.556311
35	6	0	6.303502	-2.193193	0.706367
36	8	0	5.566231	-1.060133	0.766501
37	1	0	6.568868	0.561639	-0.006276
38	1	0	7.227624	-0.563837	-2.034904
39	1	0	5.743659	-1.530482	-2.065824
40	1	0	7.069637	-3.194229	-1.016048
41	6	0	8.640123	-1.956969	-0.205019
42	1	0	3.936211	1.003629	1.153420
43	1	0	4.795278	1.009182	-1.773447
44	1	0	3.861119	-0.312331	-1.095009
45	8	0	6.252032	-3.035381	1.579650
46	1	0	9.006156	-2.718932	0.488827
47	1	0	9.248016	-1.997463	-1.113831
48	1	0	8.785964	-0.975013	0.257834
49	1	0	-1.172244	0.770431	-1.735943
50	6	0	-2.849828	-0.440753	-1.206766
51	6	0	-3.173563	-0.358233	-2.710833

52	6	0	-3.080273	-1.894562	-0.697534
53	1	0	-4.213513	-0.609831	-2.936937
54	1	0	-2.992825	0.646348	-3.102755
55	1	0	-2.538753	-1.058291	-3.266816
56	6	0	-4.477205	-2.525989	-0.840853
57	6	0	-5.397702	-2.373142	0.353815
58	8	0	-5.078296	-1.993911	1.466421
59	8	0	-6.651985	-2.767915	0.046757
60	6	0	-7.618091	-2.748065	1.120168
61	6	0	-4.755812	1.423565	-0.996097
62	1	0	-4.054992	0.120746	0.520737
63	6	0	-4.613847	2.622551	-1.581850
64	6	0	-6.117132	0.768288	-0.944401
65	1	0	-5.464145	3.120978	-2.039775
66	1	0	-3.668189	3.151950	-1.633920
67	1	0	-6.421153	0.588810	0.094352
68	1	0	-6.878416	1.391428	-1.421346
69	1	0	-6.120754	-0.205097	-1.446688
70	1	0	-4.363966	-3.611612	-0.965118
71	1	0	-5.013616	-2.200099	-1.736545
72	1	0	-2.776768	-1.956710	0.348983
73	1	0	-2.392256	-2.533857	-1.260922
74	8	0	-2.712320	3.422167	1.845123
75	1	0	-3.741169	1.716197	2.131553
76	6	0	-1.279693	0.018931	2.734809
77	1	0	-0.436198	0.693113	2.915486
78	1	0	-2.200560	0.489383	3.101780
79	1	0	-1.124780	-0.908007	3.292086
80	6	0	4.797855	2.745490	0.280918
81	1	0	5.812307	2.489176	0.602591
82	1	0	4.884341	3.272937	-0.675559
83	1	0	4.403733	3.448758	1.018945
84	1	0	-7.737819	-1.733343	1.505650
85	1	0	-8.548457	-3.101352	0.677717
86	1	0	-7.300808	-3.410833	1.928145

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.962403	0.535103	-0.821939
2	6	0	0.377817	1.122599	-0.332078
3	1	0	-0.850649	0.330634	-1.890150
4	1	0	-1.742969	1.298995	-0.731279
5	1	0	0.294207	1.497556	0.692184
6	1	0	0.636772	1.978912	-0.966841
7	6	0	3.600959	-0.998091	0.189879
8	6	0	2.423673	-2.017820	0.224511
9	6	0	1.159426	-1.140035	0.518578
10	6	0	1.459524	0.045381	-0.425588
11	6	0	2.742678	-3.180522	1.137008
12	1	0	2.244261	-2.450099	-0.762882
13	8	0	1.170276	-0.610666	1.862540
14	6	0	-2.005197	-3.135281	-0.326907
15	6	0	-2.411403	-1.727281	-0.874795
16	6	0	-1.400023	-0.757573	-0.071130
17	6	0	-0.198906	-1.707118	0.163623
18	6	0	-0.554885	-2.990190	0.039442
19	1	0	-2.595162	-3.408858	0.561362
20	1	0	-2.175489	-3.929760	-1.062751
21	6	0	-2.100930	-1.726353	-2.389132
22	6	0	-1.979162	-0.347694	1.308569
23	1	0	0.104061	-3.838447	0.193460
24	1	0	-2.354779	-0.781862	-2.877316
25	1	0	-1.039481	-1.921183	-2.570541
26	1	0	-2.666265	-2.517030	-2.891298
27	1	0	-1.226256	0.187875	1.890328
28	1	0	-2.846377	0.309710	1.200801
29	1	0	-2.289590	-1.218832	1.893609
30	6	0	-3.937811	-1.464098	-0.628151
31	6	0	-4.421624	-0.095838	-1.164602
32	6	0	-5.818062	0.333064	-0.709943
33	6	0	-6.224199	1.750959	-1.161599
34	6	0	-5.857462	2.641146	0.035949
35	6	0	-5.911760	1.665293	1.206951
36	8	0	-5.879041	0.389531	0.756542
37	1	0	-6.565872	-0.408045	-0.996463
38	1	0	-7.304257	1.794579	-1.339182
39	1	0	-5.719079	2.044121	-2.085277
40	1	0	-4.805021	2.950828	-0.036512
41	6	0	-6.722224	3.885500	0.243056
42	1	0	-4.085845	-1.462369	0.456634
43	1	0	-4.449299	-0.116400	-2.261729
44	1	0	-3.716996	0.695447	-0.890686
45	8	0	-5.962385	1.921326	2.392468
46	1	0	-6.429265	4.413839	1.154370
47	1	0	-6.610924	4.570273	-0.603169
48	1	0	-7.780470	3.616893	0.328286
49	1	0	1.369963	-0.387545	-1.432337
50	6	0	2.973473	0.405008	-0.267809
51	6	0	3.505201	0.897446	-1.626392

52	6	0	3.148725	1.502293	0.820336
53	1	0	4.574866	1.121844	-1.606740
54	1	0	3.351300	0.146921	-2.406904
55	1	0	2.977834	1.810465	-1.925026
56	6	0	4.575890	1.961917	1.186904
57	6	0	5.291844	2.864070	0.204028
58	8	0	6.438344	2.705779	-0.183801
59	8	0	4.533458	3.913925	-0.169396
60	6	0	5.139520	4.860567	-1.075756
61	6	0	4.821870	-1.514593	-0.573519
62	1	0	3.924073	-0.863457	1.230918
63	6	0	4.745047	-2.375590	-1.600207
64	6	0	6.173439	-1.030654	-0.098155
65	1	0	5.644377	-2.717855	-2.105087
66	1	0	3.807868	-2.766877	-1.981960
67	1	0	6.982838	-1.538528	-0.629744
68	1	0	6.302218	0.046880	-0.248426
69	1	0	6.300271	-1.218479	0.976100
70	1	0	5.238648	1.121016	1.395208
71	1	0	4.503270	2.540557	2.117261
72	1	0	2.683347	1.136823	1.737932
73	1	0	2.580431	2.386279	0.514035
74	8	0	2.384081	-4.330706	0.946995
75	1	0	3.382280	-2.945909	2.013049
76	6	0	0.852086	-1.490780	2.936240
77	1	0	0.654256	-0.856481	3.803653
78	1	0	-0.034004	-2.097328	2.724307
79	1	0	1.689529	-2.156819	3.180180
80	6	0	-4.828121	-2.594749	-1.189252
81	1	0	-5.867981	-2.464102	-0.874372
82	1	0	-4.818106	-2.619139	-2.284843
83	1	0	-4.513404	-3.577226	-0.828707
84	1	0	5.413316	4.367806	-2.011181
85	1	0	4.378962	5.620209	-1.251033
86	1	0	6.028736	5.304160	-0.622745

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.025670	0.533836	-0.826773
2	6	0	0.320357	1.115285	-0.346416
3	1	0	-0.918525	0.318471	-1.893260
4	1	0	-1.800758	1.303672	-0.741513
5	1	0	0.242634	1.504036	0.673062
6	1	0	0.587158	1.960651	-0.991855
7	6	0	3.540018	-1.044958	0.101984
8	6	0	2.348469	-2.025361	0.296596
9	6	0	1.084295	-1.136876	0.544108
10	6	0	1.390972	0.026548	-0.424813
11	6	0	2.641843	-3.139785	1.273115
12	1	0	2.132390	-2.555561	-0.640966
13	8	0	1.075981	-0.572077	1.874800
14	6	0	-2.098084	-3.123308	-0.291354
15	6	0	-2.487363	-1.719663	-0.861083
16	6	0	-1.472720	-0.748361	-0.063139
17	6	0	-0.277733	-1.702506	0.190345
18	6	0	-0.649009	-2.982539	0.080653
19	1	0	-2.695628	-3.379318	0.596900
20	1	0	-2.269254	-3.926450	-1.017377
21	6	0	-2.166457	-1.742992	-2.373119
22	6	0	-2.055291	-0.320891	1.309752
23	1	0	-0.010119	-3.844495	0.247177
24	1	0	-2.411009	-0.804494	-2.876938
25	1	0	-1.104930	-1.946189	-2.544786
26	1	0	-2.733395	-2.537456	-2.867445
27	1	0	-1.302739	0.220089	1.886473
28	1	0	-2.920208	0.337327	1.190288
29	1	0	-2.370419	-1.183788	1.904533
30	6	0	-4.013205	-1.441373	-0.628462
31	6	0	-4.480536	-0.073127	-1.179029
32	6	0	-5.886858	0.359895	-0.760112
33	6	0	-6.269816	1.785917	-1.206110
34	6	0	-5.930587	2.659124	0.011944
35	6	0	-6.026156	1.670128	1.169017
36	8	0	-5.990733	0.399178	0.704349
37	1	0	-6.630801	-0.372281	-1.078015
38	1	0	-7.344190	1.839585	-1.413092
39	1	0	-5.737202	2.086380	-2.111832
40	1	0	-4.874224	2.961384	-0.026576
41	6	0	-6.791460	3.907856	0.208939
42	1	0	-4.169851	-1.429071	0.455023
43	1	0	-4.480898	-0.094643	-2.276473
44	1	0	-3.780928	0.716389	-0.888214
45	8	0	-6.109120	1.912030	2.355584
46	1	0	-6.521465	4.422633	1.134969
47	1	0	-6.649570	4.601957	-0.624988
48	1	0	-7.853854	3.646851	0.259447
49	1	0	1.294795	-0.427245	-1.422866
50	6	0	2.905955	0.374903	-0.286442
51	6	0	3.411051	0.938850	-1.627184

