Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Mechanism of the Gold(I)-Catalyzed Synthesis of Imidazo-pyrimidines and Imidazo-pyrazines via [3+2] Dipolar Cycloaddition: A DFT Study

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Contents

1. The free energies and the activation barriers in the gas and solution phases

Table 1. The Relative Free Energies and Activation Free Energies in the Gas Phase and in Solution of the Structures in Figure 1, 3 and 5, the Values are Given in kcal/mol.

species	ΔG_{gas}	$\Delta G^{\ddagger}_{gas}$	ΔG_{sol}	$\Delta G^{\ddagger}_{sol}$
R1+a	0.0		0.0	
a-TS1	9.3	9.3	9.6	9.6
a-IN1	-13.4		-11.4	
a-TS2	23.5	36.9	21.2	32.6
a-IN2	16.5		13.4	
a-IN3	-64.7		-64.5	
CA+P1	-76.1		-64.8	
a-TS3	19.7	19.7	20.2	20.2
a-IN4	-18.0		-16.1	
a-TS4	25.3	43.3	24.3	40.4
a-IN5	16.3		13.2	
a-IN6	-59.3		-58.6	
CA+P2	-76.9		-65.3	
R2+a	0.0		0.0	
b-TS1	7.0	7.0	9.6	9.6
b-IN1	-13.6		-12.3	
b-TS2	19.2	32.8	17.3	29.6
b-IN2	10.4		9.9	
b-IN3	-67.7		-65.9	
CA+P3	-77.3		-65.2	
b-TS3	18.1	18.1	17.9	17.9
b-IN4	-12.8		-12.6	
b-TS4	26.8	39.6	26.2	38.8
b-IN5	15.0		13.3	
b-IN6	-56.1		-54.0	
CA+P4	-79.0		-65.1	
R1+b	0.0		0.0	
c-TS1	9.7	9.7	10.2	10.2
c-IN1	-14.4		-13.4	
c-TS2	22.3	36.7	20.6	34.0
c-IN2	17.0		14.7	
c-IN3	-74.0		-71.1	
CA+P5	-85.7		-73.0	
c-TS3	18.8	18.8	17.6	17.6
c-IN4	-17.1		-15.4	
c-TS4	26.5	43.6	25.8	41.2

c-IN5	10.7	11.6
c-IN6	-66.2	-65.4
CA+P6	-86.1	-73.1

2. The Cartesian coordinates of the stationary points discussed in the text

R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.105975	-2.600192	2.179976
2	6	0	1.839230	0.513359	0.393118
3	16	0	1.774294	-3.010813	-0.557652
4	79	0	-0.349096	0.312624	0.228839
5	6	0	2.537633	1.762844	0.119710
6	6	0	1.835917	2.967586	0.000220
7	6	0	2.519389	4.148616	-0.264384
8	6	0	3.903575	4.133976	-0.414623
9	6	0	4.609611	2.936867	-0.295999
10	6	0	3.932777	1.755883	-0.028844
11	8	0	0.612525	-2.418644	-1.186797
12	8	0	1.767808	-4.347598	-0.013333
13	6	0	3.201807	-2.741806	-1.580148
14	15	0	-2.640256	0.281430	-0.039324
15	8	0	-3.074987	-0.319948	-1.454172
16	8	0	-3.384431	-0.589827	1.076720
17	8	0	-3.266664	1.751592	0.035330
18	7	0	2.151757	-1.984030	0.833225
19	6	0	2.052710	-0.702530	0.645150
20	1	0	1.069795	-2.692376	2.512061
21	1	0	2.565040	-3.585377	2.123910
22	1	0	2.666819	-1.956652	2.855756
23	1	0	0.756467	2.976749	0.123789
24	1	0	1.971649	5.080366	-0.352497
25	1	0	4.435012	5.056553	-0.622351
26	1	0	5.688051	2.926717	-0.410122
27	1	0	4.476929	0.821212	0.069694
28	1	0	3.034945	-3.314547	-2.494368
29	1	0	3.267622	-1.676629	-1.806091
30	1	0	4.080390	-3.105845	-1.048357
31	6	0	-4.685884	-0.268112	1.599360
32	1	0	-5.460927	-0.475827	0.855903
33	1	0	-4.831271	-0.911057	2.465141

34	1	0	-4.720645	0.779932	1.903573
35	6	0	-4.406796	2.166327	-0.739070
36	1	0	-4.476408	3.245584	-0.620152
37	1	0	-4.257825	1.915171	-1.791061
38	1	0	-5.319896	1.697622	-0.361045
39	6	0	-4.252613	-1.119652	-1.660749
40	1	0	-5.147164	-0.490014	-1.656587
41	1	0	-4.135875	-1.581744	-2.638736
42	1	0	-4.325302	-1.890931	-0.891336

a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.774059	0.572423	-0.000020
2	6	0	2.684594	1.425697	-0.000056
3	6	0	1.383732	0.940779	-0.000036
4	7	0	1.140590	-0.404852	0.000003
5	6	0	2.218333	-1.255408	0.000067
6	6	0	3.511948	-0.800161	0.000044
7	7	0	-1.373549	0.918680	0.000073
8	6	0	-1.223576	-0.423921	0.000000
9	7	0	-2.264104	-1.303860	-0.000026
10	6	0	-3.476041	-0.791793	-0.000047
11	6	0	-3.739004	0.584827	0.000004
12	6	0	-2.620459	1.394549	0.000052
13	7	0	-0.028578	-1.070699	-0.000075
14	1	0	4.789078	0.950855	-0.000043
15	1	0	2.814300	2.502002	-0.000091
16	1	0	0.505267	1.565498	-0.000047
17	1	0	1.931596	-2.297571	0.000105
18	1	0	4.311949	-1.531152	0.000107
19	1	0	-4.296705	-1.508977	0.000011
20	1	0	-4.745008	0.982929	-0.000067
21	1	0	-2.712507	2.479577	0.000149

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-4.518884	-2.745943	2.801563
2	6	0	-4.395591	-2.765129	1.417579
3	6	0	-3.931228	-1.649080	0.744752
4	7	0	-3.602567	-0.526228	1.425783
5	6	0	-3.721647	-0.490573	2.773426
6	6	0	-4.168648	-1.584246	3.485316
7	7	0	-4.814369	0.500161	-0.730989
8	6	0	-3.674426	1.052816	-0.278917
9	7	0	-3.044318	2.104237	-0.857157
10	6	0	-3.583832	2.577103	-1.974201
11	6	0	-4.741589	2.056855	-2.545422
12	6	0	-5.327568	1.008313	-1.847647
13	7	0	-3.046689	0.595905	0.845745
14	6	0	-0.847911	2.019129	2.533355
15	6	0	-0.406097	-0.487502	-0.061028
16	16	0	0.294180	2.979045	0.209290
17	79	0	1.723511	-0.603472	0.003802
18	6	0	-1.194495	-1.403279	-0.894530
19	6	0	-1.947376	-0.908349	-1.966908
20	6	0	-2.723770	-1.776775	-2.728532
21	6	0	-2.755045	-3.138520	-2.427220
22	6	0	-1.980247	-3.637054	-1.380328
23	6	0	-1.187882	-2.776690	-0.626862
24	8	0	0.488055	2.419309	-1.110106
25	8	0	1.424533	3.394494	1.019623
26	6	0	-0.933089	4.258399	0.187549
27	15	0	4.034072	-0.565995	-0.038559
28	8	0	4.678266	0.756216	-0.682251
29	8	0	4.602195	-0.651583	1.455037
30	8	0	4.753554	-1.705472	-0.887171
31	7	0	-0.486443	1.723942	1.144457
32	6	0	-0.725778	0.579948	0.574225
33	1	0	-4.878183	-3.616424	3.338725
34	1	0	-4.643200	-3.645293	0.836820
35	1	0	-3.806998	-1.614590	-0.327215
36	1	0	-3.449150	0.456949	3.218134
37	1	0	-4.249194	-1.511484	4.562917
38	1	0	-3.063937	3.414692	-2.438092
39	1	0	-5.163752	2.453488	-3.458551
40	1	0	-6.252299	0.552430	-2.196774
41	1	0	-0.761044	1.098788	3.112092
42	1	0	-0.145933	2.755968	2.926951
43	1	0	-1.877083	2.385454	2.564172
44	1	0	-1.915122	0.153365	-2.191759

45	1	0	-3.307971	-1.387005	-3.555918
46	1	0	-3.364881	-3.811355	-3.020976
47	1	0	-1.983083	-4.699332	-1.158626
48	1	0	-0.575371	-3.158300	0.185088
49	1	0	-0.573780	5.011091	-0.516523
50	1	0	-1.862997	3.788441	-0.143298
51	1	0	-1.007614	4.681765	1.189470
52	6	0	6.022019	-0.693945	1.685409
53	1	0	6.162968	-0.600505	2.760286
54	1	0	6.421680	-1.650655	1.340882
55	1	0	6.515305	0.135817	1.172127
56	6	0	4.051921	2.025333	-0.399319
57	1	0	3.907086	2.158781	0.675962
58	1	0	4.728413	2.788286	-0.779764
59	1	0	3.087667	2.088461	-0.911698
60	6	0	5.928732	-1.494516	-1.693261
61	1	0	6.128988	-2.449791	-2.174300
62	1	0	5.738520	-0.723060	-2.439422
63	1	0	6.778084	-1.204119	-1.071275

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.500065	-2.544736	2.673174
2	6	0	-4.430449	-2.669303	1.291323
3	6	0	-3.807726	-1.682110	0.547007
4	7	0	-3.274754	-0.615722	1.175582
5	6	0	-3.367197	-0.447762	2.512591
6	6	0	-3.964011	-1.413917	3.292258
7	7	0	-4.805008	1.019331	-0.156160
8	6	0	-3.496894	1.234720	-0.277385
9	7	0	-2.886232	2.168354	-1.000652
10	6	0	-3.692743	2.961227	-1.705846
11	6	0	-5.078186	2.835753	-1.684497
12	6	0	-5.587074	1.832485	-0.869927
13	7	0	-2.648212	0.382918	0.433431
14	6	0	-0.096331	1.360827	2.412687
15	6	0	-0.473828	-0.574047	-0.138752
16	16	0	0.326467	2.585255	0.098132
17	79	0	1.589738	-0.582748	-0.037603
18	6	0	-1.173458	-1.605428	-0.933115

19	6	0	-1.174341	-2.951467	-0.549144
20	6	0	-1.918711	-3.887038	-1.264582
21	6	0	-2.640682	-3.496508	-2.391430
22	6	0	-2.598481	-2.165806	-2.813410
23	6	0	-1.873500	-1.224146	-2.088430
24	8	0	0.242747	2.180699	-1.293346
25	8	0	1.631071	2.684049	0.746256
26	6	0	-0.495780	4.149240	0.297443
27	15	0	3.925583	-0.408035	0.034654
28	8	0	4.590138	0.582742	-1.046361
29	8	0	4.365152	0.163774	1.469323
30	8	0	4.785634	-1.731950	-0.221492
31	7	0	-0.643441	1.561251	1.060258
32	6	0	-1.193431	0.413553	0.415865
33	1	0	-4.978709	-3.315497	3.267820
34	1	0	-4.844838	-3.524976	0.772892
35	1	0	-3.715070	-1.700028	-0.532897
36	1	0	-2.958191	0.480755	2.889055
37	1	0	-4.021782	-1.270073	4.363852
38	1	0	-3.202485	3.723464	-2.307251
39	1	0	-5.720978	3.483929	-2.265021
40	1	0	-6.657505	1.666314	-0.779612
41	1	0	0.834009	0.782037	2.397764
42	1	0	0.095585	2.324054	2.888252
43	1	0	-0.840062	0.823674	3.003153
44	1	0	-0.598907	-3.254142	0.321963
45	1	0	-1.923237	-4.926166	-0.950458
46	1	0	-3.208546	-4.228806	-2.955749
47	1	0	-3.131889	-1.864207	-3.709367
48	1	0	-1.836614	-0.182686	-2.399811
49	1	0	0.081945	4.884843	-0.263636
50	1	0	-1.503221	4.042755	-0.099653
51	1	0	-0.505852	4.402839	1.357652
52	6	0	5.753032	0.353344	1.781680
53	1	0	5.789026	0.926728	2.706183
54	1	0	6.234595	-0.616765	1.929733
55	1	0	6.253578	0.908771	0.983342
56	6	0	3.950849	1.851514	-1.288912
57	1	0	3.934753	2.452044	-0.377012
58	1	0	4.540031	2.342336	-2.061673
59	1	0	2.923008	1.702888	-1.635862
60	6	0	6.041491	-1.758882	-0.920545
61	1	0	6.327102	-2.807828	-0.974858
62	1	0	5.924921	-1.343648	-1.921789

63	1	0	6.803493	-1.195549	-0.376909

a-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.516181	1.054888	2.268570
2	6	0	-2.555989	0.864841	1.377723
3	7	0	-1.318157	1.399291	1.415421
4	6	0	-0.963035	2.103202	2.488753
5	6	0	-1.889095	2.335420	3.496057
6	6	0	-3.168889	1.806346	3.318115
7	6	0	-0.649331	-1.662164	1.757634
8	6	0	-0.557940	0.869662	-0.060350
9	16	0	-0.193737	-2.650701	-0.672395
10	79	0	1.496280	0.490545	0.134031
11	6	0	-0.877985	2.036872	-0.967150
12	6	0	-0.552053	3.352398	-0.612773
13	6	0	-0.828694	4.415239	-1.463515
14	6	0	-1.423112	4.185267	-2.703420
15	6	0	-1.725657	2.881947	-3.081983
16	6	0	-1.456432	1.817666	-2.223201
17	8	0	0.068551	-3.840748	0.128872
18	8	0	0.936489	-2.027421	-1.362773
19	6	0	-1.432027	-3.009629	-1.899127
20	15	0	3.715802	-0.237679	0.177007
21	8	0	4.795179	0.809958	0.701217
22	8	0	4.020314	-1.503452	1.113718
23	8	0	4.245718	-0.775638	-1.243280
24	7	0	-0.995509	-1.572988	0.331558
25	6	0	-1.360311	-0.327433	-0.306151
26	1	0	0.058647	2.473012	2.509823
27	1	0	-1.633068	2.917280	4.370873
28	1	0	-3.946138	1.975768	4.057945
29	1	0	-1.485534	-1.269275	2.349553
30	1	0	-0.493372	-2.705269	2.032737
31	1	0	0.244710	-1.076573	2.010583
32	1	0	-0.060058	3.546710	0.337093
33	1	0	-0.568245	5.425359	-1.164428
34	1	0	-1.631772	5.013793	-3.371726
35	1	0	-2.165481	2.688912	-4.055792
36	1	0	-1.655774	0.794169	-2.523159

37	1	0	-2.251536	-3.537651	-1.412046
38	1	0	-1.750908	-2.061015	-2.329369
39	1	0	-0.952628	-3.640431	-2.648150
40	6	0	3.613641	-0.347371	-2.461322
41	1	0	3.634076	0.742543	-2.548637
42	1	0	4.194951	-0.785752	-3.271068
43	1	0	2.585624	-0.716767	-2.496806
44	6	0	3.242985	-2.696068	0.913031
45	1	0	3.741553	-3.485476	1.472507
46	1	0	2.228099	-2.556098	1.298036
47	1	0	3.193720	-2.956130	-0.146627
48	6	0	6.181853	0.425857	0.801252
49	1	0	6.728571	1.334560	1.044637
50	1	0	6.302600	-0.315902	1.591662
51	1	0	6.527559	0.021889	-0.152594
52	7	0	-2.656350	0.079633	0.258347
53	6	0	-4.199818	-1.622518	0.816997
54	6	0	-4.462833	-0.323402	-1.147226
55	6	0	-5.320652	-2.367527	0.498089
56	1	0	-3.586019	-1.777465	1.695223
57	6	0	-5.578996	-1.049415	-1.506349
58	1	0	-4.025291	0.494013	-1.711387
59	6	0	-6.015253	-2.081277	-0.673648
60	1	0	-5.630384	-3.166162	1.160534
61	1	0	-6.100046	-0.802197	-2.422826
62	1	0	-6.892369	-2.660659	-0.940648
63	7	0	-3.814818	-0.623812	-0.001299

a-IN2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.064825	0.351505	2.641248
2	6	0	-2.315738	0.400291	1.554396
3	7	0	-1.425171	1.378329	1.274390
4	6	0	-1.235190	2.369348	2.159026
5	6	0	-1.971246	2.377374	3.325569
6	6	0	-2.891191	1.340524	3.515772
7	6	0	-1.041274	-0.445674	-2.916631
8	6	0	-0.739372	1.188084	-0.049103
9	16	0	-0.050471	-2.205293	-1.279455
10	79	0	1.259686	0.554402	0.299516

11	6	0	-0.823974	2.513386	-0.807271
12	6	0	0.225063	3.438218	-0.771859
13	6	0	0.116565	4.668834	-1.416863
14	6	0	-1.043497	4.989415	-2.114540
15	6	0	-2.094339	4.075200	-2.160634
16	6	0	-1.985034	2.850868	-1.510535
17	8	0	1.348680	-1.785021	-1.470606
18	8	0	-0.519667	-3.325321	-2.081785
19	6	0	-0.248572	-2.637258	0.440152
20	15	0	3.324504	-0.568824	0.467014
21	8	0	4.391460	0.079000	1.473980
22	8	0	3.149682	-2.079781	0.986944
23	8	0	4.125588	-0.793795	-0.909208
24	7	0	-1.188305	-0.923399	-1.532191
25	6	0	-1.621118	0.065535	-0.618394
26	1	0	-0.507526	3.123545	1.876174
27	1	0	-1.845039	3.164305	4.056326
28	1	0	-3.510727	1.304227	4.406943
29	1	0	-0.245182	0.303148	-3.005280
30	1	0	-0.825993	-1.289592	-3.575753
31	1	0	-1.984284	0.016002	-3.216965
32	1	0	1.143635	3.187477	-0.244377
33	1	0	0.944020	5.369871	-1.382102
34	1	0	-1.126859	5.942985	-2.625500
35	1	0	-3.000021	4.318177	-2.707200
36	1	0	-2.790405	2.123220	-1.550025
37	1	0	0.031144	-1.802797	1.083647
38	1	0	-1.274388	-2.965674	0.604906
39	1	0	0.442800	-3.469312	0.587895
40	6	0	3.847100	0.040211	-2.044760
41	1	0	4.017771	1.092989	-1.802283
42	1	0	4.540060	-0.269760	-2.825310
43	1	0	2.817772	-0.121043	-2.373156
44	6	0	3.631827	-3.218261	0.250607
45	1	0	3.345843	-4.091527	0.836337
46	1	0	3.167095	-3.244189	-0.736316
47	1	0	4.718919	-3.182069	0.151116
48	6	0	5.641034	-0.590595	1.714640
49	1	0	6.224161	0.064854	2.358439
50	1	0	5.459566	-1.543344	2.218046
51	1	0	6.168974	-0.753117	0.771522
52	7	0	-2.314465	-0.503053	0.525521
53	6	0	-3.948334	-2.070054	1.277440
54	6	0	-4.029467	-1.215137	-0.938953

55	6	0	-5.019746	-2.889465	1.020220
56	1	0	-3.424037	-2.028986	2.221702
57	6	0	-5.114760	-2.027894	-1.219004
58	1	0	-3.550401	-0.523113	-1.621636
59	6	0	-5.617546	-2.880223	-0.246172
60	1	0	-5.372635	-3.544327	1.807277
61	1	0	-5.537687	-1.996120	-2.215812
62	1	0	-6.442992	-3.546571	-0.468147
63	7	0	-3.500357	-1.222957	0.308267

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.281371	2.788369	2.418554
2	6	0	1.532002	1.892530	1.461675
3	7	0	1.711890	0.556346	1.727355
4	6	0	1.642864	0.075710	2.986495
5	6	0	1.383629	0.963891	3.995275
6	6	0	1.207972	2.324177	3.648860
7	6	0	2.421821	-0.355243	-2.434840
8	6	0	1.873676	-0.152758	0.481212
9	16	0	1.201069	2.063787	-2.727734
10	6	0	2.898301	-1.252432	0.522174
11	6	0	2.551115	-2.604282	0.514616
12	6	0	3.539607	-3.584242	0.584693
13	6	0	4.879706	-3.219859	0.662188
14	6	0	5.235302	-1.871409	0.676275
15	6	0	4.249934	-0.893781	0.612966
16	8	0	-0.146505	2.098916	-2.174982
17	8	0	1.411187	1.652862	-4.100617
18	6	0	2.026631	3.624116	-2.432734
19	15	0	-2.384103	-1.412495	-0.508616
20	8	0	-2.477102	-2.437932	-1.732371
21	8	0	-3.088499	-2.077372	0.759930
22	8	0	-3.419333	-0.231823	-0.838074
23	7	0	2.111366	0.924806	-1.788414
24	6	0	1.909082	0.988671	-0.437065
25	1	0	1.800306	-0.990847	3.111182
26	1	0	1.323861	0.633259	5.023248
27	1	0	1.005045	3.056131	4.426631
28	1	0	1.620961	-1.089029	-2.269814

29	1	0	2.533407	-0.176618	-3.502121
30	1	0	3.356810	-0.739298	-2.028036
31	1	0	1.505339	-2.892945	0.443314
32	1	0	3.259281	-4.632085	0.574836
33	1	0	5.648419	-3.983718	0.712322
34	1	0	6.279379	-1.583078	0.735855
35	1	0	4.525144	0.158757	0.624152
36	1	0	1.277687	4.309850	-2.039241
37	1	0	2.818834	3.479975	-1.701574
38	1	0	2.413690	3.950704	-3.397601
39	6	0	-3.143249	0.636203	-1.956430
40	1	0	-3.213634	0.075043	-2.891998
41	1	0	-3.906793	1.411874	-1.928586
42	1	0	-2.151791	1.087969	-1.861551
43	6	0	-4.489170	-1.942134	1.068218
44	1	0	-4.620107	-2.395761	2.049167
45	1	0	-4.765373	-0.887450	1.091309
46	1	0	-5.098546	-2.472680	0.333441
47	6	0	-3.733106	-3.029762	-2.111532
48	1	0	-3.579289	-3.478813	-3.090726
49	1	0	-4.005771	-3.802294	-1.388637
50	1	0	-4.515196	-2.267306	-2.171372
51	7	0	1.647544	2.154418	0.148905
52	79	0	-0.211847	-0.773816	-0.067161
53	6	0	-1.709888	2.312799	0.739367
54	6	0	-2.265712	0.777004	2.350035
55	6	0	-2.994503	2.850884	0.743670
56	1	0	-0.939475	2.702644	0.075899
57	6	0	-3.570279	1.253178	2.431104
58	1	0	-1.940332	-0.054187	2.973037
59	6	0	-3.942998	2.309896	1.604777
60	1	0	-3.236429	3.679859	0.087790
61	1	0	-4.270768	0.809285	3.130330
62	1	0	-4.951242	2.710079	1.640637
63	7	0	-1.344661	1.293609	1.527847

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.382563	1.733376	3.319430
2	6	0	3.532552	2.482185	2.501078

3	6	0	3.223913	2.033305	1.239950
4	7	0	3.726145	0.857643	0.753347
5	6	0	4.539674	0.106332	1.544484
6	6	0	4.878688	0.541532	2.818860
7	7	0	4.909212	-1.104123	-0.914609
8	6	0	3.800177	-0.428581	-1.250223
9	7	0	3.097399	-0.619541	-2.392792
10	6	0	3.578050	-1.511074	-3.244365
11	6	0	4.742137	-2.244500	-3.007018
12	6	0	5.367719	-1.993846	-1.798279
13	7	0	3.236371	0.554157	-0.477310
14	6	0	1.070011	2.203938	-2.275331
15	6	0	1.012490	-0.064499	-0.009020
16	16	0	-0.769275	3.312493	-0.651103
17	79	0	-1.635363	-0.034241	0.030479
18	6	0	1.413588	-1.352378	0.464833
19	6	0	1.441392	-2.449736	-0.413267
20	6	0	1.896339	-3.678703	0.042715
21	6	0	2.311318	-3.823718	1.367494
22	6	0	2.274295	-2.740764	2.244526
23	6	0	1.831582	-1.501819	1.798017
24	8	0	-2.070377	2.648906	-0.721194
25	8	0	-0.476750	4.433350	-1.517137
26	6	0	-0.481858	3.752169	1.048361
27	15	0	-3.730953	-0.959471	0.251393
28	8	0	-4.968325	0.043423	0.070198
29	8	0	-3.914790	-2.086724	-0.868854
30	8	0	-4.063724	-1.600951	1.668764
31	7	0	0.489426	2.190231	-0.906233
32	6	0	0.324404	0.946434	-0.321443
33	1	0	4.647588	2.077985	4.311987
34	1	0	3.115131	3.425156	2.833926
35	1	0	2.576120	2.545965	0.537898
36	1	0	4.912379	-0.804143	1.103990
37	1	0	5.539652	-0.084478	3.406628
38	1	0	3.009154	-1.652742	-4.161726
39	1	0	5.124357	-2.965759	-3.716867
40	1	0	6.273060	-2.524701	-1.512302
41	1	0	0.340131	1.844848	-3.007086
42	1	0	1.359958	3.225933	-2.510800
43	1	0	1.934964	1.543190	-2.256255
44	1	0	1.114658	-2.312181	-1.438363
45	1	0	1.923701	-4.527910	-0.631145
46	1	0	2.660756	-4.788698	1.719577

47	1	0	2.589436	-2.863253	3.275159
48	1	0	1.794306	-0.646415	2.466654
49	1	0	-1.309637	4.394451	1.351694
50	1	0	-0.465498	2.841499	1.650088
51	1	0	0.464833	4.288679	1.103229
52	6	0	-5.131779	-2.850758	-0.953008
53	1	0	-5.100798	-3.374884	-1.906189
54	1	0	-5.167913	-3.573463	-0.134430
55	1	0	-6.002338	-2.189739	-0.920493
56	6	0	-4.977473	0.932118	-1.066810
57	1	0	-4.974857	0.354168	-1.994841
58	1	0	-5.898575	1.506622	-0.992391
59	1	0	-4.113603	1.601483	-1.031154
60	6	0	-5.375353	-1.601962	2.268412
61	1	0	-5.248121	-2.054444	3.249606
62	1	0	-5.745326	-0.581108	2.362138
63	1	0	-6.071836	-2.195770	1.672973

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.851927	2.730909	2.152688
2	6	0	-3.950977	1.772704	2.604164
3	6	0	-3.229614	1.026401	1.688216
4	7	0	-3.402864	1.258972	0.374333
5	6	0	-4.259035	2.187317	-0.097992
6	6	0	-5.010590	2.936214	0.781884
7	7	0	-4.510271	-0.886063	-0.627227
8	6	0	-3.360103	-0.522074	-1.182734
9	7	0	-2.810326	-0.983751	-2.302764
10	6	0	-3.475163	-1.968567	-2.898748
11	6	0	-4.683306	-2.465116	-2.411200
12	6	0	-5.170151	-1.861899	-1.261473
13	7	0	-2.661382	0.536073	-0.566778
14	6	0	-0.607813	-2.737962	-1.038440
15	6	0	-0.470710	-0.497370	-0.141470
16	16	0	-1.047606	-2.393083	1.529717
17	79	0	1.593132	-0.389925	-0.044977
18	8	0	0.226525	-3.050661	1.770092
19	8	0	-1.467917	-1.306141	2.413178
20	6	0	-2.340530	-3.617876	1.521700

21	15	0	3.926504	-0.128858	-0.035253
22	8	0	4.466405	0.208246	1.438003
23	8	0	4.476076	1.074328	-0.967037
24	8	0	4.803865	-1.341155	-0.592818
25	7	0	-1.150248	-1.783558	-0.049642
26	6	0	-1.235622	0.585994	-0.365093
27	6	0	-0.705882	1.971246	-0.443276
28	6	0	0.105447	2.486912	0.572539
29	6	0	0.611276	3.781775	0.475361
30	6	0	0.303884	4.571379	-0.630341
31	6	0	-0.519885	4.068148	-1.636956
32	6	0	-1.030215	2.778183	-1.539510
33	1	0	-5.426139	3.319203	2.860364
34	1	0	-3.802028	1.584294	3.660111
35	1	0	-2.513799	0.247063	1.949278
36	1	0	-4.289416	2.284730	-1.175785
37	1	0	-5.697084	3.677726	0.393243
38	1	0	-3.030949	-2.364755	-3.809043
39	1	0	-5.218747	-3.260463	-2.912703
40	1	0	-6.116593	-2.164494	-0.820130
41	1	0	0.420431	-3.030513	-0.796502
42	1	0	-1.247001	-3.623389	-1.087788
43	1	0	-0.631159	-2.237509	-2.006227
44	1	0	-3.260299	-3.139582	1.184746
45	1	0	-2.056723	-4.451648	0.881040
46	1	0	-2.432137	-3.958697	2.554121
47	1	0	0.328631	1.868078	1.438140
48	1	0	1.236141	4.176925	1.270155
49	1	0	0.697284	5.579855	-0.705183
50	1	0	-0.758371	4.679971	-2.500828
51	1	0	-1.656096	2.369309	-2.329083
52	6	0	5.874461	0.332065	1.691241
53	1	0	5.975724	0.702250	2.709720
54	1	0	6.352531	-0.646968	1.605968
55	1	0	6.328314	1.040744	0.992211
56	6	0	3.796791	2.335492	-0.899905
57	1	0	3.883700	2.764562	0.103000
58	1	0	4.283461	2.987961	-1.623050
59	1	0	2.738090	2.220077	-1.158277
60	6	0	5.997564	-1.188105	-1.379561
61	1	0	6.779893	-0.682997	-0.808805
62	1	0	6.316552	-2.198002	-1.630528
63	1	0	5.781071	-0.620720	-2.285011