52	6	0	3.136302	1.415195	0.847198
53	1	0	4.490583	1.117061	-1.623505
54	1	0	3.205544	0.252947	-2.452979
55	1	0	2.918632	1.892827	-1.843417
56	6	0	4.583425	1.885170	1.087134
57	6	0	5.052809	3.006150	0.183373
58	8	0	4.372750	3.950897	-0.177898
59	8	0	6.355962	2.873349	-0.145126
60	6	0	6.932013	3.931266	-0.942438
61	6	0	4.623353	-1.599130	-0.824631
62	1	0	4.008680	-0.929622	1.084024
63	6	0	4.363949	-2.301409	-1.937631
64	6	0	6.051333	-1.315153	-0.420481
65	1	0	5.169771	-2.670688	-2.566295
66	1	0	3.356453	-2.528786	-2.274471
67	1	0	6.762860	-1.799309	-1.095234
68	1	0	6.264857	-0.239474	-0.426538
69	1	0	6.241733	-1.671724	0.599312
70	1	0	5.304758	1.066196	1.054045
71	1	0	4.645055	2.300300	2.102378
72	1	0	2.758381	0.990831	1.778396
73	1	0	2.530945	2.303944	0.640072
74	8	0	3.705967	-3.297814	1.847439
75	1	0	1.827903	-3.875335	1.425684
76	6	0	0.767755	-1.426828	2.972314
77	1	0	0.544994	-0.770295	3.816932
78	1	0	-0.105031	-2.057277	2.771646
79	1	0	1.617886	-2.062332	3.246862
80	6	0	-4.908714	-2.569235	-1.186981
81	1	0	-5.947144	-2.434452	-0.869575
82	1	0	-4.901229	-2.594430	-2.282588
83	1	0	-4.597202	-3.552790	-0.826505
84	1	0	6.411919	4.010999	-1.899408
85	1	0	6.868844	4.883579	-0.411419
86	1	0	7.971902	3.645140	-1.093917

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.135205	0.233063	1.189317
2	6	0	-0.232972	0.952757	1.196936
3	1	0	1.196072	-0.334151	2.121981
4	1	0	1.933070	0.982985	1.228689
5	1	0	-0.299482	1.694088	0.395049
6	1	0	-0.330395	1.493694	2.145955
7	6	0	-3.616663	-0.683614	0.332207
8	6	0	-2.562647	-1.689256	-0.203722
9	6	0	-1.266854	-0.808867	-0.305343
10	6	0	-1.337597	-0.095589	1.063375
11	6	0	-3.057750	-2.405207	-1.440864
12	1	0	-2.333904	-2.466661	0.532632
13	8	0	-1.395533	0.212269	-1.315900
14	6	0	1.832059	-3.021296	-0.753621
15	6	0	2.401915	-1.927440	0.208747
16	6	0	1.365030	-0.711767	-0.029968
17	6	0	0.079198	-1.490923	-0.404853
18	6	0	0.358357	-2.731810	-0.817152
19	1	0	2.278608	-2.946944	-1.757141
20	1	0	2.045571	-4.035744	-0.397807
21	6	0	2.285530	-2.488188	1.644892
22	6	0	1.780964	0.160903	-1.243438
23	1	0	-0.373591	-3.450878	-1.170130
24	1	0	2.663240	-1.800819	2.406080
25	1	0	1.244520	-2.718280	1.891580
26	1	0	2.853900	-3.418845	1.733685
27	1	0	1.007260	0.901288	-1.456829
28	1	0	2.711993	0.700794	-1.050061
29	1	0	1.922834	-0.439954	-2.147055
30	6	0	3.899817	-1.617495	-0.138048
31	6	0	4.541227	-0.564334	0.796931
32	6	0	5.902993	-0.027977	0.351631
33	6	0	6.473608	1.084995	1.254177
34	6	0	6.035915	2.385040	0.561972
35	6	0	5.866924	1.950290	-0.890273
36	8	0	5.790646	0.601560	-0.970862
37	1	0	6.617732	-0.841572	0.218715
38	1	0	7.567275	1.026929	1.277077
39	1	0	6.110744	1.002591	2.281696
40	1	0	5.029338	2.669064	0.900877
41	6	0	6.966691	3.587063	0.730226
42	1	0	3.911776	-1.206207	-1.152737
43	1	0	4.692631	-0.998581	1.793666
44	1	0	3.868431	0.288240	0.932423
45	8	0	5.790176	2.652976	-1.877158
46	1	0	6.605706	4.440159	0.149491
47	1	0	7.017716	3.883033	1.782435
48	1	0	7.980680	3.347755	0.392771
49	1	0	-1.070221	-0.888680	1.775141
50	6	0	-2.842829	0.229454	1.380492
51	6	0	-3.109543	-0.215922	2.836424

52	6	0	-3.211273	1.739620	1.321429
53	1	0	-4.139351	-0.015266	3.147952
54	1	0	-2.926839	-1.286530	2.967968
55	1	0	-2.443834	0.324497	3.520133
56	6	0	-3.179390	2.481587	-0.043225
57	6	0	-4.523544	2.619587	-0.723655
58	8	0	-4.827161	2.143037	-1.805234
59	8	0	-5.378373	3.371237	0.004548
60	6	0	-6.689479	3.592983	-0.557267
61	6	0	-4.922141	-1.309788	0.802771
62	1	0	-3.871852	-0.040665	-0.519237
63	6	0	-5.050725	-2.603875	1.133994
64	6	0	-6.120077	-0.387858	0.842719
65	1	0	-6.010248	-3.003818	1.450952
66	1	0	-4.225921	-3.308161	1.105476
67	1	0	-7.019978	-0.917800	1.166294
68	1	0	-5.961776	0.454343	1.526315
69	1	0	-6.310522	0.041261	-0.148637
70	1	0	-2.503806	1.993058	-0.744098
71	1	0	-2.817653	3.501789	0.128757
72	1	0	-2.522702	2.255742	1.998866
73	1	0	-4.201003	1.875292	1.769252
74	8	0	-2.736784	-3.538693	-1.758535
75	1	0	-3.785461	-1.847799	-2.064192
76	6	0	-1.326186	-0.176749	-2.685283
77	1	0	-1.104260	0.729849	-3.253200
78	1	0	-0.536868	-0.914175	-2.862037
79	1	0	-2.283284	-0.577831	-3.040006
80	6	0	4.771972	-2.891752	-0.174574
81	1	0	5.766785	-2.670809	-0.573183
82	1	0	4.907840	-3.325300	0.822635
83	1	0	4.341771	-3.661736	-0.819676
84	1	0	-6.608386	4.106754	-1.517593
85	1	0	-7.211281	2.643469	-0.694517
86	1	0	-7.213054	4.215641	0.166990

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.897895	0.202577	-1.136623
2	6	0	0.487500	0.873668	-1.014314
3	1	0	-0.903063	-0.348992	-2.080760
4	1	0	-1.664013	0.980981	-1.224957
5	1	0	0.516591	1.572577	-0.173227
6	1	0	0.674317	1.457837	-1.923833
7	6	0	3.750321	-1.053488	-0.127141
8	6	0	2.586257	-1.972110	0.361554
9	6	0	1.359808	-0.997441	0.463193
10	6	0	1.554376	-0.209147	-0.851668
11	6	0	2.997233	-2.754719	1.585908
12	1	0	2.317058	-2.710025	-0.399518
13	8	0	1.518759	-0.044219	1.535539
14	6	0	-1.870266	-3.050635	0.679083
15	6	0	-2.334612	-1.901728	-0.275706
16	6	0	-1.248944	-0.749311	0.045443
17	6	0	-0.026992	-1.602692	0.464233
18	6	0	-0.389211	-2.838677	0.824088
19	1	0	-2.361780	-2.980204	1.661674
20	1	0	-2.117848	-4.042389	0.283414
21	6	0	-2.181514	-2.424701	-1.722580
22	6	0	-1.682377	0.121694	1.253864
23	1	0	0.285015	-3.605593	1.191462
24	1	0	-2.488148	-1.694288	-2.475903
25	1	0	-1.143717	-2.702540	-1.930790
26	1	0	-2.792264	-3.320703	-1.867808
27	1	0	-0.874404	0.798986	1.538314
28	1	0	-2.559694	0.729996	1.016720
29	1	0	-1.922957	-0.489565	2.129389
30	6	0	-3.827670	-1.520106	0.010620
31	6	0	-4.373414	-0.424684	-0.937359
32	6	0	-5.648774	0.268030	-0.475581
33	6	0	-6.219796	1.301980	-1.461094
34	6	0	-6.849087	2.369003	-0.549713
35	6	0	-6.049672	2.214984	0.741118
36	8	0	-5.371600	1.043832	0.740932
37	1	0	-6.415456	-0.461450	-0.195024
38	1	0	-6.935543	0.847569	-2.151491
39	1	0	-5.406084	1.735497	-2.052944
40	1	0	-6.688374	3.383037	-0.927078
41	6	0	-8.353354	2.174515	-0.277667
42	1	0	-3.863007	-1.122083	1.030132
43	1	0	-4.591411	-0.862179	-1.920800
44	1	0	-3.626293	0.355966	-1.106649
45	8	0	-5.995694	2.983368	1.679786
46	1	0	-8.710359	2.901316	0.457390
47	1	0	-8.918026	2.315270	-1.204184
48	1	0	-8.568781	1.169984	0.102247
49	1	0	1.356201	-0.950606	-1.639228
50	6	0	3.074345	0.123470	-0.976696
51	6	0	3.476916	0.155588	-2.464600