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.798995	2.607099	0.218305
2	6	0	5.259696	2.428494	1.489763
3	6	0	4.084265	1.722632	1.641641
4	7	0	3.482702	1.173959	0.559571
5	6	0	3.958822	1.365261	-0.686893
6	6	0	5.128805	2.072171	-0.877183
7	7	0	3.065443	-0.739350	2.578964
8	6	0	2.196824	-0.538542	1.595850
9	7	0	1.149572	-1.323409	1.316061
10	6	0	0.880813	-2.350057	2.122676
11	6	0	1.717984	-2.632339	3.189275
12	6	0	2.825836	-1.796238	3.351682
13	7	0	2.249148	0.524140	0.722607
14	6	0	1.290063	0.478533	-0.344469
15	6	0	0.562954	-0.804021	-0.360870
16	79	0	-1.528103	-0.558237	-0.128897
17	15	0	-3.764922	0.000422	0.252123
18	8	0	-4.056488	1.582221	0.147869
19	8	0	-4.244739	-0.427261	1.722778
20	8	0	-4.842774	-0.563816	-0.781268
21	1	0	6.713887	3.172951	0.082857
22	1	0	5.729027	2.849369	2.370135
23	1	0	3.597022	1.560385	2.590949
24	1	0	3.343966	0.936128	-1.465035
25	1	0	5.498640	2.203609	-1.886392
26	1	0	0.002545	-2.941682	1.880946
27	1	0	1.536020	-3.470851	3.847560
28	1	0	3.546336	-1.977200	4.144534
29	7	0	0.982271	-1.920356	-1.113281
30	6	0	0.033261	-2.997848	-1.421144
31	1	0	-0.351115	-3.441887	-0.499208
32	1	0	-0.806380	-2.596149	-1.996615
33	1	0	0.537391	-3.776889	-1.989914
34	16	0	2.555538	-2.079265	-1.698621
35	8	0	2.753523	-3.466635	-2.071194
36	8	0	3.460445	-1.444636	-0.747157
37	6	0	2.518828	-1.105481	-3.190428
38	1	0	1.863175	-1.612358	-3.899417

39	1	0	2.128884	-0.117266	-2.939562
40	1	0	3.536343	-1.059466	-3.582032
41	6	0	0.577338	1.738438	-0.551564
42	6	0	0.761466	2.874519	0.262121
43	6	0	-0.289727	1.880789	-1.658327
44	6	0	0.102908	4.071101	-0.005738
45	1	0	1.409956	2.814063	1.131912
46	6	0	-0.967760	3.068939	-1.904613
47	1	0	-0.400197	1.047535	-2.348859
48	6	0	-0.771812	4.179970	-1.084851
49	1	0	0.269475	4.925187	0.644255
50	1	0	-1.629012	3.136005	-2.763344
51	1	0	-1.278082	5.116325	-1.292649
52	6	0	-5.981783	0.179290	-1.252811
53	1	0	-6.493474	-0.478714	-1.952663
54	1	0	-6.649347	0.435661	-0.427340
55	1	0	-5.654105	1.089869	-1.754907
56	6	0	-5.597079	-0.189017	2.147539
57	1	0	-5.630958	-0.407807	3.213150
58	1	0	-5.875063	0.854627	1.973689
59	1	0	-6.275166	-0.858211	1.611910
60	6	0	-3.178361	2.476295	0.854394
61	1	0	-3.444190	3.483244	0.538276
62	1	0	-3.325894	2.369846	1.932902
63	1	0	-2.132029	2.282512	0.591991

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.885631	2.065845	-1.402535
2	6	0	-5.258591	1.535782	-2.535290
3	6	0	-4.054116	0.886664	-2.409220
4	7	0	-3.502488	0.720369	-1.176291
5	6	0	-4.057206	1.262026	-0.069460
6	6	0	-5.268821	1.921521	-0.166740
7	7	0	-2.801256	-1.740964	-2.368140
8	6	0	-2.062709	-1.106914	-1.476565
9	7	0	-1.056651	-1.663404	-0.771005
10	6	0	-0.709327	-2.942312	-1.002641
11	6	0	-1.408914	-3.657649	-1.944084
12	6	0	-2.478025	-3.009327	-2.588942

13	7	0	-2.182435	0.206175	-1.103234
14	6	0	-1.330156	0.469342	-0.000482
15	6	0	-0.553334	-0.774360	0.339201
16	79	0	1.526468	-0.370162	0.068038
17	15	0	3.769702	0.151849	-0.394793
18	8	0	4.513841	0.857717	0.842970
19	8	0	3.949582	1.154199	-1.638097
20	8	0	4.662311	-1.139350	-0.749196
21	1	0	-6.823586	2.601115	-1.493077
22	1	0	-5.692041	1.639313	-3.522272
23	1	0	-3.495344	0.470358	-3.235017
24	1	0	-3.498722	1.108224	0.842198
25	1	0	-5.706296	2.330434	0.735644
26	1	0	0.099162	-3.333402	-0.393939
27	1	0	-1.162843	-4.688342	-2.159198
28	1	0	-3.088932	-3.540600	-3.312902
29	7	0	-0.839805	-1.503744	1.589713
30	6	0	0.212876	-1.794432	2.566092
31	1	0	1.014475	-2.358153	2.083480
32	1	0	0.640962	-0.880679	2.996860
33	1	0	-0.206760	-2.415206	3.358738
34	16	0	-2.410810	-1.580234	2.146791
35	8	0	-2.535392	-2.740011	3.009776
36	8	0	-3.270922	-1.448343	0.971631
37	6	0	-2.615313	-0.132890	3.172654
38	1	0	-1.985031	-0.257050	4.054834
39	1	0	-2.313076	0.754306	2.612326
40	1	0	-3.664022	-0.090530	3.472027
41	6	0	-1.000932	1.804388	0.364107
42	6	0	-1.488175	2.939067	-0.331767
43	6	0	-0.205543	2.049280	1.515404
44	6	0	-1.176747	4.225701	0.090484
45	1	0	-2.054354	2.811325	-1.250031
46	6	0	0.107851	3.340317	1.912490
47	1	0	0.143834	1.206386	2.107919
48	6	0	-0.379799	4.444094	1.211383
49	1	0	-1.553379	5.071749	-0.476813
50	1	0	0.725075	3.487977	2.793848
51	1	0	-0.144312	5.451678	1.533930
52	6	0	6.044826	-1.274151	-0.389030
53	1	0	6.306830	-2.315282	-0.569027
54	1	0	6.673279	-0.629761	-1.011368
55	1	0	6.187594	-1.032942	0.666589
56	6	0	5.051350	1.112677	-2.555159

57	1	0	4.764127	1.727015	-3.406515
58	1	0	5.953495	1.528146	-2.095679
59	1	0	5.234129	0.086982	-2.883939
60	6	0	5.507212	1.883293	0.700889
61	1	0	5.639921	2.319589	1.689085
62	1	0	6.456220	1.457225	0.360856
63	1	0	5.164510	2.648465	0.000976

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.002290	3.593352	0.929595
2	6	0	-1.236709	2.301990	0.706494
3	7	0	-1.333301	1.778706	-0.552533
4	6	0	-1.260980	2.554870	-1.648718
5	6	0	-1.049225	3.896643	-1.464426
6	6	0	-0.914014	4.363955	-0.138401
7	7	0	-1.407113	1.353906	1.661027
8	6	0	-1.656327	0.226857	1.024218
9	6	0	-1.508701	0.340043	-0.434750
10	15	0	2.636978	-1.486204	-0.611067
11	8	0	3.674963	-0.491005	-1.318700
12	8	0	2.644265	-2.887614	-1.357090
13	8	0	3.328799	-1.865277	0.790297
14	1	0	-1.392652	2.066496	-2.609090
15	1	0	-0.998364	4.572414	-2.307226
16	1	0	-0.735045	5.420220	0.045402
17	7	0	-2.425974	-0.262459	-1.324710
18	6	0	-2.067727	-0.969522	-2.561393
19	1	0	-2.471818	-0.454201	-3.435263
20	1	0	-0.980699	-1.016238	-2.635347
21	1	0	-2.451488	-1.995134	-2.544179
22	16	0	-4.048624	0.223440	-1.187572
23	8	0	-4.513883	0.531377	-2.527547
24	8	0	-4.062503	1.218869	-0.128580
25	6	0	-4.898426	-1.233123	-0.619560
26	1	0	-4.735710	-2.038172	-1.337107
27	1	0	-4.519746	-1.492104	0.369683
28	1	0	-5.957946	-0.974729	-0.581424
29	6	0	-2.050791	-0.997284	1.730161
30	6	0	-2.552014	-0.877535	3.032280

31	6	0	-1.984444	-2.260416	1.123306
32	6	0	-2.983499	-2.007469	3.716407
33	1	0	-2.609571	0.108064	3.481603
34	6	0	-2.415281	-3.386070	1.814311
35	1	0	-1.592040	-2.362101	0.114645
36	6	0	-2.916353	-3.260275	3.110112
37	1	0	-3.377973	-1.910277	4.721965
38	1	0	-2.355396	-4.362789	1.346137
39	1	0	-3.252795	-4.141168	3.646974
40	6	0	3.349017	-0.866893	1.825083
41	1	0	2.329562	-0.659316	2.164554
42	1	0	3.933313	-1.284612	2.642859
43	1	0	3.813199	0.057795	1.463982
44	6	0	3.784297	-3.771172	-1.371233
45	1	0	3.417708	-4.726401	-1.740742
46	1	0	4.544545	-3.382734	-2.052401
47	1	0	4.187229	-3.887390	-0.363996
48	6	0	5.105151	-0.634764	-1.246162
49	1	0	5.514236	0.360684	-1.070465
50	1	0	5.393390	-1.298898	-0.427807
51	1	0	5.470284	-1.021472	-2.198648
52	79	0	0.552747	-0.501744	-0.501777
53	6	0	1.738746	2.187687	1.964006
54	6	0	2.709961	2.242138	-0.112739
55	6	0	2.872580	2.730692	2.562246
56	1	0	0.854082	1.949489	2.551263
57	6	0	3.883503	2.796921	0.391858
58	1	0	2.614335	2.026761	-1.174882
59	6	0	3.966668	3.041553	1.759785
60	1	0	2.886288	2.915352	3.630318
61	1	0	4.702357	3.041576	-0.275924
62	1	0	4.863508	3.475034	2.190651
63	7	0	1.654078	1.937342	0.650572

CA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.976178	-0.024613	-0.080416
2	8	0	-2.458369	1.475975	-0.309802
3	8	0	-2.602775	-0.960549	-1.190797
4	8	0	-2.721077	-0.541620	1.238950

5	6	0	-2.360035	0.029237	2.509036
6	1	0	-2.536217	1.107768	2.506372
7	1	0	-2.992897	-0.451477	3.251933
8	1	0	-1.308506	-0.179603	2.728938
9	6	0	-3.875907	-1.637120	-1.074931
10	1	0	-3.958803	-2.252354	-1.967907
11	1	0	-3.886170	-2.256341	-0.178598
12	1	0	-4.691879	-0.913051	-1.042956
13	6	0	-3.859059	1.787086	-0.471110
14	1	0	-3.945777	2.866909	-0.372214
15	1	0	-4.187395	1.478027	-1.465552
16	1	0	-4.451311	1.293236	0.304013
17	79	0	0.294830	-0.025929	-0.060364
18	6	0	3.135223	-1.127822	0.191270
19	6	0	3.100474	1.144984	-0.269181
20	6	0	4.521220	-1.143653	0.206007
21	1	0	2.559210	-2.029568	0.368842
22	6	0	4.485199	1.206552	-0.269192
23	1	0	2.496802	2.026842	-0.455079
24	6	0	5.208949	0.043092	-0.027645
25	1	0	5.043809	-2.073019	0.397619
26	1	0	4.978943	2.152499	-0.456113
27	1	0	6.293572	0.060872	-0.021917
28	7	0	2.437013	-0.002530	-0.042104

P1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.031590	-3.204789	0.066786
2	6	0	1.265856	-2.106712	0.207873
3	7	0	1.797676	-0.812171	0.043190
4	6	0	3.102836	-0.635591	-0.311888
5	6	0	3.879938	-1.743174	-0.459324
6	6	0	3.289069	-3.021604	-0.246334
7	6	0	-1.819179	0.830025	1.761510
8	6	0	0.762317	0.081323	0.229101
9	16	0	-2.801554	-0.558999	-0.326022
10	6	0	0.882296	1.532691	0.043378
11	6	0	-0.024421	2.188149	-0.799667
12	6	0	0.059579	3.565954	-0.970824
13	6	0	1.053320	4.296787	-0.322455

14	6	0	1.960999	3.648451	0.511120
15	6	0	1.872075	2.273129	0.701005
16	8	0	-2.224341	-0.316711	-1.642496
17	8	0	-3.967410	0.191304	0.114091
18	6	0	-3.129423	-2.300900	-0.183249
19	7	0	-1.625965	-0.307052	0.853426
20	6	0	-0.322104	-0.728558	0.526726
21	1	0	3.434063	0.385062	-0.464174
22	1	0	4.920144	-1.649933	-0.741057
23	1	0	3.897950	-3.916530	-0.352135
24	1	0	-1.685439	1.799496	1.272597
25	1	0	-2.823749	0.775154	2.178409
26	1	0	-1.084698	0.726165	2.561560
27	1	0	-0.783168	1.604104	-1.316174
28	1	0	-0.648395	4.068538	-1.621752
29	1	0	1.119039	5.370576	-0.465008
30	1	0	2.730285	4.214987	1.025817
31	1	0	2.555785	1.772712	1.382314
32	1	0	-2.182303	-2.832025	-0.281008
33	1	0	-3.575445	-2.475134	0.794994
34	1	0	-3.822916	-2.555528	-0.985547
35	7	0	-0.016334	-2.050303	0.512731