52	6	0	3.397991	1.505042	-0.340225
53	1	0	4.562253	0.176003	-2.596520
54	1	0	3.093064	-0.709419	-3.011796
55	1	0	3.065817	1.051340	-2.944609
56	6	0	4.873585	1.958035	-0.443046
57	6	0	5.076362	3.253995	0.306428
58	8	0	5.353377	3.342970	1.491058
59	8	0	4.880890	4.330918	-0.483594
60	6	0	4.996743	5.624462	0.148570
61	6	0	4.894472	-1.842962	-0.756361
62	1	0	4.163675	-0.577339	0.768800
63	6	0	6.161888	-1.628602	-0.369879
64	6	0	4.580775	-2.928067	-1.765383
65	1	0	6.988721	-2.187417	-0.800645
66	1	0	6.415547	-0.897222	0.392888
67	1	0	5.493016	-3.273739	-2.258999
68	1	0	4.122405	-3.796719	-1.276447
69	1	0	3.880568	-2.596037	-2.536869
70	1	0	5.166225	2.100237	-1.485943
71	1	0	5.538385	1.218722	0.008166
72	1	0	3.103104	1.485872	0.711364
73	1	0	2.779367	2.263809	-0.833562
74	8	0	2.690551	-3.916612	1.798593
75	1	0	3.658355	-2.224175	2.300258
76	6	0	1.290775	-0.477330	2.873727
77	1	0	0.388688	-1.090576	2.961102
78	1	0	2.144630	-1.039063	3.272492
79	1	0	1.167952	0.429097	3.471295
80	6	0	-4.765195	-2.747168	-0.012289
81	1	0	-5.779929	-2.466954	0.287541
82	1	0	-4.832755	-3.192817	-1.010841
83	1	0	-4.436654	-3.524900	0.681749
84	1	0	4.801674	6.350166	-0.639744
85	1	0	4.262564	5.721023	0.951277
86	1	0	6.001668	5.758798	0.554549

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.966100	0.219786	-1.149812
2	6	0	0.431303	0.869918	-1.053402
3	1	0	-0.986776	-0.355610	-2.079538
4	1	0	-1.719568	1.008580	-1.253663
5	1	0	0.479215	1.590915	-0.232166
6	1	0	0.622485	1.426221	-1.979289
7	6	0	3.666011	-1.084408	-0.132227
8	6	0	2.490987	-1.972940	0.385068
9	6	0	1.281176	-0.975821	0.468375
10	6	0	1.479937	-0.226858	-0.868571
11	6	0	2.895854	-2.729448	1.627254
12	1	0	2.205805	-2.725958	-0.355099
13	8	0	1.462765	0.001678	1.515139
14	6	0	-1.981189	-2.968183	0.757129
15	6	0	-2.431422	-1.838043	-0.226387
16	6	0	-1.325715	-0.695395	0.058680
17	6	0	-0.115307	-1.557674	0.493603
18	6	0	-0.496012	-2.777276	0.888707
19	1	0	-2.466203	-2.862647	1.739796
20	1	0	-2.247361	-3.965939	0.389635
21	6	0	-2.293320	-2.402704	-1.659041
22	6	0	-1.737077	0.213449	1.246786
23	1	0	0.167061	-3.545496	1.273172
24	1	0	-2.593712	-1.689152	-2.430808
25	1	0	-1.260426	-2.700152	-1.864473
26	1	0	-2.917114	-3.293865	-1.776564
27	1	0	-0.917555	0.886684	1.507120
28	1	0	-2.607394	0.828062	1.000305
29	1	0	-1.979836	-0.371217	2.139699
30	6	0	-3.916476	-1.424443	0.056599
31	6	0	-4.446946	-0.342025	-0.914194
32	6	0	-5.723135	0.364974	-0.477205
33	6	0	-6.266858	1.400173	-1.476747
34	6	0	-6.903556	2.475620	-0.580512
35	6	0	-6.129501	2.319186	0.725455
36	8	0	-5.460371	1.142940	0.740984
37	1	0	-6.501856	-0.356007	-0.207991
38	1	0	-6.973873	0.949570	-2.178542
39	1	0	-5.438751	1.824575	-2.055022
40	1	0	-6.727434	3.486989	-0.958095
41	6	0	-8.414079	2.294015	-0.335743
42	1	0	-3.939904	-1.001376	1.066384
43	1	0	-4.657904	-0.793401	-1.892885
44	1	0	-3.693234	0.431212	-1.087860
45	8	0	-6.087747	3.089460	1.663154
46	1	0	-8.779133	3.026250	0.389901
47	1	0	-8.960313	2.435384	-1.273159
48	1	0	-8.644026	1.292539	0.043735
49	1	0	1.261726	-0.986577	-1.633107
50	6	0	3.003811	0.076241	-1.015205
51	6	0	3.391842	0.047684	-2.507840

52	6	0	3.357935	1.474116	-0.433412
53	1	0	4.475846	0.041977	-2.652217
54	1	0	2.985742	-0.827768	-3.021601
55	1	0	2.992205	0.934044	-3.014314
56	6	0	4.831498	1.883493	-0.544239
57	6	0	5.104056	3.260335	0.023542
58	8	0	4.267463	4.109369	0.275605
59	8	0	6.427978	3.459852	0.204664
60	6	0	6.822622	4.758679	0.697533
61	6	0	4.800295	-1.905926	-0.737281
62	1	0	4.084842	-0.587427	0.749882
63	6	0	6.070333	-1.696075	-0.356763
64	6	0	4.473982	-3.014565	-1.716096
65	1	0	6.890720	-2.276150	-0.771392
66	1	0	6.332810	-0.945861	0.384484
67	1	0	5.382252	-3.385402	-2.198680
68	1	0	4.003899	-3.863399	-1.204078
69	1	0	3.779100	-2.694399	-2.497247
70	1	0	5.163922	1.913143	-1.589589
71	1	0	5.499062	1.177240	-0.042895
72	1	0	3.052359	1.510492	0.614624
73	1	0	2.758195	2.227127	-0.955440
74	8	0	2.577193	-3.882209	1.870093
75	1	0	3.564276	-2.188618	2.327139
76	6	0	1.233034	-0.392605	2.864774
77	1	0	1.110933	0.530305	3.436876
78	1	0	0.330091	-1.001860	2.969315
79	1	0	2.085815	-0.944688	3.279514
80	6	0	-4.874458	-2.635778	0.067979
81	1	0	-5.879413	-2.334102	0.379340
82	1	0	-4.965212	-3.096656	-0.921877
83	1	0	-4.547697	-3.407626	0.769346
84	1	0	6.377796	4.943984	1.677553
85	1	0	7.908697	4.722255	0.770621
86	1	0	6.510438	5.540081	0.001198

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.896417	0.027357	-1.187229
2	6	0	0.471910	0.745744	-1.179569
3	1	0	-0.930549	-0.574374	-2.099433
4	1	0	-1.692617	0.774692	-1.277848
5	1	0	0.514976	1.509428	-0.397995
6	1	0	0.599799	1.260394	-2.139281
7	6	0	3.826904	-0.892369	-0.195800
8	6	0	2.753454	-1.880586	0.344771
9	6	0	1.466371	-0.976318	0.398806
10	6	0	1.570273	-0.300213	-0.986583
11	6	0	3.213152	-2.557480	1.613550
12	1	0	2.537814	-2.678441	-0.373319
13	8	0	1.597473	0.072004	1.381630
14	6	0	-1.656058	-3.152958	0.853031
15	6	0	-2.197488	-2.090032	-0.159603
16	6	0	-1.160158	-0.871384	0.059827
17	6	0	0.112536	-1.642706	0.492904
18	6	0	-0.183189	-2.866812	0.942238
19	1	0	-2.126757	-3.044014	1.842260
20	1	0	-1.864722	-4.178025	0.525986
21	6	0	-2.050606	-2.700595	-1.572477
22	6	0	-1.598684	0.045457	1.232043
23	1	0	0.535168	-3.578342	1.336355
24	1	0	-2.407396	-2.038297	-2.365316
25	1	0	-1.005075	-2.942302	-1.786929
26	1	0	-2.620750	-3.631773	-1.642123
27	1	0	-0.825369	0.787980	1.440205
28	1	0	-2.520054	0.585350	0.997396
29	1	0	-1.768028	-0.523744	2.151150
30	6	0	-3.701126	-1.762544	0.142837
31	6	0	-4.313940	-0.730765	-0.833673
32	6	0	-5.697895	-0.201846	-0.452491
33	6	0	-6.229581	0.911432	-1.378241
34	6	0	-5.837995	2.211773	-0.659195
35	6	0	-5.734101	1.771562	0.797401
36	8	0	-5.652962	0.423111	0.876066
37	1	0	-6.413807	-1.019649	-0.357480
38	1	0	-7.320131	0.845571	-1.457735
39	1	0	-5.813836	0.836489	-2.386089
40	1	0	-4.819467	2.508021	-0.948058
41	6	0	-6.772085	3.405391	-0.865265
42	1	0	-3.733689	-1.323739	1.145520
43	1	0	-4.421488	-1.180232	-1.829326
44	1	0	-3.644243	0.126318	-0.954967
45	8	0	-5.708145	2.470367	1.789740
46	1	0	-6.448740	4.258226	-0.262388
47	1	0	-6.774961	3.707884	-1.916836
48	1	0	-7.798711	3.153375	-0.579128
49	1	0	1.317101	-1.112643	-1.681687
50	6	0	3.080453	0.007912	-1.273242
51	6	0	3.377276	-0.420647	-2.728895

52	6	0	3.503779	1.500651	-1.196544
53	1	0	4.436865	-0.304176	-2.977324
54	1	0	3.093444	-1.460023	-2.916101
55	1	0	2.802035	0.203587	-3.422732
56	6	0	3.431308	2.238320	0.145024
57	6	0	3.655508	3.728090	0.001871
58	8	0	3.582766	4.371055	-1.031285
59	8	0	3.930399	4.295503	1.197043
60	6	0	4.110826	5.728109	1.205111
61	6	0	5.148589	-1.527001	-0.612517
62	1	0	4.060755	-0.231096	0.643250
63	6	0	6.303705	-0.898094	-0.341573
64	6	0	5.152897	-2.876969	-1.296361
65	1	0	7.262001	-1.316290	-0.638510
66	1	0	6.328135	0.053566	0.183313
67	1	0	6.168612	-3.159144	-1.586574
68	1	0	4.768546	-3.660523	-0.631965
69	1	0	4.527674	-2.893800	-2.194408
70	1	0	4.163293	1.864941	0.867445
71	1	0	2.458108	2.102266	0.627658
72	1	0	2.900222	2.054417	-1.923179
73	1	0	4.535611	1.567894	-1.564723
74	8	0	2.960702	-3.714139	1.910308
75	1	0	3.858990	-1.952717	2.281297
76	6	0	1.453342	-0.261652	2.759693
77	1	0	2.376134	-0.687360	3.172838
78	1	0	1.242849	0.674073	3.283352
79	1	0	0.629043	-0.960948	2.930338
80	6	0	-4.581222	-3.030811	0.194662
81	1	0	-5.579035	-2.795865	0.577293
82	1	0	-4.707974	-3.484120	-0.794971
83	1	0	-4.162901	-3.789957	0.860043
84	1	0	4.314159	5.987828	2.243134
85	1	0	4.952011	6.008654	0.567534
86	1	0	3.204652	6.227341	0.854978

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.812626	0.147667	-1.064949
2	6	0	0.550431	0.834719	-0.828151
3	1	0	-0.774803	-0.294383	-2.064417
4	1	0	-1.597091	0.912399	-1.092279
5	1	0	0.537548	1.442209	0.082117
6	1	0	0.735520	1.511534	-1.669795
7	6	0	3.823842	-1.076144	0.031227
8	6	0	2.684357	-2.098176	0.296485
9	6	0	1.424498	-1.171694	0.454377
10	6	0	1.648518	-0.228580	-0.750074
11	6	0	3.046858	-3.032029	1.426278
12	1	0	2.487868	-2.728007	-0.576634
13	8	0	1.513574	-0.338207	1.630644
14	6	0	-1.748338	-3.317861	0.314046
15	6	0	-2.223563	-2.067967	-0.498436
16	6	0	-1.173519	-0.940731	-0.012342
17	6	0	0.058270	-1.809008	0.335682
18	6	0	-0.278329	-3.089100	0.526739
19	1	0	-2.265158	-3.387998	1.283307
20	1	0	-1.956084	-4.256288	-0.212868
21	6	0	-2.028759	-2.403595	-1.995181
22	6	0	-1.658406	-0.228929	1.278045
23	1	0	0.407135	-3.879565	0.814123
24	1	0	-2.333284	-1.590301	-2.658974
25	1	0	-0.981118	-2.634829	-2.211598
26	1	0	-2.617043	-3.285626	-2.265599
27	1	0	-0.878646	0.433063	1.659741
28	1	0	-2.547905	0.379203	1.091417
29	1	0	-1.901606	-0.944251	2.069754
30	6	0	-3.731802	-1.761667	-0.197707
31	6	0	-4.283906	-0.552435	-0.989744
32	6	0	-5.659031	-0.048244	-0.547872
33	6	0	-6.131988	1.227199	-1.274619
34	6	0	-5.705721	2.367393	-0.337074
35	6	0	-5.657065	1.680144	1.023699
36	8	0	-5.625718	0.335938	0.869848
37	1	0	-6.403895	-0.843270	-0.608540
38	1	0	-7.222681	1.219215	-1.376768
39	1	0	-5.700978	1.309849	-2.275426
40	1	0	-4.668302	2.660801	-0.552848
41	6	0	-6.583703	3.619671	-0.352355
42	1	0	-3.797640	-1.512370	0.866484
43	1	0	-4.379731	-0.817273	-2.050747
44	1	0	-3.583348	0.287305	-0.944384
45	8	0	-5.632492	2.196601	2.121953
46	1	0	-6.244490	4.339138	0.397758
47	1	0	-6.542571	4.099968	-1.334649
48	1	0	-7.627884	3.368500	-0.138022
49	1	0	1.497129	-0.875901	-1.626348
50	6	0	3.168541	0.138801	-0.781902
51	6	0	3.634983	0.220793	-2.247501

52	6	0	3.577930	1.436875	-0.026032
53	1	0	4.703939	0.446719	-2.320363
54	1	0	3.448802	-0.713492	-2.783377
55	1	0	3.088018	1.004673	-2.781933
56	6	0	3.284910	2.782882	-0.701070
57	6	0	3.796999	3.959239	0.104613
58	8	0	4.561890	3.903052	1.051066
59	8	0	3.308369	5.124154	-0.374553
60	6	0	3.756723	6.330118	0.281464
61	6	0	5.109613	-1.679355	-0.519963
62	1	0	4.080882	-0.659196	1.010512
63	6	0	6.297815	-1.251367	-0.063480
64	6	0	5.037720	-2.792398	-1.543174
65	1	0	7.232081	-1.653302	-0.447188
66	1	0	6.373685	-0.488352	0.706816
67	1	0	6.034164	-3.033940	-1.922974
68	1	0	4.621723	-3.706516	-1.101587
69	1	0	4.401173	-2.541344	-2.397297
70	1	0	2.219366	2.945757	-0.879214
71	1	0	3.768310	2.854824	-1.683210
72	1	0	4.660723	1.386889	0.137877
73	1	0	3.115200	1.423082	0.964231
74	8	0	2.779822	-4.222720	1.451763
75	1	0	3.635442	-2.588276	2.253940
76	6	0	1.273564	-0.928528	2.905582
77	1	0	1.013914	-0.110442	3.581953
78	1	0	0.447941	-1.646646	2.879030
79	1	0	2.169828	-1.426105	3.296453
80	6	0	-4.637448	-2.993639	-0.416047
81	1	0	-5.647627	-2.804975	-0.040474
82	1	0	-4.725994	-3.255696	-1.476391
83	1	0	-4.265049	-3.871933	0.116785
84	1	0	4.841626	6.426107	0.199368
85	1	0	3.259526	7.145654	-0.241924
86	1	0	3.469614	6.318514	1.335021

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.969899	-0.050773	-1.173262
2	6	0	0.401830	0.657211	-1.199901
3	1	0	-1.021032	-0.673192	-2.070543
4	1	0	-1.762358	0.699712	-1.269552
5	1	0	0.460833	1.439551	-0.438096
6	1	0	0.520264	1.146979	-2.173695
7	6	0	3.775178	-1.008086	-0.274963
8	6	0	2.704012	-1.923544	0.366847
9	6	0	1.411553	-1.030308	0.408088
10	6	0	1.496923	-0.388342	-0.993616
11	6	0	3.150203	-2.565164	1.660567
12	1	0	2.447382	-2.764799	-0.292448
13	8	0	1.550036	0.042717	1.362793
14	6	0	-1.733241	-3.173282	0.948760
15	6	0	-2.275627	-2.129132	-0.081009
16	6	0	-1.222155	-0.917506	0.097401
17	6	0	0.052095	-1.689193	0.531696
18	6	0	-0.256835	-2.898987	1.010361
19	1	0	-2.187714	-3.035386	1.941695
20	1	0	-1.956942	-4.203529	0.649189
21	6	0	-2.153065	-2.773733	-1.481282
22	6	0	-1.636607	0.029955	1.253698
23	1	0	0.446503	-3.618828	1.417384
24	1	0	-2.513064	-2.125858	-2.284402
25	1	0	-1.112677	-3.030472	-1.703582
26	1	0	-2.732950	-3.700664	-1.523222
27	1	0	-0.854100	0.769453	1.435976
28	1	0	-2.555902	0.572042	1.016594
29	1	0	-1.800870	-0.516251	2.187663
30	6	0	-3.771439	-1.776445	0.231693
31	6	0	-4.390679	-0.779945	-0.777342
32	6	0	-5.737553	-0.180234	-0.368902
33	6	0	-6.283465	0.880955	-1.346194
34	6	0	-5.809646	2.214809	-0.748104
35	6	0	-5.645158	1.878727	0.730508
36	8	0	-5.604734	0.537247	0.905924
37	1	0	-6.471649	-0.964663	-0.177983
38	1	0	-7.378354	0.849627	-1.361915
39	1	0	-5.927333	0.717069	-2.366322
40	1	0	-4.797695	2.447905	-1.108673
41	6	0	-6.709976	3.426029	-0.996948
42	1	0	-3.784715	-1.297150	1.216092
43	1	0	-4.555855	-1.281968	-1.739348
44	1	0	-3.698683	0.044110	-0.976286
45	8	0	-5.543812	2.646491	1.665151
46	1	0	-6.328869	4.305632	-0.471151
47	1	0	-6.752112	3.654486	-2.066197
48	1	0	-7.730006	3.233732	-0.647895
49	1	0	1.237250	-1.218736	-1.665614
50	6	0	3.000224	-0.079831	-1.313635
51	6	0	3.244629	-0.502835	-2.780409

52	6	0	3.408137	1.419013	-1.238223
53	1	0	4.276399	-0.320307	-3.095990
54	1	0	3.035833	-1.565366	-2.933647
55	1	0	2.587068	0.070102	-3.445205
56	6	0	3.403584	2.135853	0.115445
57	6	0	3.698054	3.614345	-0.009885
58	8	0	3.723935	4.259565	-1.044146
59	8	0	3.920334	4.169704	1.201972
60	6	0	4.175729	5.590299	1.223613
61	6	0	5.010697	-1.717917	-0.813526
62	1	0	4.128462	-0.363536	0.535265
63	6	0	5.020005	-2.982967	-1.256654
64	6	0	6.276496	-0.891867	-0.814232
65	1	0	5.933087	-3.436467	-1.633070
66	1	0	4.136559	-3.614342	-1.260467
67	1	0	7.122990	-1.451738	-1.221428
68	1	0	6.159848	0.024286	-1.406132
69	1	0	6.528830	-0.577227	0.206379
70	1	0	4.136505	1.715621	0.811521
71	1	0	2.439786	2.033332	0.623097
72	1	0	2.757109	1.974235	-1.922098
73	1	0	4.414016	1.512530	-1.664514
74	8	0	4.212652	-2.347881	2.216926
75	1	0	2.449480	-3.303161	2.098562
76	6	0	1.431969	-0.257375	2.752835
77	1	0	2.350990	-0.697213	3.153066
78	1	0	1.257145	0.696664	3.256191
79	1	0	0.589430	-0.926051	2.957245
80	6	0	-4.661918	-3.032951	0.347238
81	1	0	-5.660487	-2.769429	0.708853
82	1	0	-4.786571	-3.539225	-0.616582
83	1	0	-4.254655	-3.757368	1.056910
84	1	0	4.324876	5.841234	2.272956
85	1	0	5.070258	5.824688	0.642318
86	1	0	3.322068	6.136508	0.816157