P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.361242	-3.004888	-0.256866
2	6	0	-1.380864	-2.099007	-0.067225
3	7	0	-1.672920	-0.764901	0.244906
4	6	0	-2.956839	-0.318930	0.330798
5	6	0	-3.951833	-1.229447	0.145795
6	6	0	-3.593172	-2.576768	-0.145755
7	7	0	-0.077400	-2.296506	-0.139565
8	6	0	0.502932	-1.095734	0.129198
9	6	0	-0.454356	-0.116993	0.369938
10	1	0	-3.097268	0.740357	0.509064
11	1	0	-4.989172	-0.928493	0.201488
12	1	0	-4.376940	-3.315081	-0.298764
13	7	0	-0.342601	1.232972	0.711943
14	6	0	-0.493985	1.635234	2.116562
15	1	0	-1.508082	1.454490	2.488654

16	1	0	0.213287	1.050795	2.709707
17	1	0	-0.262365	2.695935	2.206079
18	16	0	-0.633216	2.359375	-0.507680
19	8	0	-0.577876	3.666373	0.126637
20	8	0	-1.812490	1.954954	-1.260798
21	6	0	0.784406	2.141623	-1.563087
22	1	0	1.675294	2.439019	-1.011722
23	1	0	0.839507	1.092778	-1.857547
24	1	0	0.623990	2.778112	-2.434059
25	6	0	1.969444	-0.952497	0.113788
26	6	0	2.733268	-1.971915	-0.465961
27	6	0	2.621449	0.161078	0.658311
28	6	0	4.118467	-1.872275	-0.512082
29	1	0	2.218290	-2.836207	-0.871337
30	6	0	4.008257	0.256071	0.609123
31	1	0	2.044373	0.950555	1.128376
32	6	0	4.760938	-0.757345	0.021503
33	1	0	4.698858	-2.668707	-0.966841
34	1	0	4.502220	1.121301	1.039924
35	1	0	5.842869	-0.680759	-0.015214

R2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.334484	-2.484150	2.171508
2	6	0	1.700010	0.627019	0.386232
3	16	0	2.024936	-2.862166	-0.572035
4	79	0	-0.455716	0.348813	0.218801
5	8	0	0.877531	-2.320883	-1.266261
6	8	0	2.054795	-4.196569	-0.023193
7	6	0	3.499194	-2.516104	-1.499386
8	15	0	-2.743211	0.168328	-0.034780
9	8	0	-3.156495	-0.259800	-1.517862
10	8	0	-3.375571	-0.920809	0.951067
11	8	0	-3.500927	1.546665	0.259314
12	7	0	2.252873	-1.818980	0.850191
13	6	0	2.040775	-0.558419	0.682411
14	1	0	1.378166	-2.954051	2.405278
15	1	0	3.115174	-3.242750	2.138397
16	1	0	2.576117	-1.718678	2.906751
17	1	0	3.429881	-3.104438	-2.416422

18	1	0	3.517220	-1.450374	-1.731160
19	1	0	4.361039	-2.823162	-0.907406
20	6	0	-4.690100	-0.812194	1.526184
21	1	0	-5.457480	-0.990006	0.767436
22	1	0	-4.750390	-1.583278	2.291556
23	1	0	-4.822692	0.172679	1.978586
24	6	0	-4.697198	1.952618	-0.430250
25	1	0	-4.858725	2.995923	-0.166862
26	1	0	-4.560318	1.856637	-1.509260
27	1	0	-5.552972	1.356335	-0.101088
28	6	0	-4.262054	-1.126302	-1.827927
29	1	0	-5.210428	-0.595377	-1.703088
30	1	0	-4.138281	-1.412020	-2.870467
31	1	0	-4.235806	-2.014362	-1.193485
32	6	0	2.313956	1.890821	0.089888
33	6	0	1.688890	3.087886	-0.171542
34	16	0	4.041815	2.059641	0.004399
35	6	0	2.602342	4.138193	-0.441487
36	1	0	0.610343	3.200451	-0.162681
37	6	0	3.904364	3.723915	-0.381350
38	1	0	2.312093	5.155688	-0.667833
39	1	0	4.796022	4.314386	-0.541192

b-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.856455	-3.929372	1.720439
2	6	0	-3.726405	-3.465004	0.740963
3	6	0	-3.828201	-2.111259	0.481123
4	7	0	-3.085386	-1.215918	1.183070
5	6	0	-2.250468	-1.655495	2.158056
6	6	0	-2.113911	-2.997912	2.440599
7	7	0	-5.306522	0.236239	0.469678
8	6	0	-4.082563	0.791636	0.464654
9	7	0	-3.811684	2.067303	0.095760
10	6	0	-4.852255	2.809012	-0.263745
11	6	0	-6.163047	2.340921	-0.273802
12	6	0	-6.322900	1.016261	0.109056
13	7	0	-2.977538	0.117254	0.898516
14	6	0	-1.203133	2.277912	2.047595
15	6	0	-0.339775	-0.494249	-0.224591

16	16	0	-0.033214	2.986828	-0.356761
17	79	0	1.777966	-0.464373	-0.017881
18	8	0	0.545992	2.226512	-1.444201
19	8	0	0.781478	3.839446	0.484382
20	6	0	-1.460189	3.870771	-0.928499
21	15	0	4.074298	-0.245115	0.125142
22	8	0	4.673656	1.060355	-0.592757
23	8	0	4.510383	-0.137283	1.661226
24	8	0	4.948219	-1.395116	-0.544443
25	7	0	-0.716030	1.798844	0.744975
26	6	0	-0.805168	0.568570	0.343403
27	1	0	-2.766123	-4.989776	1.926079
28	1	0	-4.330796	-4.144314	0.152361
29	1	0	-4.488400	-1.700132	-0.263563
30	1	0	-1.712658	-0.870831	2.670226
31	1	0	-1.432870	-3.298177	3.227491
32	1	0	-4.629576	3.833873	-0.561297
33	1	0	-6.997256	2.963337	-0.567210
34	1	0	-7.307578	0.553399	0.128148
35	1	0	-0.997538	1.513540	2.795851
36	1	0	-0.653575	3.184382	2.301431
37	1	0	-2.277075	2.459498	1.971853
38	1	0	-1.084899	4.640049	-1.605853
39	1	0	-2.116608	3.159065	-1.427463
40	1	0	-1.958148	4.314076	-0.065408
41	6	0	5.900572	-0.024911	2.016046
42	1	0	5.929374	0.225269	3.074676
43	1	0	6.400428	-0.981918	1.848560
44	1	0	6.380519	0.767226	1.434851
45	6	0	3.960755	2.306526	-0.453738
46	1	0	3.790771	2.538179	0.601503
47	1	0	4.595187	3.069873	-0.900038
48	1	0	3.005870	2.253574	-0.984529
49	6	0	6.186283	-1.168172	-1.247027
50	1	0	6.029654	-0.465307	-2.065123
51	1	0	6.949775	-0.781769	-0.568516
52	1	0	6.488369	-2.140324	-1.630924
53	6	0	-1.013751	-1.485806	-1.036739
54	6	0	-0.771263	-2.835653	-1.100297
55	16	0	-2.272229	-1.027367	-2.143297
56	6	0	-1.626970	-3.507766	-2.016270
57	1	0	-0.007221	-3.319122	-0.501709
58	6	0	-2.480785	-2.653974	-2.656713
59	1	0	-1.594776	-4.572852	-2.208078

60	1	0	-3.201482	-2.889556	-3.427629

b-IN1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.468012	-2.598378	2.751082
2	6	0	-4.366786	-2.753910	1.374231
3	6	0	-3.764046	-1.764152	0.616909
4	7	0	-3.279484	-0.665317	1.228974
5	6	0	-3.405165	-0.467932	2.559481
6	6	0	-3.984540	-1.434582	3.351817
7	7	0	-4.798226	0.832409	-0.292770
8	6	0	-3.500540	1.121197	-0.312662
9	7	0	-2.882422	2.071839	-1.005172
10	6	0	-3.666376	2.796502	-1.802517
11	6	0	-5.039363	2.588894	-1.895247
12	6	0	-5.560444	1.581478	-1.094181
13	7	0	-2.661418	0.335560	0.483147
14	6	0	-0.133226	1.273221	2.511461
15	6	0	-0.466982	-0.582479	-0.082628
16	16	0	0.266717	2.605079	0.246468
17	79	0	1.601588	-0.564287	-0.001262
18	8	0	0.256827	2.214036	-1.150951
19	8	0	1.536750	2.764420	0.947878
20	6	0	-0.647417	4.119788	0.429022
21	15	0	3.938138	-0.408024	0.003672
22	8	0	4.566567	0.715352	-0.961845
23	8	0	4.457361	-0.046649	1.479152
24	8	0	4.759205	-1.693924	-0.475262
25	7	0	-0.676307	1.516504	1.163716
26	6	0	-1.209278	0.385039	0.480080
27	1	0	-4.932021	-3.370478	3.355560
28	1	0	-4.744397	-3.634922	0.870340
29	1	0	-3.665766	-1.802120	-0.460997
30	1	0	-3.032725	0.482404	2.919584
31	1	0	-4.069006	-1.266472	4.418098
32	1	0	-3.169393	3.571301	-2.381490
33	1	0	-5.665511	3.183591	-2.546853
34	1	0	-6.623924	1.357208	-1.088249
35	1	0	0.802348	0.703741	2.480830
36	1	0	0.047866	2.221051	3.019972

37	1	0	-0.874155	0.707238	3.078406
38	1	0	-0.094219	4.891488	-0.107726
39	1	0	-1.633878	3.960229	-0.001903
40	1	0	-0.704963	4.361470	1.490480
41	6	0	5.862752	0.091700	1.738353
42	1	0	5.955618	0.513873	2.737265
43	1	0	6.343210	-0.889671	1.706238
44	1	0	6.321555	0.764844	1.008586
45	6	0	3.915646	2.001671	-1.009117
46	1	0	3.827512	2.427144	-0.007050
47	1	0	4.540759	2.632090	-1.639064
48	1	0	2.916400	1.903780	-1.444873
49	6	0	5.963751	-1.637866	-1.258607
50	1	0	6.246452	-2.673299	-1.440022
51	1	0	5.775949	-1.124204	-2.201836
52	1	0	6.760645	-1.124718	-0.715668
53	6	0	-1.119205	-1.626253	-0.884654
54	6	0	-1.160219	-2.979992	-0.669603
55	16	0	-2.000270	-1.204053	-2.325946
56	6	0	-1.945282	-3.676784	-1.637607
57	1	0	-0.646703	-3.452237	0.160206
58	6	0	-2.461508	-2.847172	-2.590247
59	1	0	-2.094130	-4.749679	-1.638746
60	1	0	-3.039434	-3.113819	-3.464022

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.038876	0.147816	2.503564
2	6	0	-2.252454	0.360623	1.461167
3	7	0	-1.015303	0.875819	1.498896
4	6	0	-0.451808	1.101790	2.681421
5	6	0	-1.177546	0.876502	3.841549
6	6	0	-2.487513	0.418523	3.688262
7	6	0	-0.610280	-1.334857	-2.548357
8	6	0	-0.519240	1.017553	-0.189588
9	16	0	-0.461964	-2.355954	-0.121503
10	79	0	1.508995	0.486074	-0.211673
11	8	0	-0.962805	-2.000543	1.211542
12	8	0	0.981017	-2.531938	-0.310785
13	6	0	-1.216184	-3.910027	-0.580577

14	15	0	3.703706	-0.293000	0.009531
15	8	0	4.844314	0.808084	-0.138629
16	8	0	4.034801	-0.911762	1.452430
17	8	0	4.121885	-1.521897	-0.942945
18	7	0	-1.158285	-1.249920	-1.188710
19	6	0	-1.487420	0.103354	-0.789052
20	1	0	0.567422	1.479240	2.670599
21	1	0	-0.754244	1.068410	4.817945
22	1	0	-3.120430	0.250282	4.555298
23	1	0	0.346390	-0.804471	-2.633242
24	1	0	-0.459126	-2.376699	-2.844984
25	1	0	-1.330593	-0.868635	-3.219278
26	1	0	-2.299698	-3.806635	-0.532681
27	1	0	-0.895212	-4.191102	-1.582759
28	1	0	-0.861289	-4.645846	0.142507
29	6	0	3.504081	-1.660804	-2.230538
30	1	0	3.598323	-0.739810	-2.813954
31	1	0	4.035676	-2.464072	-2.738289
32	1	0	2.452770	-1.930772	-2.101454
33	6	0	3.205386	-1.980664	1.934614
34	1	0	3.239896	-2.827963	1.246807
35	1	0	3.607360	-2.262183	2.906426
36	1	0	2.167508	-1.644229	2.037706
37	6	0	6.226110	0.453751	0.076942
38	1	0	6.809253	1.321526	-0.223858
39	1	0	6.387539	0.232980	1.132869
40	1	0	6.491724	-0.410711	-0.534994
41	7	0	-2.595723	0.118691	0.153087
42	6	0	-4.079029	-1.685001	0.466355
43	6	0	-4.548883	0.025235	-1.109327
44	6	0	-5.254228	-2.335679	0.134456
45	1	0	-3.351943	-2.032728	1.192760
46	6	0	-5.717157	-0.606420	-1.479154
47	1	0	-4.164851	0.950330	-1.525572
48	6	0	-6.080842	-1.796498	-0.846023
49	1	0	-5.501661	-3.261965	0.638132
50	1	0	-6.336781	-0.160785	-2.247334
51	1	0	-7.001317	-2.300128	-1.120642
52	7	0	-3.778283	-0.520371	-0.144102
53	6	0	-0.805191	2.463366	-0.414835
54	6	0	-0.196038	3.561365	0.131769
55	16	0	-2.063252	2.951161	-1.511359
56	6	0	-0.760068	4.796338	-0.301732
57	1	0	0.645119	3.486388	0.813619

58	6	0	-1.779442	4.619047	-1.189578
59	1	0	-0.405813	5.768921	0.016128
60	1	0	-2.350666	5.377725	-1.705447