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.088419	0.139022	-1.140020
2	6	0	0.305630	0.796688	-1.063215
3	1	0	-1.111045	-0.452566	-2.059396
4	1	0	-1.848335	0.920223	-1.253910
5	1	0	0.355152	1.533236	-0.256250
6	1	0	0.490206	1.335216	-2.000696
7	6	0	3.563512	-1.171384	-0.204937
8	6	0	2.406797	-1.979648	0.452179
9	6	0	1.176147	-1.006411	0.497814
10	6	0	1.359055	-0.292201	-0.860266
11	6	0	2.800336	-2.674975	1.734662
12	1	0	2.079727	-2.795946	-0.206542
13	8	0	1.331133	0.004462	1.516806
14	6	0	-2.082854	-3.018826	0.823028
15	6	0	-2.536482	-1.909264	-0.181655
16	6	0	-1.436438	-0.757840	0.084866
17	6	0	-0.217487	-1.603612	0.534935
18	6	0	-0.599366	-2.815385	0.952301
19	1	0	-2.571108	-2.899666	1.802319
20	1	0	-2.339637	-4.024755	0.471829
21	6	0	-2.392823	-2.502883	-1.602062
22	6	0	-1.847777	0.163855	1.263172
23	1	0	0.054432	-3.581653	1.357200
24	1	0	-2.693017	-1.807261	-2.389826
25	1	0	-1.358547	-2.801271	-1.799333
26	1	0	-3.014524	-3.397758	-1.701393
27	1	0	-1.031871	0.845872	1.510527
28	1	0	-2.722368	0.770680	1.013204
29	1	0	-2.084279	-0.410185	2.164301
30	6	0	-4.024586	-1.499329	0.093940
31	6	0	-4.553425	-0.412888	-0.871641
32	6	0	-5.920600	0.175998	-0.517415
33	6	0	-6.345033	1.366836	-1.401324
34	6	0	-5.907782	2.600332	-0.595930
35	6	0	-5.901574	2.079209	0.837277
36	8	0	-5.899498	0.725587	0.844353
37	1	0	-6.685774	-0.601728	-0.497937
38	1	0	-7.433090	1.372624	-1.528337
39	1	0	-5.890556	1.319509	-2.394066
40	1	0	-4.859729	2.842567	-0.822732
41	6	0	-6.752791	3.862276	-0.777421
42	1	0	-4.053915	-1.079710	1.104680
43	1	0	-4.653137	-0.829606	-1.882264
44	1	0	-3.837942	0.411382	-0.949840
45	8	0	-5.886636	2.721607	1.866971
46	1	0	-6.405086	4.658614	-0.113860
47	1	0	-6.685503	4.219375	-1.809524
48	1	0	-7.806051	3.664585	-0.551854
49	1	0	1.137386	-1.073940	-1.602683
50	6	0	2.877189	0.013909	-1.035046
51	6	0	3.223496	0.027667	-2.538080

52	6	0	3.247830	1.396331	-0.426001
53	1	0	4.301769	0.066235	-2.711885
54	1	0	2.840802	-0.855195	-3.057483
55	1	0	2.775853	0.906456	-3.016696
56	6	0	4.720296	1.805125	-0.554720
57	6	0	5.001692	3.177517	0.019696
58	8	0	4.171760	4.035218	0.265213
59	8	0	6.325765	3.363480	0.212815
60	6	0	6.728897	4.656744	0.712824
61	6	0	4.558671	-2.052022	-0.956468
62	1	0	4.122694	-0.709956	0.613005
63	6	0	5.879094	-1.853953	-0.830438
64	6	0	4.043610	-3.184900	-1.820673
65	1	0	6.598774	-2.463850	-1.370712
66	1	0	6.285604	-1.088075	-0.176052
67	1	0	4.837157	-3.572891	-2.465090
68	1	0	3.687284	-4.020621	-1.204749
69	1	0	3.205496	-2.884980	-2.458089
70	1	0	5.039422	1.843831	-1.603949
71	1	0	5.393334	1.095316	-0.065380
72	1	0	2.965418	1.407787	0.628586
73	1	0	2.640010	2.163922	-0.916784
74	8	0	3.891580	-2.585567	2.270858
75	1	0	2.030895	-3.337611	2.178247
76	6	0	1.141200	-0.366202	2.880157
77	1	0	2.011856	-0.893933	3.284654
78	1	0	1.017672	0.567429	3.434222
79	1	0	0.247055	-0.982890	3.018385
80	6	0	-4.979892	-2.713127	0.098884
81	1	0	-5.966041	-2.428453	0.477668
82	1	0	-5.121575	-3.129306	-0.905009
83	1	0	-4.616347	-3.515401	0.745703
84	1	0	6.430790	5.443344	0.016085
85	1	0	6.277267	4.843531	1.689438
86	1	0	7.813858	4.609223	0.795592

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.891370	0.191293	1.141609
2	6	0	-0.496099	0.854591	1.006103
3	1	0	0.895601	-0.349685	2.091785
4	1	0	1.653332	0.974449	1.224138
5	1	0	-0.523626	1.543627	0.157010
6	1	0	-0.688396	1.448744	1.908007
7	6	0	-3.747385	-1.103049	0.138538
8	6	0	-2.577296	-2.015020	-0.335855
9	6	0	-1.354743	-1.039752	-0.450953
10	6	0	-1.558480	-0.234213	0.851397
11	6	0	-2.983120	-2.830688	-1.542231
12	1	0	-2.295035	-2.734948	0.435980
13	8	0	-1.512480	-0.103995	-1.538800
14	6	0	1.888807	-3.077527	-0.628767
15	6	0	2.344009	-1.912459	0.310493
16	6	0	1.251084	-0.772002	-0.028108
17	6	0	0.035602	-1.638548	-0.438472
18	6	0	0.406785	-2.877020	-0.780376
19	1	0	2.382183	-3.018455	-1.611196
20	1	0	2.141611	-4.062061	-0.218475
21	6	0	2.192678	-2.416801	1.764227
22	6	0	1.680603	0.086171	-1.247061
23	1	0	-0.262162	-3.652266	-1.139333
24	1	0	2.491814	-1.673648	2.508060
25	1	0	1.156881	-2.700562	1.974509
26	1	0	2.810642	-3.305619	1.922528
27	1	0	0.866242	0.749914	-1.544750
28	1	0	2.550627	0.707211	-1.015580
29	1	0	1.930886	-0.535484	-2.112573
30	6	0	3.834793	-1.524190	0.021193
31	6	0	4.371629	-0.413158	0.956045
32	6	0	5.641592	0.284089	0.486190
33	6	0	6.201863	1.337405	1.457346
34	6	0	6.822627	2.397038	0.531579
35	6	0	6.027400	2.216406	-0.758417
36	8	0	5.359532	1.039594	-0.741860
37	1	0	6.415010	-0.442741	0.217321
38	1	0	6.920821	0.899797	2.155224
39	1	0	5.383326	1.771837	2.041831
40	1	0	6.651210	3.414858	0.893727
41	6	0	8.329347	2.213372	0.265603
42	1	0	3.868647	-1.138533	-1.003079
43	1	0	4.592923	-0.836935	1.944768
44	1	0	3.618170	0.363368	1.115797
45	8	0	5.968798	2.970011	-1.708749
46	1	0	8.681026	2.932909	-0.479112
47	1	0	8.890509	2.373006	1.191199
48	1	0	8.555403	1.205576	-0.099218
49	1	0	-1.365463	-0.963151	1.651738
50	6	0	-3.081141	0.101618	0.960491
51	6	0	-3.478217	0.124858	2.448404

52	6	0	-3.372634	1.483555	0.310260
53	1	0	-4.543785	0.318367	2.599139
54	1	0	-3.249978	-0.826903	2.936274
55	1	0	-2.923416	0.913575	2.969866
56	6	0	-4.849525	1.936877	0.273739
57	6	0	-4.963093	3.286676	-0.396664
58	8	0	-5.060483	3.464358	-1.599342
59	8	0	-4.912794	4.299512	0.493642
60	6	0	-4.962271	5.637943	-0.047879
61	6	0	-4.882332	-1.873150	0.814272
62	1	0	-4.175934	-0.655906	-0.768307
63	6	0	-4.706728	-3.024045	1.481836
64	6	0	-6.271979	-1.291232	0.677259
65	1	0	-5.550476	-3.534139	1.938735
66	1	0	-3.739979	-3.500463	1.606120
67	1	0	-6.523780	-1.118834	-0.376966
68	1	0	-7.024073	-1.961135	1.102545
69	1	0	-6.361737	-0.324668	1.185265
70	1	0	-5.268226	2.004924	1.280623
71	1	0	-5.450552	1.241050	-0.315175
72	1	0	-2.986627	1.475380	-0.711233
73	1	0	-2.803808	2.240481	0.863057
74	8	0	-2.606636	-3.968595	-1.768744
75	1	0	-3.705186	-2.346489	-2.231625
76	6	0	-1.303708	-0.569482	-2.868582
77	1	0	-1.201344	0.322117	-3.491663
78	1	0	-2.158824	-1.150390	-3.236914
79	1	0	-0.396821	-1.176065	-2.955837
80	6	0	4.780794	-2.744240	0.060598
81	1	0	5.794332	-2.460407	-0.239912
82	1	0	4.848845	-3.177924	1.064376
83	1	0	4.459121	-3.532108	-0.625176
84	1	0	-5.897311	5.791911	-0.590655
85	1	0	-4.905820	6.300783	0.814397
86	1	0	-4.117695	5.806661	-0.719329

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.936633	0.149331	-1.129585
2	6	0	0.449769	0.819043	-1.022032
3	1	0	-0.947261	-0.413544	-2.066971
4	1	0	-1.702271	0.927451	-1.223237
5	1	0	0.482941	1.530297	-0.191694
6	1	0	0.633455	1.389384	-1.940726
7	6	0	3.719873	-1.139307	-0.196655
8	6	0	2.565118	-1.985050	0.407913
9	6	0	1.327425	-1.029567	0.482256
10	6	0	1.515023	-0.262938	-0.845957
11	6	0	2.965403	-2.741024	1.653494
12	1	0	2.259499	-2.776586	-0.290155
13	8	0	1.466887	-0.053770	1.538357
14	6	0	-1.916580	-3.075287	0.729530
15	6	0	-2.375683	-1.938291	-0.240577
16	6	0	-1.284275	-0.787376	0.065083
17	6	0	-0.061406	-1.638301	0.491418
18	6	0	-0.434436	-2.866557	0.866801
19	1	0	-2.405011	-2.987402	1.712123
20	1	0	-2.169200	-4.071512	0.348761
21	6	0	-2.225915	-2.482341	-1.680072
22	6	0	-1.709742	0.096916	1.266699
23	1	0	0.224544	-3.641085	1.246624
24	1	0	-2.531756	-1.762027	-2.443182
25	1	0	-1.189161	-2.765362	-1.886448
26	1	0	-2.839456	-3.378574	-1.811622
27	1	0	-0.898182	0.773979	1.540486
28	1	0	-2.586741	0.704576	1.026822
29	1	0	-1.948020	-0.505248	2.149214
30	6	0	-3.866882	-1.545994	0.041648
31	6	0	-4.407607	-0.460788	-0.920601
32	6	0	-5.684363	0.238569	-0.472921
33	6	0	-6.244451	1.266675	-1.470869
34	6	0	-6.876119	2.343461	-0.572724
35	6	0	-6.087708	2.196190	0.725641
36	8	0	-5.413814	1.022471	0.739631
37	1	0	-6.455465	-0.486500	-0.192984
38	1	0	-6.957081	0.809391	-2.162577
39	1	0	-5.424962	1.692246	-2.060461
40	1	0	-6.707917	3.353785	-0.956709
41	6	0	-8.383306	2.157493	-0.311356
42	1	0	-3.899525	-1.134092	1.055708
43	1	0	-4.621335	-0.908445	-1.900368
44	1	0	-3.658995	0.317265	-1.094406
45	8	0	-6.038584	2.971099	1.659084
46	1	0	-8.743233	2.891570	0.414973
47	1	0	-8.939775	2.293145	-1.243575
48	1	0	-8.605835	1.156855	0.074669
49	1	0	1.315339	-1.018604	-1.620549
50	6	0	3.034081	0.070281	-0.989420
51	6	0	3.390157	0.125422	-2.487655