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.182872	0.465982	2.572840
2	6	0	-2.370650	0.394474	1.529499
3	7	0	-1.309786	1.213114	1.322001
4	6	0	-0.980627	2.114528	2.259750
5	6	0	-1.759602	2.221743	3.393000
6	6	0	-2.877616	1.382212	3.487140
7	6	0	-0.677931	-1.196893	-2.607412
8	6	0	-0.687614	1.020733	-0.053670
9	16	0	0.024779	-2.501122	-0.473878
10	79	0	1.390447	0.613262	0.078300
11	8	0	1.440902	-2.225860	-0.773059
12	8	0	-0.485814	-3.813718	-0.840001
13	6	0	-0.199979	-2.289313	1.285766
14	15	0	3.571092	-0.238388	0.227028
15	8	0	4.674994	0.797586	0.751523
16	8	0	3.653212	-1.461642	1.261475
17	8	0	4.198135	-0.886963	-1.103382
18	7	0	-1.014135	-1.326285	-1.183502
19	6	0	-1.521685	-0.155982	-0.566419
20	1	0	-0.116411	2.732180	2.037784
21	1	0	-1.527815	2.944534	4.163096
22	1	0	-3.549471	1.447996	4.338109
23	1	0	0.175009	-0.524507	-2.766006
24	1	0	-0.448136	-2.180473	-3.025920
25	1	0	-1.546027	-0.781389	-3.121356
26	1	0	0.060320	-1.273026	1.587075
27	1	0	-1.223152	-2.552319	1.549416
28	1	0	0.502246	-2.996828	1.730572
29	6	0	3.633034	-0.594019	-2.390740
30	1	0	3.551058	0.486258	-2.543461
31	1	0	4.319707	-1.011251	-3.125500
32	1	0	2.654520	-1.072151	-2.473348
33	6	0	4.110917	-2.775589	0.893687
34	1	0	4.003658	-3.385102	1.790332

35	1	0	3.495290	-3.170673	0.084726
36	1	0	5.159765	-2.745899	0.590711
37	6	0	6.016150	0.339401	0.997008
38	1	0	6.596043	1.217789	1.272929
39	1	0	6.015637	-0.381626	1.817930
40	1	0	6.430657	-0.112693	0.092580
41	7	0	-2.447410	-0.487608	0.495094
42	6	0	-4.369767	-1.761780	1.122082
43	6	0	-4.092150	-1.019874	-1.112529
44	6	0	-5.531405	-2.416974	0.778548
45	1	0	-3.947663	-1.755436	2.116605
46	6	0	-5.258779	-1.660102	-1.483467
47	1	0	-3.420162	-0.457862	-1.756848
48	6	0	-5.989648	-2.373142	-0.539044
49	1	0	-6.059770	-2.970811	1.544587
50	1	0	-5.570224	-1.610351	-2.519716
51	1	0	-6.888234	-2.907811	-0.825004
52	7	0	-3.699245	-1.051435	0.180173
53	6	0	-0.921176	2.299053	-0.808300
54	6	0	-0.178008	3.449429	-0.824807
55	16	0	-2.378004	2.492292	-1.740674
56	6	0	-0.786305	4.501847	-1.573416
57	1	0	0.788888	3.531875	-0.337885
58	6	0	-1.977984	4.126834	-2.117196
59	1	0	-0.342550	5.479165	-1.717152
60	1	0	-2.625603	4.708749	-2.758087

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.086153	3.510742	-0.824855
2	6	0	-1.401093	2.273386	-0.432700
3	7	0	-1.529159	1.231798	-1.319218
4	6	0	-1.374724	1.410841	-2.648949
5	6	0	-1.061918	2.668632	-3.088671
6	6	0	-0.919515	3.690551	-2.119387
7	6	0	-2.503093	-1.561443	1.824597
8	6	0	-1.764721	0.015903	-0.576972
9	16	0	-1.373390	0.388553	3.357566
10	8	0	-0.008565	0.752131	3.004998
11	8	0	-1.619354	-0.671125	4.312685

12	6	0	-2.279600	1.837465	3.831145
13	15	0	2.465978	-1.605445	-0.159608
14	8	0	2.575964	-3.158223	0.200572
15	8	0	3.267300	-1.372858	-1.523402
16	8	0	3.415726	-0.833645	0.876071
17	7	0	-2.171694	-0.133107	1.907815
18	6	0	-1.889496	0.576584	0.773155
19	1	0	-1.507896	0.534483	-3.275750
20	1	0	-0.928750	2.870888	-4.142670
21	1	0	-0.662030	4.698818	-2.433819
22	1	0	-1.675881	-2.134102	1.384024
23	1	0	-2.695871	-1.923613	2.831758
24	1	0	-3.397630	-1.683203	1.214391
25	1	0	-2.177986	2.578548	3.039982
26	1	0	-3.316011	1.542412	3.993042
27	1	0	-1.826343	2.176336	4.764647
28	6	0	2.926614	-0.583472	2.209778
29	1	0	2.739162	-1.528158	2.727204
30	1	0	3.714307	-0.033466	2.721039
31	1	0	2.011539	0.014138	2.176248
32	6	0	4.624599	-0.891677	-1.577903
33	1	0	4.915135	-0.948437	-2.625468
34	1	0	4.664103	0.140224	-1.223701
35	1	0	5.286519	-1.513116	-0.971817
36	6	0	3.863153	-3.803918	0.241039
37	1	0	3.696722	-4.793776	0.660733
38	1	0	4.262363	-3.891291	-0.772222
39	1	0	4.550286	-3.240041	0.877570
40	7	0	-1.618593	1.877200	0.830926
41	79	0	0.301527	-0.829745	-0.284732
42	6	0	1.595745	2.570433	0.718865
43	6	0	2.260741	1.940001	-1.387008
44	6	0	2.424812	3.688635	0.694326
45	1	0	0.963737	2.349327	1.576749
46	6	0	3.113638	3.032752	-1.505191
47	1	0	2.174395	1.209128	-2.190804
48	6	0	3.193633	3.926059	-0.439788
49	1	0	2.456047	4.357955	1.546240
50	1	0	3.696253	3.176791	-2.408433
51	1	0	3.845915	4.791722	-0.493158
52	7	0	1.510233	1.711291	-0.303791
53	6	0	-2.692241	-0.947023	-1.216826
54	6	0	-2.429591	-2.176995	-1.757334
55	16	0	-4.377829	-0.544523	-1.387498

56	6	0	-3.585824	-2.806118	-2.302993
57	1	0	-1.439605	-2.621339	-1.748058
58	6	0	-4.705462	-2.038693	-2.172408
59	1	0	-3.582757	-3.782815	-2.769303
60	1	0	-5.711503	-2.267515	-2.495755

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.416779	-0.911853	-3.158357
2	6	0	-5.049149	0.431608	-3.093261
3	6	0	-4.385347	0.901456	-1.981252
4	7	0	-4.068884	0.081876	-0.946686
5	6	0	-4.397277	-1.232697	-1.005115
6	6	0	-5.080600	-1.741031	-2.096931
7	7	0	-4.724343	-0.435060	1.612556
8	6	0	-3.619744	0.275002	1.328960
9	7	0	-2.729148	0.725639	2.238930
10	6	0	-3.000933	0.465064	3.511545
11	6	0	-4.128605	-0.243994	3.919708
12	6	0	-4.964276	-0.677575	2.899762
13	7	0	-3.310194	0.644936	0.041453
14	6	0	-1.626534	3.193157	0.289790
15	6	0	-0.984069	0.143515	-0.259102
16	16	0	1.027462	3.499662	-0.182847
17	79	0	1.654178	0.028779	-0.117899
18	8	0	2.211966	2.683788	0.053658
19	8	0	0.810896	4.726152	0.550190
20	6	0	0.946005	3.841617	-1.928640
21	15	0	3.648186	-1.093135	-0.045069
22	8	0	4.950450	-0.177947	0.149120
23	8	0	3.647821	-2.119793	1.181273
24	8	0	4.035590	-1.898651	-1.363161
25	7	0	-0.329217	2.520803	0.097950
26	6	0	-0.262754	1.180309	-0.118284
27	1	0	-5.951659	-1.298651	-4.018172
28	1	0	-5.286474	1.124413	-3.891315
29	1	0	-4.083024	1.929466	-1.835356
30	1	0	-4.106745	-1.834710	-0.157226
31	1	0	-5.329988	-2.795327	-2.101116
32	1	0	-2.281643	0.837428	4.238036

33	1	0	-4.335145	-0.448991	4.961524
34	1	0	-5.866419	-1.245631	3.117742
35	1	0	-1.432183	4.211539	0.622215
36	1	0	-2.199752	3.188480	-0.641403
37	1	0	-2.169167	2.642980	1.056358
38	1	0	1.794705	4.482988	-2.170143
39	1	0	1.010831	2.895884	-2.468295
40	1	0	0.008302	4.358560	-2.135484
41	6	0	4.785176	-2.969058	1.418685
42	1	0	4.648409	-3.398288	2.409118
43	1	0	4.810189	-3.765446	0.670921
44	1	0	5.710191	-2.386610	1.390853
45	6	0	4.925192	0.852853	1.157698
46	1	0	4.772623	0.409605	2.145253
47	1	0	5.898549	1.337821	1.116714
48	1	0	4.136581	1.578216	0.937602
49	6	0	5.381276	-2.042982	-1.859981
50	1	0	5.286652	-2.548957	-2.818704
51	1	0	5.841403	-1.063507	-1.988853
52	1	0	5.982176	-2.648769	-1.178538
53	6	0	-1.296538	-1.229909	-0.348011
54	6	0	-1.480435	-1.976389	-1.495826
55	16	0	-1.468797	-2.222207	1.076480
56	6	0	-1.747403	-3.342096	-1.226668
57	1	0	-1.404465	-1.541164	-2.485543
58	6	0	-1.773104	-3.609554	0.117314
59	1	0	-1.908364	-4.093738	-1.988684
60	1	0	-1.952924	-4.563788	0.594181

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.098934	2.351565	2.234860
2	6	0	-4.053278	1.544510	2.668884
3	6	0	-3.269731	0.881068	1.740398
4	7	0	-3.528519	1.045503	0.430444
5	6	0	-4.524133	1.832078	-0.026044
6	6	0	-5.339049	2.492401	0.868050
7	7	0	-4.414950	-1.212102	-0.519287
8	6	0	-3.333219	-0.728932	-1.120034
9	7	0	-2.778566	-1.139304	-2.256777

10	6	0	-3.352238	-2.198072	-2.819683
11	6	0	-4.478832	-2.819832	-2.283245
12	6	0	-4.986849	-2.261131	-1.120926
13	7	0	-2.734291	0.405679	-0.529073
14	6	0	-0.379577	-2.666209	-1.072781
15	6	0	-0.432421	-0.408349	-0.195431
16	16	0	-0.834224	-2.347128	1.496162
17	79	0	1.614825	-0.146035	-0.139506
18	8	0	0.461825	-2.968973	1.712190
19	8	0	-1.268283	-1.270786	2.385167
20	6	0	-2.091791	-3.608225	1.518683
21	15	0	3.958554	0.072611	-0.052953
22	8	0	4.498216	0.539129	1.390413
23	8	0	4.562131	1.145432	-1.091080
24	8	0	4.722271	-1.307582	-0.372989
25	7	0	-0.984621	-1.751825	-0.083849
26	6	0	-1.314124	0.596800	-0.361952
27	1	0	-5.722072	2.873198	2.953321
28	1	0	-3.837005	1.410478	3.721436
29	1	0	-2.441458	0.218545	1.988345
30	1	0	-4.608661	1.896231	-1.103601
31	1	0	-6.136903	3.120417	0.492263
32	1	0	-2.900779	-2.552962	-3.743430
33	1	0	-4.941962	-3.674408	-2.758579
34	1	0	-5.877361	-2.660620	-0.641944
35	1	0	0.673842	-2.867008	-0.847691
36	1	0	-0.939115	-3.605148	-1.099579
37	1	0	-0.465225	-2.181797	-2.045187
38	1	0	-3.038605	-3.146691	1.237531
39	1	0	-1.817244	-4.415965	0.841354
40	1	0	-2.125056	-3.979303	2.544122
41	6	0	5.708178	0.057833	1.988345
42	1	0	5.664668	0.339214	3.039070
43	1	0	5.771215	-1.028919	1.900392
44	1	0	6.582168	0.525393	1.523461
45	6	0	5.722534	1.942343	-0.823522
46	1	0	5.638270	2.418003	0.156203
47	1	0	6.631689	1.334520	-0.868237
48	1	0	5.758332	2.702811	-1.601903
49	6	0	5.992412	-1.380684	-1.031947
50	1	0	6.795463	-1.044309	-0.368400
51	1	0	6.147896	-2.428698	-1.282307
52	1	0	5.982809	-0.779826	-1.944186
53	6	0	-0.940372	2.015724	-0.362739

54	6	0	-0.113252	2.666183	0.514273
55	16	0	-1.584129	3.115548	-1.543629
56	6	0	0.019037	4.056332	0.225102
57	1	0	0.362546	2.159225	1.346695
58	6	0	-0.725563	4.438347	-0.850733
59	1	0	0.628122	4.740268	0.802368
60	1	0	-0.816819	5.424346	-1.283897

b-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.838009	2.510777	-0.224322
2	6	0	5.212593	2.642745	1.012046
3	6	0	4.026639	1.977555	1.248975
4	7	0	3.506503	1.174242	0.293900
5	6	0	4.069709	1.051774	-0.924697
6	6	0	5.249576	1.710998	-1.200809
7	7	0	3.072882	-0.365924	2.591493
8	6	0	2.201797	-0.327292	1.590894
9	7	0	1.139059	-1.127885	1.451430
10	6	0	0.866555	-2.007425	2.415360
11	6	0	1.707786	-2.117991	3.509255
12	6	0	2.823082	-1.275376	3.530541
13	7	0	2.274812	0.560714	0.544986
14	6	0	1.296061	0.363456	-0.490096
15	6	0	0.527857	-0.876479	-0.261996
16	79	0	-1.556179	-0.511621	-0.099166
17	15	0	-3.798435	0.088960	0.164779
18	8	0	-4.817279	-0.478273	-0.925923
19	8	0	-4.081059	1.671188	0.037345
20	8	0	-4.361566	-0.329860	1.607844
21	1	0	6.761081	3.040442	-0.431492
22	1	0	5.619785	3.275933	1.790159
23	1	0	3.461251	2.046332	2.167008
24	1	0	3.518208	0.424806	-1.609505
25	1	0	5.694932	1.594211	-2.180834
26	1	0	-0.016901	-2.624287	2.275106
27	1	0	1.524405	-2.837660	4.295225
28	1	0	3.541949	-1.329070	4.343639
29	7	0	0.884600	-2.121084	-0.829617
30	6	0	-0.135058	-3.159195	-1.032010

31	1	0	-0.618352	-3.399598	-0.081987
32	1	0	-0.895605	-2.808085	-1.736687
33	1	0	0.338478	-4.062337	-1.413085
34	16	0	2.434866	-2.440510	-1.398307
35	8	0	2.571392	-3.876194	-1.546053
36	8	0	3.376112	-1.702285	-0.562504
37	6	0	2.426241	-1.713999	-3.026918
38	1	0	1.734519	-2.290764	-3.642165
39	1	0	2.093008	-0.678450	-2.932194
40	1	0	3.438324	-1.788744	-3.428292
41	6	0	-5.735864	-0.089449	1.953647
42	1	0	-5.828107	-0.289573	3.019460
43	1	0	-6.006120	0.950074	1.746572
44	1	0	-6.381068	-0.770329	1.392890
45	6	0	-3.210033	2.565509	0.750420
46	1	0	-2.164031	2.379025	0.483276
47	1	0	-3.484022	3.573045	0.442747
48	1	0	-3.353999	2.451164	1.828597
49	6	0	-5.930906	0.260287	-1.460940
50	1	0	-6.666532	0.473272	-0.682177
51	1	0	-5.584861	1.193936	-1.904682
52	1	0	-6.372556	-0.381992	-2.220447
53	6	0	0.589509	1.591960	-0.809576
54	6	0	-0.278873	1.846889	-1.848786
55	16	0	0.780810	3.040206	0.168750
56	6	0	-0.784571	3.183411	-1.854987
57	1	0	-0.496753	1.111201	-2.614730
58	6	0	-0.282745	3.953153	-0.850515
59	1	0	-1.463041	3.565184	-2.608800
60	1	0	-0.440174	5.005859	-0.666155

b-IN5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.898478	2.157992	-1.060278
2	6	0	-5.224987	1.874901	-2.251465
3	6	0	-4.007115	1.237219	-2.211761
4	7	0	-3.491832	0.846916	-1.016904
5	6	0	-4.092343	1.148482	0.155046
6	6	0	-5.316429	1.788731	0.146651
7	7	0	-2.785325	-1.412195	-2.553096

8	6	0	-2.049882	-0.918663	-1.575776
9	7	0	-1.039069	-1.568313	-0.960502
10	6	0	-0.684412	-2.795058	-1.383721
11	6	0	-1.379484	-3.361865	-2.424344
12	6	0	-2.452366	-2.629867	-2.965409
13	7	0	-2.176481	0.322775	-1.009603
14	6	0	-1.322690	0.420509	0.118416
15	6	0	-0.526765	-0.846510	0.260179
16	79	0	1.546752	-0.366986	0.040363
17	15	0	3.786015	0.228125	-0.347264
18	8	0	4.611163	0.422530	1.018859
19	8	0	3.950288	1.607540	-1.154742
20	8	0	4.611900	-0.866723	-1.189730
21	1	0	-6.846973	2.682161	-1.077381
22	1	0	-5.629757	2.163983	-3.213368
23	1	0	-3.409217	1.001349	-3.080499
24	1	0	-3.553849	0.831533	1.036639
25	1	0	-5.793217	2.004509	1.094742
26	1	0	0.125870	-3.270608	-0.841690
27	1	0	-1.126882	-4.346564	-2.792614
28	1	0	-3.058982	-3.047803	-3.763387
29	7	0	-0.787047	-1.753603	1.393467
30	6	0	0.278710	-2.126856	2.327098
31	1	0	1.092958	-2.603776	1.777173
32	1	0	0.681978	-1.259095	2.863966
33	1	0	-0.118684	-2.851210	3.038997
34	16	0	-2.348275	-1.895234	1.967880
35	8	0	-2.457685	-3.147351	2.692205
36	8	0	-3.228291	-1.629492	0.830143
37	6	0	-2.529712	-0.576141	3.158647
38	1	0	-1.892462	-0.809505	4.013244
39	1	0	-2.226812	0.371647	2.705964
40	1	0	-3.574334	-0.564201	3.475082
41	6	0	6.003393	-1.147001	-0.979006
42	1	0	6.221367	-2.054351	-1.539502
43	1	0	6.626155	-0.329693	-1.355813
44	1	0	6.200637	-1.310443	0.082783
45	6	0	5.012950	1.881792	-2.077584
46	1	0	4.720685	2.777559	-2.622640
47	1	0	5.950251	2.070567	-1.544970
48	1	0	5.136168	1.049046	-2.773832
49	6	0	5.637061	1.407967	1.204407
50	1	0	5.830142	1.450692	2.274790
51	1	0	6.553318	1.116103	0.681654

52	1	0	5.294991	2.382802	0.850273
53	6	0	-0.962396	1.673613	0.659672
54	6	0	-0.158662	1.921335	1.767325
55	16	0	-1.533820	3.189892	-0.014084
56	6	0	0.004783	3.311060	2.034380
57	1	0	0.258622	1.129562	2.379524
58	6	0	-0.681711	4.118429	1.181199
59	1	0	0.596263	3.695231	2.857023
60	1	0	-0.765835	5.194475	1.183892

b-IN6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.915903	3.343536	0.969584
2	6	0	-1.188553	2.063845	0.723147
3	7	0	-1.261989	1.564018	-0.551725
4	6	0	-1.175840	2.363563	-1.630930
5	6	0	-0.937843	3.697244	-1.418576
6	6	0	-0.790819	4.130768	-0.083632
7	7	0	-1.419760	1.110379	1.656285
8	6	0	-1.684874	0.000660	0.992605
9	6	0	-1.469619	0.118272	-0.461601
10	15	0	2.811902	-1.277717	-0.421924
11	8	0	3.361322	-1.192825	1.078039
12	8	0	3.769044	-0.277333	-1.240985
13	8	0	3.169390	-2.756148	-0.930761
14	1	0	-1.323535	1.904473	-2.602860
15	1	0	-0.873358	4.389146	-2.247186
16	1	0	-0.574338	5.175882	0.123974
17	7	0	-2.365446	-0.465860	-1.388684
18	6	0	-1.884526	-1.081668	-2.631055
19	1	0	-1.289835	-0.392425	-3.239476
20	1	0	-1.278774	-1.957501	-2.384705
21	1	0	-2.739307	-1.398688	-3.230113
22	16	0	-3.932701	0.198860	-1.427144
23	8	0	-4.159598	0.715936	-2.765858
24	8	0	-4.008737	1.061806	-0.260814
25	6	0	-4.977405	-1.216531	-1.166142
26	1	0	-4.802595	-1.943516	-1.959833
27	1	0	-4.740470	-1.628029	-0.184477
28	1	0	-6.006784	-0.856838	-1.205206

29	6	0	4.364067	-3.430331	-0.496432
30	1	0	4.339842	-4.417419	-0.954162
31	1	0	5.257315	-2.893703	-0.830708
32	1	0	4.365243	-3.520253	0.591420
33	6	0	4.623444	-0.662533	-2.326871
34	1	0	4.582064	0.137065	-3.065402
35	1	0	5.647243	-0.766100	-1.958037
36	1	0	4.291545	-1.600181	-2.777934
37	6	0	4.593367	-0.536936	1.422033
38	1	0	4.678710	-0.613898	2.504534
39	1	0	5.444174	-1.035955	0.949508
40	1	0	4.555060	0.509657	1.115743
41	79	0	0.574807	-0.694257	-0.511206
42	6	0	1.835852	1.695529	1.922139
43	6	0	2.440871	2.667904	-0.065404
44	6	0	1.917612	2.907515	2.600275
45	1	0	1.549071	0.782309	2.440378
46	6	0	2.558030	3.922652	0.525858
47	1	0	2.648482	2.524694	-1.123864
48	6	0	2.290030	4.041881	1.886845
49	1	0	1.686824	2.955670	3.657943
50	1	0	2.857080	4.779851	-0.067455
51	1	0	2.369374	5.003879	2.382876
52	7	0	2.092310	1.570847	0.614229
53	6	0	-2.112197	-1.206394	1.655610
54	6	0	-2.289757	-2.466011	1.120461
55	16	0	-2.493470	-1.171883	3.342029
56	6	0	-2.739546	-3.402749	2.081637
57	1	0	-2.088354	-2.698282	0.080363
58	6	0	-2.891657	-2.834711	3.320709
59	1	0	-2.938610	-4.445742	1.872621
60	1	0	-3.225306	-3.317391	4.229169

P3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.216712	-2.113843	0.148032
2	6	0	2.057353	-1.437360	0.237614
3	7	0	1.997740	-0.043716	0.023225
4	6	0	3.134550	0.669709	-0.225607
5	6	0	4.310242	-0.010395	-0.306666

6	6	0	4.294701	-1.422823	-0.123486
7	6	0	-1.694087	-1.852783	1.881999
8	6	0	0.682479	0.339606	0.188423
9	16	0	-2.322198	-1.094965	-0.608110
10	8	0	-1.872703	-0.074941	-1.536150
11	8	0	-3.692707	-1.142823	-0.131211
12	6	0	-1.909330	-2.692069	-1.297108
13	7	0	-1.346404	-0.961763	0.766662
14	6	0	0.034492	-0.845057	0.497501
15	1	0	3.024431	1.742368	-0.326664
16	1	0	5.235285	0.515913	-0.499981
17	1	0	5.223918	-1.982522	-0.199885
18	1	0	-2.776926	-1.842297	1.999502
19	1	0	-1.327545	-2.872577	1.723452
20	1	0	-1.230551	-1.450390	2.784163
21	1	0	-2.238223	-3.466184	-0.603627
22	1	0	-2.442646	-2.776168	-2.244476
23	1	0	-0.829949	-2.736630	-1.446428
24	7	0	0.860840	-1.919269	0.520276
25	6	0	0.197933	1.697480	0.033657
26	6	0	0.588504	2.644162	-0.880090
27	16	0	-1.057921	2.304315	1.059719
28	6	0	-0.119900	3.870830	-0.741803
29	1	0	1.316884	2.453306	-1.659601
30	6	0	-1.038069	3.828341	0.265250
31	1	0	0.036506	4.734691	-1.375240
32	1	0	-1.721427	4.605283	0.576463

P4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.959558	-3.196821	-0.263678
2	6	0	-1.105223	-2.173623	-0.071822
3	7	0	-1.568604	-0.885932	0.238113
4	6	0	-2.899231	-0.612301	0.331836
5	6	0	-3.767001	-1.645744	0.147822
6	6	0	-3.237172	-2.932967	-0.149503
7	7	0	0.214973	-2.203218	-0.136974
8	6	0	0.626664	-0.936100	0.129215
9	6	0	-0.444992	-0.084709	0.360220
10	1	0	-3.173430	0.419609	0.515372

11	1	0	-4.834413	-1.483430	0.210621
12	1	0	-3.918676	-3.766452	-0.304075
13	7	0	-0.478931	1.261971	0.718508
14	6	0	-0.505859	1.638946	2.137863
15	1	0	-1.444382	1.341739	2.616570
16	1	0	0.327552	1.137431	2.635462
17	1	0	-0.386981	2.718917	2.217811
18	16	0	-0.938641	2.368406	-0.462249
19	8	0	-0.977602	3.666766	0.189983
20	8	0	-2.110104	1.854185	-1.159015
21	6	0	0.429027	2.306502	-1.601512
22	1	0	1.308437	2.719345	-1.109523
23	1	0	0.594035	1.266771	-1.888062
24	1	0	0.142325	2.903753	-2.467594
25	6	0	2.039886	-0.591818	0.148379
26	6	0	2.653972	0.572194	0.541957
27	16	0	3.197133	-1.762876	-0.388214
28	6	0	4.069216	0.519392	0.404506
29	1	0	2.110541	1.428219	0.924571
30	6	0	4.497117	-0.679511	-0.088881
31	1	0	4.734028	1.333342	0.664989
32	1	0	5.513157	-0.988910	-0.288747

b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.664381	0.687812	-0.088070
2	6	0	-2.551676	1.333982	-0.615599
3	6	0	-1.309510	0.732930	-0.594767
4	7	0	-1.124918	-0.504919	-0.038887
5	6	0	-2.218176	-1.152079	0.468453
6	6	0	-3.472241	-0.583772	0.447354
7	6	0	1.196242	-0.507530	-0.022692
8	7	0	2.244952	-1.152263	-0.559211
9	6	0	3.430347	-0.556912	-0.465602
10	6	0	3.613197	0.674432	0.152988
11	7	0	0.010323	-1.208171	-0.049247
12	1	0	-4.642988	1.151136	-0.102327
13	1	0	-2.633049	2.314531	-1.070670
14	1	0	-0.429808	1.184101	-1.030787
15	1	0	-1.988335	-2.129291	0.869839

16	1	0	-4.295346	-1.149648	0.868056
17	1	0	4.274910	-1.085568	-0.903231
18	1	0	4.590785	1.142722	0.212474
19	6	0	1.400158	0.734097	0.636879
20	1	0	0.573160	1.243192	1.128030
21	7	0	2.584915	1.315506	0.720911

c-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.205438	-3.040957	2.666201
2	6	0	-4.223357	-2.923850	1.279733
3	6	0	-3.862991	-1.732684	0.680319
4	7	0	-3.515831	-0.654995	1.429199
5	6	0	-3.499134	-0.754093	2.780442
6	6	0	-3.827186	-1.933477	3.419463
7	6	0	-3.759306	1.046357	-0.152115
8	7	0	-3.124364	2.028421	-0.814857
9	6	0	-3.756745	2.581446	-1.850605
10	6	0	-5.023994	2.183440	-2.253334
11	7	0	-3.046973	0.525419	0.902994
12	6	0	-0.829390	1.965763	2.569722
13	6	0	-0.404325	-0.484421	-0.084484
14	16	0	0.269283	2.971233	0.240883
15	79	0	1.727637	-0.580438	-0.024088
16	6	0	-1.185982	-1.377935	-0.947659
17	6	0	-1.955673	-0.845644	-1.990220
18	6	0	-2.728897	-1.688991	-2.783077
19	6	0	-2.737683	-3.063649	-2.543215
20	6	0	-1.943044	-3.598106	-1.529249
21	6	0	-1.154783	-2.761756	-0.744589
22	8	0	0.488119	2.415680	-1.076407
23	8	0	1.381261	3.412035	1.062906
24	6	0	-0.987399	4.220818	0.202409
25	15	0	4.037375	-0.519327	-0.067169
26	8	0	4.669160	0.816689	-0.693986
27	8	0	4.606875	-0.618714	1.425040
28	8	0	4.765182	-1.641575	-0.930813
29	7	0	-0.494255	1.698954	1.168157
30	6	0	-0.733187	0.562470	0.580926
31	1	0	-4.477034	-3.972779	3.148662