52	6	0	3.360972	1.439606	-0.328483
53	1	0	4.459620	0.273854	-2.661027
54	1	0	3.106442	-0.796457	-3.001739
55	1	0	2.859981	0.957347	-2.965772
56	6	0	4.842939	1.878869	-0.367167
57	6	0	5.007889	3.215076	0.319289
58	8	0	5.153376	3.373671	1.519591
59	8	0	4.943719	4.242986	-0.554004
60	6	0	5.039580	5.571261	0.005243
61	6	0	4.743022	-1.974839	-0.966672
62	1	0	4.256168	-0.706176	0.653247
63	6	0	4.420129	-3.019067	-1.743940
64	6	0	6.187686	-1.562815	-0.806285
65	1	0	5.186017	-3.578509	-2.274415
66	1	0	3.397834	-3.355075	-1.892313
67	1	0	6.859326	-2.235402	-1.346883
68	1	0	6.359618	-0.545821	-1.178699
69	1	0	6.473020	-1.564336	0.252949
70	1	0	5.205621	1.961969	-1.394361
71	1	0	5.468737	1.165106	0.173913
72	1	0	3.032186	1.415144	0.712144
73	1	0	2.768105	2.210423	-0.835401
74	8	0	4.081563	-2.729931	2.143957
75	1	0	2.179389	-3.375866	2.107120
76	6	0	1.300497	-0.483879	2.886444
77	1	0	0.412659	-1.113054	3.010909
78	1	0	2.181679	-1.021422	3.255232
79	1	0	1.179742	0.423802	3.482495
80	6	0	-4.809925	-2.769024	0.036075
81	1	0	-5.822049	-2.480653	0.336688
82	1	0	-4.883598	-3.225759	-0.957032
83	1	0	-4.482659	-3.540430	0.737802
84	1	0	4.965919	6.248665	-0.844403
85	1	0	4.223076	5.746473	0.709073
86	1	0	5.996211	5.698518	0.516448

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.126052	-0.247861	1.234811
2	6	0	0.224585	-0.995115	1.276918
3	1	0	-1.149969	0.416585	2.102799
4	1	0	-1.937950	-0.970871	1.372572
5	1	0	0.258585	-1.794780	0.531693
6	1	0	0.332000	-1.466986	2.261424
7	6	0	3.631587	0.644638	0.349030
8	6	0	2.547325	1.535243	-0.335208
9	6	0	1.272738	0.618936	-0.376171
10	6	0	1.356568	0.005452	1.039471
11	6	0	3.066893	2.120009	-1.626907
12	1	0	2.275703	2.385451	0.296833
13	8	0	1.419460	-0.475311	-1.303480
14	6	0	-1.816951	2.795920	-1.022117
15	6	0	-2.391577	1.805632	0.043628
16	6	0	-1.362966	0.564982	-0.073065
17	6	0	-0.074332	1.291848	-0.529860
18	6	0	-0.346077	2.488652	-1.060939
19	1	0	-2.266330	2.627840	-2.012751
20	1	0	-2.022540	3.841878	-0.766376
21	6	0	-2.270276	2.502291	1.418780
22	6	0	-1.793076	-0.427047	-1.185660
23	1	0	0.388583	3.164985	-1.486002
24	1	0	-2.650132	1.892304	2.242468
25	1	0	-1.227202	2.748275	1.640685
26	1	0	-2.831871	3.441453	1.419672
27	1	0	-1.019619	-1.182946	-1.338474
28	1	0	-2.719761	-0.944997	-0.923376
29	1	0	-1.950076	0.080956	-2.142489
30	6	0	-3.890698	1.470638	-0.268268
31	6	0	-4.545589	0.550759	0.790651
32	6	0	-5.835780	-0.132971	0.357938
33	6	0	-6.514223	-0.988160	1.441535
34	6	0	-7.165381	-2.133870	0.648794
35	6	0	-6.295629	-2.205224	-0.603149
36	8	0	-5.546619	-1.084716	-0.723579
37	1	0	-6.543855	0.588767	-0.062325
38	1	0	-7.231933	-0.404766	2.024606
39	1	0	-5.757227	-1.380290	2.129776
40	1	0	-7.088880	-3.093381	1.168269
41	6	0	-8.638860	-1.892171	0.267753
42	1	0	-3.903619	0.934623	-1.223128
43	1	0	-4.784318	1.133974	1.690062
44	1	0	-3.853962	-0.234969	1.107760
45	8	0	-6.243603	-3.099151	-1.423338
46	1	0	-9.006509	-2.690932	-0.382465
47	1	0	-9.255867	-1.871085	1.171061
48	1	0	-8.769412	-0.938524	-0.254923
49	1	0	1.158203	0.854012	1.710220
50	6	0	2.846307	-0.380625	1.296253
51	6	0	3.155338	-0.227368	2.799462

52	6	0	3.126004	-1.854021	0.879325
53	1	0	4.220094	-0.343904	3.020530
54	1	0	2.845704	0.746755	3.187125
55	1	0	2.612634	-0.990688	3.369094
56	6	0	4.578069	-2.356723	1.014697
57	6	0	5.358899	-2.437489	-0.282765
58	8	0	4.915507	-2.281348	-1.406439
59	8	0	6.652599	-2.744446	-0.043966
60	6	0	7.502917	-2.908024	-1.199926
61	6	0	4.766216	1.461121	0.962393
62	1	0	4.081331	0.038663	-0.442921
63	6	0	6.044784	1.105537	0.760583
64	6	0	4.444708	2.714201	1.750075
65	1	0	6.866394	1.672809	1.190418
66	1	0	6.314413	0.242832	0.158372
67	1	0	5.330912	3.078154	2.277022
68	1	0	4.103880	3.518327	1.086208
69	1	0	3.651173	2.558343	2.486817
70	1	0	4.587189	-3.377124	1.418764
71	1	0	5.172190	-1.769128	1.720757
72	1	0	2.796518	-2.003460	-0.150158
73	1	0	2.494052	-2.490402	1.508062
74	8	0	2.834205	3.254183	-2.014124
75	1	0	3.739111	1.467868	-2.219506
76	6	0	1.303781	-0.207384	-2.697441
77	1	0	0.463743	0.457755	-2.921629
78	1	0	2.224397	0.227112	-3.106068
79	1	0	1.137663	-1.172448	-3.181889
80	6	0	-4.750840	2.737321	-0.466979
81	1	0	-5.768114	2.471960	-0.771772
82	1	0	-4.831597	3.328232	0.452151
83	1	0	-4.347881	3.385321	-1.249446
84	1	0	8.485512	-3.157939	-0.802123
85	1	0	7.129158	-3.713831	-1.835337
86	1	0	7.546615	-1.980232	-1.774513

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.939266	0.536055	-0.799997
2	6	0	0.397776	1.123826	-0.301541
3	1	0	-0.824202	0.342838	-1.869950
4	1	0	-1.723111	1.295840	-0.703603
5	1	0	0.311737	1.489085	0.726040
6	1	0	0.655830	1.986387	-0.928194
7	6	0	3.624030	-0.981261	0.238097
8	6	0	2.454215	-2.015068	0.249383
9	6	0	1.184005	-1.140249	0.536763
10	6	0	1.482530	0.050828	-0.401621
11	6	0	2.768119	-3.172226	1.167911
12	1	0	2.297764	-2.445609	-0.743869
13	8	0	1.188990	-0.613867	1.881676
14	6	0	-1.965311	-3.145095	-0.339828
15	6	0	-2.375072	-1.735106	-0.880457
16	6	0	-1.374375	-0.765788	-0.062958
17	6	0	-0.169729	-1.711098	0.172662
18	6	0	-0.518180	-2.995030	0.037342
19	1	0	-2.559756	-3.427713	0.542558
20	1	0	-2.126514	-3.935176	-1.082375
21	6	0	-2.054397	-1.720865	-2.392535
22	6	0	-1.965612	-0.369120	1.315485
23	1	0	0.143366	-3.841836	0.189303
24	1	0	-2.311304	-0.774235	-2.874928
25	1	0	-0.990499	-1.907348	-2.568342
26	1	0	-2.611105	-2.511215	-2.904743
27	1	0	-1.221266	0.169721	1.905213
28	1	0	-2.837098	0.282046	1.205422
29	1	0	-2.273456	-1.245842	1.893449
30	6	0	-3.904413	-1.481612	-0.641905
31	6	0	-4.392046	-0.111703	-1.170598
32	6	0	-5.790936	0.308898	-0.715523
33	6	0	-6.201935	1.728079	-1.158756
34	6	0	-5.841232	2.612056	0.045236
35	6	0	-5.892611	1.628349	1.209778
36	8	0	-5.854396	0.355623	0.751143
37	1	0	-6.535351	-0.433341	-1.007967
38	1	0	-7.281792	1.768459	-1.338243
39	1	0	-5.696114	2.029226	-2.079467
40	1	0	-4.790245	2.927433	-0.023532
41	6	0	-6.712368	3.850782	0.259385
42	1	0	-4.059259	-1.489200	0.441884
43	1	0	-4.417551	-0.125251	-2.267889
44	1	0	-3.690996	0.680436	-0.890213
45	8	0	-5.945342	1.876424	2.396872
46	1	0	-6.423050	4.374526	1.174495
47	1	0	-6.603411	4.541639	-0.582180
48	1	0	-7.769383	3.576432	0.341558
49	1	0	1.392665	-0.377599	-1.410324
50	6	0	2.993952	0.410122	-0.243250
51	6	0	3.539831	0.925093	-1.589070