32	1	0	-4.492630	-3.756651	0.641173
33	1	0	-3.823358	-1.599125	-0.393787
34	1	0	-3.221580	0.159109	3.289004
35	1	0	-3.798471	-1.965965	4.501751
36	1	0	-3.227584	3.372269	-2.378400
37	1	0	-5.518644	2.631250	-3.108423
38	1	0	-0.159591	2.740700	2.945647
39	1	0	-1.876376	2.271568	2.635678
40	1	0	-0.667186	1.050740	3.141271
41	1	0	-1.938347	0.225230	-2.163749
42	1	0	-3.327677	-1.271112	-3.585992
43	1	0	-3.344409	-3.717705	-3.160715
44	1	0	-1.926944	-4.669644	-1.358232
45	1	0	-0.527662	-3.171560	0.042201
46	1	0	-0.632808	4.989662	-0.486385
47	1	0	-1.897541	3.732737	-0.153846
48	1	0	-1.097593	4.631633	1.206288
49	6	0	6.027393	-0.650611	1.654072
50	1	0	6.168378	-0.564079	2.729511
51	1	0	6.434747	-1.601266	1.301969
52	1	0	6.513248	0.187214	1.146802
53	6	0	4.035318	2.077418	-0.390893
54	1	0	3.895676	2.195522	0.686967
55	1	0	4.704470	2.850114	-0.764609
56	1	0	3.067952	2.140408	-0.897366
57	6	0	5.938549	-1.411278	-1.734713
58	1	0	5.741587	-0.632116	-2.471075
59	1	0	6.785713	-1.121904	-1.109314
60	1	0	6.146166	-2.358881	-2.227597
61	6	0	-5.080685	0.693727	-0.535528
62	1	0	-5.654054	-0.038481	0.027336
63	7	0	-5.689734	1.246637	-1.568917

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.968649	-3.302619	1.869870
2	6	0	-4.440532	-2.775856	0.671893
3	6	0	-4.004322	-1.531091	0.260511
4	7	0	-3.153068	-0.824380	1.035835
5	6	0	-2.684120	-1.310334	2.204903

6	6	0	-3.076715	-2.558481	2.640583
7	6	0	-3.584099	1.313355	0.058249
8	7	0	-3.164447	2.053233	-0.957437
9	6	0	-4.037472	2.940447	-1.441991
10	6	0	-5.322901	3.068685	-0.924653
11	7	0	-2.657427	0.398876	0.598986
12	6	0	-0.423048	1.766957	2.308566
13	6	0	-0.490971	-0.531916	-0.122030
14	16	0	0.264220	2.647223	-0.123272
15	79	0	1.572578	-0.497277	-0.007746
16	6	0	-1.172306	-1.631905	-0.836716
17	6	0	-1.062711	-2.965254	-0.421860
18	6	0	-1.750003	-3.971947	-1.094105
19	6	0	-2.527507	-3.668424	-2.212331
20	6	0	-2.607872	-2.350418	-2.659000
21	6	0	-1.943327	-1.335567	-1.972612
22	8	0	0.202433	2.128058	-1.476165
23	8	0	1.548752	2.810134	0.547382
24	6	0	-0.575551	4.216268	-0.078531
25	15	0	3.908871	-0.339566	0.063120
26	8	0	4.578362	0.601559	-1.058709
27	8	0	4.373863	0.272896	1.472399
28	8	0	4.743630	-1.686905	-0.152794
29	7	0	-0.722686	1.703288	0.876791
30	6	0	-1.219701	0.475796	0.380306
31	1	0	-4.288389	-4.284869	2.199711
32	1	0	-5.118039	-3.327664	0.032432
33	1	0	-4.288716	-1.070010	-0.675602
34	1	0	-1.987332	-0.669502	2.730080
35	1	0	-2.688556	-2.931997	3.579905
36	1	0	-3.700043	3.553686	-2.272928
37	1	0	-6.027872	3.783969	-1.335275
38	1	0	0.372373	1.061298	2.577421
39	1	0	-0.104070	2.771886	2.587688
40	1	0	-1.341207	1.539944	2.859720
41	1	0	-0.432293	-3.205322	0.431086
42	1	0	-1.660783	-5.001009	-0.759445
43	1	0	-3.041236	-4.459208	-2.749163
44	1	0	-3.182662	-2.111808	-3.548716
45	1	0	-1.991974	-0.302589	-2.311646
46	1	0	0.030411	4.913437	-0.658697
47	1	0	-1.557471	4.077677	-0.527510
48	1	0	-0.651893	4.553037	0.955495
49	6	0	5.768983	0.442833	1.764408

50	1	0	5.826164	1.032853	2.677277
51	1	0	6.234815	-0.532847	1.925468
52	1	0	6.269316	0.973550	0.949453
53	6	0	3.943146	1.861918	-1.350178
54	1	0	3.907562	2.489131	-0.456823
55	1	0	4.547664	2.331844	-2.124113
56	1	0	2.923395	1.699998	-1.714354
57	6	0	5.984973	-1.763986	-0.874009
58	1	0	6.245932	-2.820343	-0.901469
59	1	0	5.859238	-1.376424	-1.885182
60	1	0	6.769421	-1.202261	-0.361425
61	6	0	-4.868377	1.458161	0.608048
62	1	0	-5.191136	0.866355	1.462492
63	7	0	-5.734467	2.323885	0.105656

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.554191	0.910983	1.371560
2	7	0	-1.314988	1.421316	1.400989
3	6	0	-0.914334	2.139408	2.451408
4	6	0	-1.815993	2.399286	3.475545
5	6	0	-0.671359	-1.621133	1.791394
6	6	0	-0.560450	0.880937	-0.054759
7	16	0	-0.233281	-2.658090	-0.622369
8	79	0	1.493999	0.486732	0.125786
9	6	0	-0.874039	2.043343	-0.973407
10	6	0	-0.491551	3.351516	-0.650432
11	6	0	-0.771501	4.412829	-1.502566
12	6	0	-1.425243	4.187231	-2.712684
13	6	0	-1.784833	2.889672	-3.061058
14	6	0	-1.513350	1.828136	-2.200047
15	8	0	-0.003649	-3.844562	0.193696
16	8	0	0.914771	-2.062856	-1.307031
17	6	0	-1.467616	-3.004503	-1.856602
18	15	0	3.707165	-0.257739	0.148738
19	8	0	4.802526	0.801660	0.610432
20	8	0	4.023736	-1.492230	1.122180
21	8	0	4.199808	-0.853438	-1.261658
22	7	0	-1.024929	-1.552106	0.364968
23	6	0	-1.369732	-0.313415	-0.295408

24	1	0	0.112409	2.491083	2.445224
25	1	0	-1.522235	2.981829	4.340929
26	1	0	-1.510399	-1.237932	2.386255
27	1	0	-0.492623	-2.658237	2.075721
28	1	0	0.211228	-1.014095	2.032079
29	1	0	0.047344	3.541556	0.274549
30	1	0	-0.466983	5.417447	-1.227843
31	1	0	-1.635743	5.013903	-3.382716
32	1	0	-2.270362	2.699134	-4.013403
33	1	0	-1.759016	0.808208	-2.477422
34	1	0	-2.298272	-3.519413	-1.374023
35	1	0	-1.768832	-2.053815	-2.294996
36	1	0	-0.991155	-3.646890	-2.597676
37	6	0	3.573074	-0.428712	-2.483479
38	1	0	3.647353	0.655893	-2.602483
39	1	0	4.119526	-0.918996	-3.287533
40	1	0	2.527513	-0.746810	-2.495504
41	6	0	3.233924	-2.684972	0.981296
42	1	0	3.743005	-3.459641	1.551827
43	1	0	2.231736	-2.524354	1.391615
44	1	0	3.152727	-2.978046	-0.067733
45	6	0	6.189242	0.413802	0.698714
46	1	0	6.743466	1.326691	0.906776
47	1	0	6.319448	-0.305549	1.508108
48	1	0	6.516967	-0.019184	-0.248805
49	7	0	-2.670966	0.124612	0.243491
50	6	0	-4.094182	-1.699366	0.757813
51	6	0	-4.528119	-0.282882	-1.094635
52	6	0	-5.181692	-2.490202	0.431353
53	1	0	-3.422033	-1.883881	1.587061
54	6	0	-5.613302	-1.052227	-1.458941
55	1	0	-4.164618	0.593684	-1.621340
56	6	0	-5.947053	-2.166041	-0.686067
57	1	0	-5.410515	-3.353525	1.044033
58	1	0	-6.188491	-0.776850	-2.334145
59	1	0	-6.798740	-2.780162	-0.957998
60	7	0	-3.811943	-0.615920	0.002402
61	6	0	-3.461534	1.229976	2.391799
62	1	0	-4.488466	0.874729	2.370351
63	7	0	-3.079987	1.960146	3.427166

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.328545	0.419482	1.560900
2	7	0	-1.461775	1.403219	1.269288
3	6	0	-1.291268	2.436976	2.113614
4	6	0	-2.053198	2.480573	3.263162
5	6	0	-1.108119	-0.403597	-2.907020
6	6	0	-0.749977	1.191992	-0.033035
7	16	0	-0.033674	-2.177652	-1.332828
8	79	0	1.249184	0.565288	0.346772
9	6	0	-0.834859	2.494717	-0.828180
10	6	0	0.235343	3.392874	-0.874561
11	6	0	0.123367	4.602936	-1.557215
12	6	0	-1.062241	4.929009	-2.207232
13	6	0	-2.136239	4.041151	-2.169704
14	6	0	-2.021838	2.836893	-1.484727
15	8	0	1.346922	-1.707897	-1.533768
16	8	0	-0.489258	-3.283790	-2.160816
17	6	0	-0.191923	-2.659304	0.377350
18	15	0	3.310050	-0.566818	0.484483
19	8	0	4.369887	0.030901	1.527364
20	8	0	3.125433	-2.101637	0.926951
21	8	0	4.119364	-0.726346	-0.895821
22	7	0	-1.210125	-0.914148	-1.528835
23	6	0	-1.605014	0.043801	-0.577106
24	1	0	-0.570196	3.189363	1.814828
25	1	0	-1.942837	3.297696	3.966232
26	1	0	-0.313830	0.345423	-3.004461
27	1	0	-0.916268	-1.233919	-3.589911
28	1	0	-2.059980	0.064943	-3.165573
29	1	0	1.170268	3.140423	-0.377998
30	1	0	0.966984	5.284584	-1.586259
31	1	0	-1.148852	5.867508	-2.744771
32	1	0	-3.063122	4.289404	-2.676816
33	1	0	-2.847632	2.131167	-1.458127
34	1	0	0.050945	-1.827039	1.038367
35	1	0	-1.198569	-3.043508	0.540218
36	1	0	0.543159	-3.457071	0.501043
37	6	0	3.842458	0.150503	-1.999157
38	1	0	3.988610	1.195209	-1.709562
39	1	0	4.554104	-0.111677	-2.780467
40	1	0	2.821905	-0.015731	-2.351467
41	6	0	3.636708	-3.201908	0.152758

42	1	0	3.352692	-4.102716	0.696436
43	1	0	3.190034	-3.191723	-0.842854
44	1	0	4.724695	-3.147944	0.074106
45	6	0	5.619414	-0.647283	1.745442
46	1	0	6.203649	-0.012321	2.408414
47	1	0	5.437390	-1.614742	2.219591
48	1	0	6.146334	-0.780516	0.797135
49	7	0	-2.272699	-0.532658	0.567021
50	6	0	-3.798059	-2.222832	1.269122
51	6	0	-4.024183	-1.239321	-0.882303
52	6	0	-4.831585	-3.086161	1.009900
53	1	0	-3.198651	-2.244020	2.171142
54	6	0	-5.074220	-2.096614	-1.165460
55	1	0	-3.607213	-0.493174	-1.548534
56	6	0	-5.489631	-3.032300	-0.228002
57	1	0	-5.102556	-3.815835	1.763443
58	1	0	-5.538903	-2.033856	-2.142237
59	1	0	-6.281873	-3.734561	-0.458744
60	7	0	-3.451945	-1.274772	0.347586
61	6	0	-3.110926	0.523021	2.722120
62	1	0	-3.867312	-0.217771	2.960278
63	7	0	-2.966606	1.538628	3.549841

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.601521	2.266550	0.205516
2	7	0	-1.779450	1.426697	-0.853679
3	6	0	-1.826208	1.892147	-2.132275
4	6	0	-1.640612	3.233641	-2.320733
5	6	0	-2.293371	-1.999160	1.699090
6	6	0	-1.863274	0.088092	-0.364122
7	16	0	-0.814817	-0.450027	3.362887
8	6	0	-2.784381	-0.820852	-1.124991
9	6	0	-2.333316	-1.877981	-1.917152
10	6	0	-3.244498	-2.669913	-2.612974
11	6	0	-4.608173	-2.409370	-2.525126
12	6	0	-5.066337	-1.349593	-1.743511
13	6	0	-4.159071	-0.556762	-1.051188
14	8	0	0.435072	0.067984	2.815624
15	8	0	-0.822688	-1.729161	4.043700

16	6	0	-1.569186	0.784130	4.388468
17	15	0	2.473225	-1.435468	-0.602525
18	8	0	2.502529	-2.941919	-1.141420
19	8	0	3.321565	-0.558668	-1.632614
20	8	0	3.432490	-1.403917	0.682419
21	7	0	-1.932869	-0.621277	2.061406
22	6	0	-1.835816	0.332933	1.069319
23	1	0	-2.001478	1.166103	-2.917218
24	1	0	-1.668825	3.650121	-3.320843
25	1	0	-1.557563	-2.440543	1.013358
26	1	0	-2.337728	-2.591658	2.609825
27	1	0	-3.272139	-1.985850	1.220235
28	1	0	-1.269565	-2.091254	-1.981055
29	1	0	-2.885534	-3.492449	-3.222165
30	1	0	-5.315207	-3.030158	-3.065067
31	1	0	-6.128765	-1.142676	-1.672328
32	1	0	-4.512395	0.269923	-0.438904
33	1	0	-1.685731	1.688891	3.793638
34	1	0	-2.525914	0.390878	4.730826
35	1	0	-0.889281	0.936090	5.228517
36	6	0	2.968913	-2.013565	1.904935
37	1	0	2.777708	-3.078145	1.745560
38	1	0	3.772181	-1.887522	2.628073
39	1	0	2.067559	-1.505535	2.258048
40	6	0	4.673247	-0.123110	-1.393164
41	1	0	4.961312	0.440757	-2.278307
42	1	0	4.709122	0.512490	-0.507660
43	1	0	5.338666	-0.978812	-1.260214
44	6	0	3.760844	-3.552414	-1.487201
45	1	0	3.548636	-4.600875	-1.685696
46	1	0	4.165853	-3.077865	-2.384102
47	1	0	4.467189	-3.465607	-0.657131
48	7	0	-1.631158	1.616912	1.376137
49	79	0	0.342720	-0.608582	-0.352560
50	6	0	1.544228	2.562916	0.961156
51	6	0	1.622231	2.559473	-1.336028
52	6	0	1.972452	3.886019	1.017571
53	1	0	1.317366	1.996281	1.861258
54	6	0	2.043846	3.884459	-1.378442
55	1	0	1.480158	1.989020	-2.252479
56	6	0	2.218382	4.560935	-0.175107
57	1	0	2.104789	4.372855	1.977268
58	1	0	2.224364	4.370126	-2.330580
59	1	0	2.543181	5.596278	-0.167194