52	6	0	3.195332	1.502935	0.845421
53	1	0	4.629464	1.019702	-1.583117
54	1	0	3.272131	0.264867	-2.418273
55	1	0	3.116685	1.910943	-1.810422
56	6	0	4.640400	1.981097	1.106199
57	6	0	5.232613	2.993557	0.147319
58	8	0	6.377913	2.966615	-0.272045
59	8	0	4.370450	3.986786	-0.152960
60	6	0	4.868183	5.034660	-1.012093
61	6	0	4.865489	-1.512668	-0.473628
62	1	0	3.914278	-0.831568	1.284139
63	6	0	6.071842	-1.425192	0.108017
64	6	0	4.716282	-2.215875	-1.806828
65	1	0	6.966232	-1.802981	-0.380306
66	1	0	6.207827	-0.977482	1.088778
67	1	0	5.693499	-2.380512	-2.268571
68	1	0	4.243002	-3.197656	-1.680948
69	1	0	4.096336	-1.656807	-2.513144
70	1	0	5.346788	1.151309	1.161110
71	1	0	4.658725	2.473384	2.088077
72	1	0	2.795409	1.119600	1.786524
73	1	0	2.590165	2.376505	0.584198
74	8	0	2.487816	-4.336563	0.933866
75	1	0	3.331536	-2.920995	2.089243
76	6	0	0.841514	-1.486145	2.953492
77	1	0	0.627397	-0.845393	3.812266
78	1	0	-0.042824	-2.088875	2.725359
79	1	0	1.668993	-2.155287	3.220496
80	6	0	-4.785126	-2.612295	-1.217751
81	1	0	-5.828175	-2.487735	-0.911025
82	1	0	-4.765736	-2.629549	-2.313334
83	1	0	-4.469582	-3.595821	-0.860764
84	1	0	4.035456	5.725388	-1.137957
85	1	0	5.717240	5.537535	-0.544113
86	1	0	5.174787	4.621938	-1.975641

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908920	0.609335	-0.809492
2	6	0	0.440705	1.182538	-0.328681
3	1	0	-0.803327	0.393305	-1.876135
4	1	0	-1.677840	1.385207	-0.722706
5	1	0	0.365442	1.566322	0.692879
6	1	0	0.709721	2.030423	-0.970210
7	6	0	3.637853	-0.982136	0.186276
8	6	0	2.443893	-1.982509	0.246972
9	6	0	1.194981	-1.082246	0.540349
10	6	0	1.507415	0.090183	-0.416101
11	6	0	2.753610	-3.135652	1.173849
12	1	0	2.249509	-2.426466	-0.732210
13	8	0	1.221964	-0.543115	1.879962
14	6	0	-1.998383	-3.043028	-0.273481
15	6	0	-2.389126	-1.635576	-0.832866
16	6	0	-1.362101	-0.669559	-0.043499
17	6	0	-0.173082	-1.632737	0.196691
18	6	0	-0.544916	-2.912485	0.085250
19	1	0	-2.587284	-3.300426	0.620342
20	1	0	-2.183143	-3.842184	-1.000867
21	6	0	-2.086861	-1.651104	-2.348746
22	6	0	-1.933450	-0.232766	1.331171
23	1	0	0.104127	-3.767443	0.244649
24	1	0	-2.335007	-0.708157	-2.842873
25	1	0	-1.028111	-1.856758	-2.533841
26	1	0	-2.661553	-2.440905	-2.841659
27	1	0	-1.172224	0.301514	1.903436
28	1	0	-2.793140	0.433004	1.214694
29	1	0	-2.252485	-1.091914	1.929707
30	6	0	-3.910216	-1.350188	-0.582946
31	6	0	-4.381805	0.008568	-1.155572
32	6	0	-5.711764	0.521979	-0.619871
33	6	0	-6.194770	1.843595	-1.241955
34	6	0	-6.933072	2.544808	-0.089434
35	6	0	-6.276813	1.934363	1.145622
36	8	0	-5.580585	0.823044	0.812170
37	1	0	-6.489933	-0.244676	-0.692410
38	1	0	-6.828067	1.668863	-2.115878
39	1	0	-5.332084	2.437986	-1.562704
40	1	0	-6.745108	3.622271	-0.072403
41	6	0	-8.455439	2.307687	-0.064491
42	1	0	-4.051286	-1.317839	0.502492
43	1	0	-4.491370	-0.067657	-2.245513
44	1	0	-3.637759	0.789294	-0.974510
45	8	0	-6.339707	2.327482	2.292869
46	1	0	-8.900451	2.743511	0.834447
47	1	0	-8.916929	2.775706	-0.939237
48	1	0	-8.698614	1.239771	-0.083018
49	1	0	1.408447	-0.351238	-1.418472
50	6	0	3.025418	0.430801	-0.266177
51	6	0	3.560194	0.918479	-1.624751

52	6	0	3.225498	1.522831	0.823198
53	1	0	4.633596	1.128400	-1.603042
54	1	0	3.396795	0.171165	-2.406323
55	1	0	3.049030	1.840749	-1.920645
56	6	0	4.660645	1.993020	1.124072
57	6	0	5.205981	3.036842	0.171745
58	8	0	4.570286	3.970393	-0.285769
59	8	0	6.519372	2.849623	-0.081120
60	6	0	7.163117	3.836215	-0.917773
61	6	0	4.833557	-1.525325	-0.598776
62	1	0	3.984909	-0.847704	1.219537
63	6	0	4.721515	-2.380446	-1.626949
64	6	0	6.204876	-1.075205	-0.145858
65	1	0	5.604614	-2.742298	-2.146630
66	1	0	3.769640	-2.747806	-1.995750
67	1	0	6.993052	-1.612708	-0.680138
68	1	0	6.361034	-0.004052	-0.315796
69	1	0	6.340436	-1.248617	0.929439
70	1	0	5.368996	1.167345	1.206305
71	1	0	4.655670	2.486539	2.105552
72	1	0	2.791285	1.151287	1.752946
73	1	0	2.646279	2.407485	0.538911
74	8	0	2.392994	-4.286993	0.994094
75	1	0	3.389024	-2.893448	2.050925
76	6	0	0.881780	-1.404987	2.961362
77	1	0	0.717105	-0.758599	3.826765
78	1	0	-0.028672	-1.978601	2.761980
79	1	0	1.695175	-2.101635	3.201215
80	6	0	-4.817647	-2.483472	-1.109396
81	1	0	-5.861176	-2.307386	-0.829776
82	1	0	-4.782187	-2.562465	-2.201671
83	1	0	-4.540487	-3.455111	-0.692711
84	1	0	7.094489	4.824843	-0.458859
85	1	0	8.202274	3.518597	-0.991221
86	1	0	6.696951	3.858093	-1.905105

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.888804	0.066209	-1.159500
2	6	0	0.470162	0.799072	-1.099000
3	1	0	-0.901237	-0.499941	-2.094799
4	1	0	-1.692713	0.806978	-1.232889
5	1	0	0.492197	1.525326	-0.281979
6	1	0	0.605837	1.359886	-2.031732
7	6	0	3.832542	-0.881241	-0.178951
8	6	0	2.754263	-1.889639	0.314429
9	6	0	1.465980	-0.989654	0.407636
10	6	0	1.578955	-0.241327	-0.939195
11	6	0	3.213700	-2.621358	1.552427
12	1	0	2.538793	-2.656208	-0.436993
13	8	0	1.591069	0.006187	1.442495
14	6	0	-1.650975	-3.195828	0.743773
15	6	0	-2.189679	-2.095205	-0.229000
16	6	0	-1.159025	-0.882903	0.047341
17	6	0	0.113963	-1.665328	0.458277
18	6	0	-0.179849	-2.908220	0.854333
19	1	0	-2.128185	-3.127015	1.733504
20	1	0	-1.854173	-4.207881	0.375535
21	6	0	-2.030698	-2.647254	-1.664426
22	6	0	-1.611002	-0.014758	1.251275
23	1	0	0.538464	-3.632847	1.224089
24	1	0	-2.382427	-1.953511	-2.432193
25	1	0	-0.983442	-2.879583	-1.880775
26	1	0	-2.599249	-3.575179	-1.776925
27	1	0	-0.840911	0.719484	1.496766
28	1	0	-2.530732	0.533107	1.028788
29	1	0	-1.789083	-0.619778	2.145507
30	6	0	-3.697062	-1.785644	0.074979
31	6	0	-4.308488	-0.722564	-0.868525
32	6	0	-5.694711	-0.208524	-0.475528
33	6	0	-6.228133	0.927108	-1.372538
34	6	0	-5.837330	2.208913	-0.620829
35	6	0	-5.735171	1.732107	0.824334
36	8	0	-5.653462	0.381903	0.868951
37	1	0	-6.408504	-1.030459	-0.403089
38	1	0	-7.318662	0.862075	-1.452976
39	1	0	-5.812977	0.878201	-2.382216
40	1	0	-4.818318	2.511814	-0.901115
41	6	0	-6.770870	3.407558	-0.798083
42	1	0	-3.738823	-1.383769	1.092577
43	1	0	-4.411176	-1.139501	-1.878734
44	1	0	-3.640386	0.139671	-0.959247
45	8	0	-5.710833	2.405798	1.833853
46	1	0	-6.447707	4.245161	-0.174122
47	1	0	-6.772924	3.735835	-1.841920
48	1	0	-7.797787	3.149010	-0.518933
49	1	0	1.350322	-1.020495	-1.679915
50	6	0	3.085839	0.100317	-1.183896
51	6	0	3.403287	-0.191491	-2.668579

52	6	0	3.516806	1.579729	-0.969919
53	1	0	4.464594	-0.045551	-2.891206
54	1	0	3.130692	-1.211484	-2.952776
55	1	0	2.830371	0.487452	-3.310794
56	6	0	3.343959	2.241890	0.414286
57	6	0	3.933936	3.633854	0.394340
58	8	0	5.126636	3.886740	0.343851
59	8	0	2.983829	4.592444	0.420275
60	6	0	3.447153	5.960117	0.378987
61	6	0	5.137552	-1.506494	-0.658697
62	1	0	4.092933	-0.278106	0.695698
63	6	0	6.306291	-0.910525	-0.372836
64	6	0	5.106754	-2.811508	-1.424189
65	1	0	7.252095	-1.322214	-0.715513
66	1	0	6.355087	0.006764	0.208284
67	1	0	6.108210	-3.079735	-1.771513
68	1	0	4.743793	-3.632853	-0.794208
69	1	0	4.445546	-2.769525	-2.295205
70	1	0	3.884423	1.682675	1.182873
71	1	0	2.297886	2.285563	0.710559
72	1	0	2.979520	2.189080	-1.707753
73	1	0	4.578266	1.645883	-1.238888
74	8	0	2.971722	-3.793311	1.792453
75	1	0	3.849813	-2.042034	2.251323
76	6	0	1.424288	-0.394047	2.799740
77	1	0	0.577634	-1.075284	2.928492
78	1	0	2.328793	-0.869526	3.199111
79	1	0	1.238026	0.520076	3.368779
80	6	0	-4.571307	-3.059189	0.073434
81	1	0	-5.574625	-2.842234	0.452229
82	1	0	-4.684239	-3.478722	-0.932594
83	1	0	-4.157017	-3.838788	0.717334
84	1	0	4.085614	6.169710	1.239807
85	1	0	4.004298	6.143778	-0.542251
86	1	0	2.546481	6.571557	0.411571

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891719	0.616218	-0.786071
2	6	0	0.461246	1.177546	-0.300004
3	1	0	-0.788556	0.415710	-1.855964
4	1	0	-1.657699	1.393481	-0.686754
5	1	0	0.390835	1.549032	0.726466
6	1	0	0.733375	2.031649	-0.931910
7	6	0	3.644620	-0.991680	0.233919
8	6	0	2.454141	-2.001563	0.252899
9	6	0	1.205146	-1.097540	0.545630
10	6	0	1.521974	0.081184	-0.402174
11	6	0	2.749131	-3.161812	1.173002
12	1	0	2.283254	-2.430624	-0.738654
13	8	0	1.234847	-0.564094	1.887235
14	6	0	-1.989382	-3.042229	-0.296991
15	6	0	-2.374635	-1.627766	-0.843036
16	6	0	-1.349684	-0.672350	-0.038246
17	6	0	-0.163339	-1.640787	0.195800
18	6	0	-0.537217	-2.918484	0.069445
19	1	0	-2.582872	-3.307778	0.591352
20	1	0	-2.172403	-3.833139	-1.033727
21	6	0	-2.065197	-1.627093	-2.357441
22	6	0	-1.926815	-0.250744	1.338816
23	1	0	0.108810	-3.777196	0.221386
24	1	0	-2.310603	-0.678603	-2.842181
25	1	0	-1.005734	-1.831475	-2.539883
26	1	0	-2.638095	-2.411008	-2.861695
27	1	0	-1.168776	0.279204	1.919317
28	1	0	-2.786660	0.415248	1.225607
29	1	0	-2.247628	-1.116040	1.927423
30	6	0	-3.896310	-1.342609	-0.596878
31	6	0	-4.363081	0.023809	-1.155030
32	6	0	-5.693926	0.532939	-0.617389
33	6	0	-6.173310	1.862557	-1.225114
34	6	0	-6.914408	2.550698	-0.066504
35	6	0	-6.262354	1.924990	1.163095
36	8	0	-5.566539	0.816795	0.818461
37	1	0	-6.472934	-0.231710	-0.701369
38	1	0	-6.804055	1.699161	-2.103064
39	1	0	-5.308854	2.459620	-1.535991
40	1	0	-6.725649	3.627718	-0.036143
41	6	0	-8.437043	2.314501	-0.048914
42	1	0	-4.042247	-1.323209	0.488208
43	1	0	-4.469188	-0.039402	-2.246131
44	1	0	-3.618159	0.800877	-0.962162
45	8	0	-6.327950	2.304501	2.314745
46	1	0	-8.884333	2.739676	0.853987
47	1	0	-8.895611	2.793558	-0.919208
48	1	0	-8.681004	1.247086	-0.081186
49	1	0	1.415159	-0.351297	-1.407635
50	6	0	3.041294	0.408998	-0.256223
51	6	0	3.587977	0.901870	-1.609937

52	6	0	3.280953	1.505037	0.821093
53	1	0	4.678949	0.990427	-1.606488
54	1	0	3.315516	0.231601	-2.429459
55	1	0	3.173194	1.888049	-1.842105
56	6	0	4.739143	1.960439	1.021525
57	6	0	5.181241	3.106935	0.134708
58	8	0	4.463021	3.995486	-0.289433
59	8	0	6.511090	3.068471	-0.094841
60	6	0	7.065991	4.160073	-0.860646
61	6	0	4.876762	-1.554545	-0.469486
62	1	0	3.936386	-0.839378	1.279002
63	6	0	6.081377	-1.493558	0.120125
64	6	0	4.719528	-2.261623	-1.799559
65	1	0	6.969325	-1.897147	-0.359486
66	1	0	6.220146	-1.046488	1.100990
67	1	0	5.695734	-2.459654	-2.250354
68	1	0	4.215137	-3.227414	-1.671524
69	1	0	4.123795	-1.688887	-2.515531
70	1	0	5.455247	1.142525	0.920351
71	1	0	4.855326	2.339667	2.046210
72	1	0	2.895925	1.136139	1.773592
73	1	0	2.688526	2.389449	0.565285
74	8	0	2.454850	-4.322803	0.938611
75	1	0	3.312552	-2.917614	2.096203
76	6	0	0.867535	-1.418598	2.966253
77	1	0	-0.045485	-1.982999	2.753961
78	1	0	1.669066	-2.122796	3.222243
79	1	0	0.695171	-0.767162	3.826378
80	6	0	-4.803088	-2.467798	-1.141443
81	1	0	-5.847427	-2.293908	-0.863568
82	1	0	-4.763481	-2.532493	-2.234529
83	1	0	-4.528876	-3.445163	-0.736356
84	1	0	6.883195	5.110695	-0.354878
85	1	0	8.134283	3.956746	-0.920771
86	1	0	6.623572	4.186312	-1.858822

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856796	0.081493	-1.083501
2	6	0	0.508287	0.770536	-0.875917
3	1	0	-0.827663	-0.390046	-2.069513
4	1	0	-1.640582	0.846061	-1.126925
5	1	0	0.501924	1.400653	0.018577
6	1	0	0.691380	1.425548	-1.735185
7	6	0	3.801633	-1.156642	-0.075221
8	6	0	2.658690	-2.112316	0.340545
9	6	0	1.394135	-1.194344	0.462698
10	6	0	1.603900	-0.292560	-0.773868
11	6	0	3.010580	-2.992484	1.518566
12	1	0	2.413592	-2.819253	-0.464614
13	8	0	1.483735	-0.317629	1.608591
14	6	0	-1.797659	-3.336122	0.400370
15	6	0	-2.269764	-2.108582	-0.445358
16	6	0	-1.211402	-0.973647	0.003504
17	6	0	0.022204	-1.834361	0.371362
18	6	0	-0.326156	-3.105619	0.598318
19	1	0	-2.309905	-3.376405	1.373658
20	1	0	-2.010533	-4.288658	-0.098323
21	6	0	-2.084739	-2.489517	-1.932605
22	6	0	-1.685245	-0.225206	1.276933
23	1	0	0.343866	-3.902176	0.905814
24	1	0	-2.388272	-1.694654	-2.618592
25	1	0	-1.039838	-2.733455	-2.148465
26	1	0	-2.680237	-3.375296	-2.172969
27	1	0	-0.898547	0.439896	1.637766
28	1	0	-2.570927	0.384310	1.077570
29	1	0	-1.930339	-0.917895	2.087993
30	6	0	-3.775371	-1.786594	-0.146479
31	6	0	-4.325579	-0.596734	-0.968686
32	6	0	-5.699705	-0.078758	-0.539474
33	6	0	-6.165877	1.183659	-1.292993
34	6	0	-5.738788	2.340796	-0.376778
35	6	0	-5.696144	1.680588	0.997409
36	8	0	-5.667621	0.333339	0.870232
37	1	0	-6.447535	-0.871961	-0.586109
38	1	0	-7.256184	1.177259	-1.399015
39	1	0	-5.730903	1.244800	-2.293619
40	1	0	-4.699779	2.626498	-0.594959
41	6	0	-6.612347	3.595516	-0.419347
42	1	0	-3.835371	-1.507907	0.910635
43	1	0	-4.422115	-0.887557	-2.022817
44	1	0	-3.623804	0.242820	-0.944547
45	8	0	-5.673560	2.218306	2.085372
46	1	0	-6.272143	4.328732	0.316893
47	1	0	-6.567312	4.055784	-1.411003
48	1	0	-7.657894	3.352485	-0.202358
49	1	0	1.445191	-0.970033	-1.626639
50	6	0	3.121518	0.077738	-0.841338
51	6	0	3.529579	0.178337	-2.323467

52	6	0	3.545169	1.369225	-0.081135
53	1	0	4.571012	0.495684	-2.444185
54	1	0	3.416707	-0.782314	-2.832473
55	1	0	2.898687	0.904973	-2.846865
56	6	0	3.193830	2.724547	-0.714606
57	6	0	3.845953	3.883431	0.011308
58	8	0	4.898568	3.839498	0.623723
59	8	0	3.126261	5.018103	-0.126156
60	6	0	3.681410	6.209603	0.472918
61	6	0	4.977065	-1.821176	-0.781277
62	1	0	4.203975	-0.752689	0.859496
63	6	0	4.869850	-2.899599	-1.570910
64	6	0	6.323725	-1.183061	-0.528856
65	1	0	5.744846	-3.328582	-2.052019
66	1	0	3.924795	-3.396059	-1.770969
67	1	0	6.565755	-1.214455	0.540948
68	1	0	7.120766	-1.691081	-1.078953
69	1	0	6.330155	-0.125562	-0.819815
70	1	0	2.119789	2.910704	-0.754222
71	1	0	3.557093	2.782212	-1.749111
72	1	0	4.634499	1.340130	0.028022
73	1	0	3.131958	1.328080	0.930336
74	8	0	4.083986	-2.985823	2.096187
75	1	0	2.228630	-3.708807	1.836829
76	6	0	1.285213	-0.874235	2.906112
77	1	0	2.174306	-1.407029	3.261294
78	1	0	1.100668	-0.030301	3.575289
79	1	0	0.421774	-1.547410	2.936904
80	6	0	-4.687354	-3.020062	-0.327040
81	1	0	-5.694823	-2.816596	0.047921
82	1	0	-4.781831	-3.310607	-1.379389
83	1	0	-4.316529	-3.885271	0.227956
84	1	0	4.653778	6.438775	0.031357
85	1	0	2.965966	7.001802	0.256691
86	1	0	3.792123	6.075415	1.550981