60	7	0	1.367456	1.910680	-0.195404
61	6	0	-1.401490	3.643102	-0.076416
62	1	0	-1.226750	4.329626	0.747012
63	7	0	-1.416895	4.104889	-1.299347

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.019848	-1.717448	-2.876253
2	6	0	-4.450339	-0.480053	-3.165423
3	6	0	-3.918414	0.287901	-2.150063
4	7	0	-3.925992	-0.139149	-0.859796
5	6	0	-4.449825	-1.361377	-0.568452
6	6	0	-5.009967	-2.150017	-1.554444
7	6	0	-3.699530	0.599550	1.338212
8	7	0	-2.766610	0.825382	2.271848
9	6	0	-3.180404	0.909087	3.538221
10	6	0	-4.512406	0.753352	3.898208
11	7	0	-3.249350	0.636065	0.025708
12	6	0	-1.544944	3.204697	0.189208
13	6	0	-0.976698	0.098230	-0.170094
14	16	0	0.960143	3.404538	-0.835939
15	79	0	1.656177	0.007540	-0.023364
16	6	0	-1.297832	-1.304674	-0.208805
17	6	0	-1.546242	-2.015462	0.977094
18	6	0	-1.871171	-3.365012	0.913261
19	6	0	-1.945030	-4.013243	-0.321435
20	6	0	-1.700690	-3.310696	-1.499671
21	6	0	-1.382602	-1.957532	-1.447753
22	8	0	2.180586	2.620170	-0.692371
23	8	0	0.857515	4.737037	-0.286224
24	6	0	0.558380	3.456902	-2.570229
25	15	0	3.665711	-1.046007	0.293910
26	8	0	4.972109	-0.225448	-0.144584
27	8	0	3.847369	-1.357833	1.852077
28	8	0	3.880573	-2.404318	-0.508743
29	7	0	-0.296132	2.503209	-0.154036
30	6	0	-0.264018	1.140398	-0.228452
31	1	0	-5.455684	-2.326733	-3.659079
32	1	0	-4.426179	-0.090506	-4.176109
33	1	0	-3.471478	1.263475	-2.286029

34	1	0	-4.379730	-1.671894	0.465157
35	1	0	-5.417181	-3.113129	-1.269927
36	1	0	-2.417856	1.102337	4.288041
37	1	0	-4.832006	0.812715	4.933369
38	1	0	-1.293039	4.230895	0.451383
39	1	0	-2.257293	3.176314	-0.639794
40	1	0	-1.974378	2.694449	1.050663
41	1	0	-1.483492	-1.489685	1.924675
42	1	0	-2.056751	-3.917591	1.828329
43	1	0	-2.188914	-5.069917	-0.361928
44	1	0	-1.756174	-3.815963	-2.458200
45	1	0	-1.183223	-1.397215	-2.356321
46	1	0	1.344536	4.027733	-3.066260
47	1	0	0.530420	2.433388	-2.946011
48	1	0	-0.404147	3.956046	-2.687009
49	6	0	5.014901	-2.053685	2.324989
50	1	0	4.994284	-1.986090	3.410745
51	1	0	4.968079	-3.101246	2.018049
52	1	0	5.923343	-1.581589	1.940283
53	6	0	5.109675	1.140055	0.300222
54	1	0	5.176859	1.174174	1.390813
55	1	0	6.034485	1.508736	-0.138965
56	1	0	4.264077	1.741282	-0.045938
57	6	0	5.147104	-2.824720	-1.053890
58	1	0	4.955745	-3.781996	-1.534549
59	1	0	5.501608	-2.095163	-1.781930
60	1	0	5.890752	-2.946825	-0.263805
61	6	0	-5.059327	0.470700	1.713498
62	1	0	-5.833631	0.329681	0.962053
63	7	0	-5.454598	0.539861	2.972207

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.862220	3.214632	-1.560732
2	6	0	3.813643	2.552601	-2.185334
3	6	0	3.067275	1.622078	-1.480630
4	7	0	3.359848	1.382463	-0.186299
5	6	0	4.351920	2.041076	0.460523
6	6	0	5.135513	2.946752	-0.217421
7	6	0	3.244506	-0.581596	1.159429

8	7	0	2.748407	-1.001491	2.314181
9	6	0	3.341381	-2.063624	2.854164
10	6	0	4.436293	-2.682718	2.251296
11	7	0	2.571740	0.517765	0.572179
12	6	0	0.364421	-2.954851	0.594006
13	6	0	0.427127	-0.575477	0.082332
14	16	0	1.592511	-2.159216	-1.612469
15	79	0	-1.639417	-0.467048	0.006781
16	8	0	0.451710	-2.431543	-2.471306
17	8	0	2.510270	-1.074645	-1.971671
18	6	0	2.565094	-3.642336	-1.452827
19	15	0	-3.970298	-0.188039	0.034205
20	8	0	-4.529237	0.174533	-1.425612
21	8	0	-4.493791	1.005326	0.992294
22	8	0	-4.848368	-1.401842	0.587570
23	7	0	1.113064	-1.848321	-0.022243
24	6	0	1.165202	0.533778	0.298503
25	6	0	0.589319	1.902067	0.375039
26	6	0	-0.225296	2.403800	-0.645916
27	6	0	-0.767585	3.683982	-0.546548
28	6	0	-0.494183	4.473935	0.567333
29	6	0	0.330734	3.984998	1.580564
30	6	0	0.878037	2.710856	1.480436
31	1	0	5.457660	3.938302	-2.106296
32	1	0	3.567922	2.732116	-3.224583
33	1	0	2.271351	1.019791	-1.901622
34	1	0	4.461194	1.800843	1.511027
35	1	0	5.932383	3.453459	0.312478
36	1	0	2.940222	-2.426305	3.796223
37	1	0	4.907843	-3.551874	2.699213
38	1	0	-0.548687	-3.199712	0.035956
39	1	0	1.004601	-3.835276	0.677170
40	1	0	0.097939	-2.634796	1.601887
41	1	0	3.305672	-3.506043	-0.663509
42	1	0	1.915063	-4.496169	-1.268829
43	1	0	3.058201	-3.756142	-2.419670
44	1	0	-0.427014	1.786068	-1.517852
45	1	0	-1.394026	4.066538	-1.346236
46	1	0	-0.913932	5.471613	0.643910
47	1	0	0.543197	4.596964	2.451108
48	1	0	1.508298	2.314479	2.272739
49	6	0	-5.939961	0.317828	-1.654759
50	1	0	-6.052751	0.708403	-2.664341
51	1	0	-6.426803	-0.657756	-1.580642

52	1	0	-6.375475	1.017712	-0.935598
53	6	0	-3.801751	2.260432	0.937501
54	1	0	-3.887633	2.702202	-0.059943
55	1	0	-4.279132	2.909197	1.670097
56	1	0	-2.743487	2.130660	1.190668
57	6	0	-6.030205	-1.250993	1.393455
58	1	0	-6.820362	-0.743089	0.836234
59	1	0	-6.346343	-2.261583	1.645038
60	1	0	-5.799360	-0.687524	2.297729
61	6	0	4.352784	-1.180114	0.550307
62	1	0	4.736509	-0.827888	-0.403560
63	7	0	4.945741	-2.232794	1.103246

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.748747	2.694478	0.329407
2	6	0	5.088912	2.610942	1.554162
3	6	0	3.936401	1.860916	1.652368
4	7	0	3.479776	1.165719	0.581217
5	6	0	4.071721	1.265870	-0.627218
6	6	0	5.220160	2.019347	-0.767540
7	6	0	2.190006	-0.563191	1.602340
8	7	0	1.131943	-1.321813	1.328823
9	6	0	0.796701	-2.331530	2.135611
10	6	0	1.604002	-2.630782	3.219189
11	7	0	2.261433	0.491206	0.713696
12	6	0	1.315041	0.451256	-0.358598
13	6	0	0.564855	-0.815139	-0.370170
14	79	0	-1.522411	-0.534245	-0.147226
15	15	0	-3.752792	0.029365	0.257954
16	8	0	-4.079065	1.594700	0.053965
17	8	0	-4.160746	-0.294450	1.775924
18	8	0	-4.856289	-0.626442	-0.688854
19	1	0	6.643772	3.297734	0.227523
20	1	0	5.439268	3.147475	2.427362
21	1	0	3.330322	1.796641	2.547369
22	1	0	3.572786	0.722404	-1.415567
23	1	0	5.688618	2.073802	-1.742531
24	1	0	-0.095104	-2.895081	1.882434
25	1	0	1.367584	-3.449259	3.889246

26	7	0	0.972734	-1.953798	-1.092632
27	6	0	0.003568	-3.014533	-1.400373
28	1	0	-0.406400	-3.430590	-0.477083
29	1	0	-0.815332	-2.604266	-1.999416
30	1	0	0.500302	-3.815752	-1.944097
31	16	0	2.539254	-2.139372	-1.688345
32	8	0	2.714280	-3.530235	-2.056515
33	8	0	3.461735	-1.512535	-0.747734
34	6	0	2.508630	-1.169678	-3.183164
35	1	0	1.815159	-1.648634	-3.875492
36	1	0	2.169454	-0.163946	-2.927092
37	1	0	3.517590	-1.170880	-3.599237
38	6	0	0.629089	1.719102	-0.602331
39	6	0	0.792634	2.861417	0.206825
40	6	0	-0.198121	1.855293	-1.739642
41	6	0	0.158795	4.061983	-0.099935
42	1	0	1.399020	2.801803	1.106532
43	6	0	-0.851545	3.047982	-2.026230
44	1	0	-0.298084	1.011582	-2.418813
45	6	0	-0.671199	4.167282	-1.214303
46	1	0	0.306795	4.921430	0.547431
47	1	0	-1.482197	3.110610	-2.907909
48	1	0	-1.158862	5.106379	-1.451945
49	6	0	-6.042547	0.049605	-1.145812
50	1	0	-6.553121	-0.658676	-1.795499
51	1	0	-6.687995	0.314970	-0.305883
52	1	0	-5.771650	0.948793	-1.699356
53	6	0	-5.491094	-0.031231	2.251869
54	1	0	-5.460168	-0.139100	3.334543
55	1	0	-5.798872	0.985251	1.989687
56	1	0	-6.185561	-0.761059	1.828879
57	6	0	-3.204626	2.549652	0.680335
58	1	0	-3.499998	3.528458	0.306827
59	1	0	-3.324888	2.510615	1.766706
60	1	0	-2.160441	2.359963	0.406710
61	6	0	3.034958	-0.927181	2.671354
62	1	0	3.963600	-0.403753	2.875524
63	7	0	2.732514	-1.944390	3.453909

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.795728	2.066068	-1.642551
2	6	0	-5.055075	1.618962	-2.744459
3	6	0	-3.881094	0.936824	-2.544336
4	7	0	-3.472934	0.633058	-1.275150
5	6	0	-4.132672	1.110059	-0.189252
6	6	0	-5.313213	1.806920	-0.364529
7	6	0	-2.020120	-1.202108	-1.461871
8	7	0	-1.007196	-1.707186	-0.740797
9	6	0	-0.606105	-2.984891	-0.924087
10	6	0	-1.286297	-3.756837	-1.832773
11	7	0	-2.163033	0.121489	-1.135877
12	6	0	-1.323896	0.442851	-0.053088
13	6	0	-0.527149	-0.769776	0.340856
14	79	0	1.543460	-0.327579	0.061795
15	15	0	3.778185	0.223750	-0.405388
16	8	0	4.518535	0.930019	0.833783
17	8	0	3.948387	1.232211	-1.644705
18	8	0	4.674513	-1.061530	-0.767026
19	1	0	-6.709273	2.630465	-1.786117
20	1	0	-5.371198	1.824602	-3.759970
21	1	0	-3.214638	0.620326	-3.336906
22	1	0	-3.691202	0.855402	0.763417
23	1	0	-5.840903	2.150224	0.517021
24	1	0	0.220373	-3.326631	-0.312726
25	1	0	-0.992497	-4.783242	-2.016346
26	7	0	-0.800923	-1.428327	1.626514
27	6	0	0.269616	-1.756333	2.571135
28	1	0	1.026461	-2.372196	2.079367
29	1	0	0.754788	-0.854526	2.963860
30	1	0	-0.151173	-2.336253	3.393404
31	16	0	-2.367876	-1.582053	2.178960
32	8	0	-2.448592	-2.758691	3.022688
33	8	0	-3.232488	-1.458913	1.005996
34	6	0	-2.636934	-0.159838	3.222261
35	1	0	-1.959048	-0.231645	4.074507
36	1	0	-2.432983	0.750133	2.653762
37	1	0	-3.671117	-0.201932	3.568126
38	6	0	-1.129600	1.776478	0.391753
39	6	0	-1.694891	2.907491	-0.251136
40	6	0	-0.371459	2.016852	1.570518
41	6	0	-1.501035	4.187764	0.254497
42	1	0	-2.220105	2.795736	-1.194712
43	6	0	-0.177762	3.301632	2.050188

44	1	0	0.046769	1.171707	2.112055
45	6	0	-0.748601	4.401540	1.405488
46	1	0	-1.935756	5.032374	-0.271456
47	1	0	0.412746	3.448164	2.949606
48	1	0	-0.605364	5.403298	1.793617
49	6	0	6.058598	-1.195307	-0.411460
50	1	0	6.321242	-2.235551	-0.595293
51	1	0	6.683836	-0.548255	-1.034189
52	1	0	6.204015	-0.957065	0.644468
53	6	0	5.045263	1.195173	-2.568595
54	1	0	4.753303	1.814232	-3.414878
55	1	0	5.949966	1.607904	-2.111797
56	1	0	5.225566	0.171206	-2.903795
57	6	0	5.514513	1.953756	0.693132
58	1	0	5.648455	2.387832	1.682107
59	1	0	6.462360	1.526279	0.351950
60	1	0	5.173101	2.720831	-0.005324
61	6	0	-2.729918	-2.045097	-2.334220
62	1	0	-3.605341	-1.690502	-2.870091
63	7	0	-2.359333	-3.292669	-2.513076

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204293	2.317874	0.605012
2	7	0	-1.220904	1.737174	-0.618543
3	6	0	-1.027483	2.451365	-1.752234
4	6	0	-0.753393	3.787837	-1.614577
5	7	0	-1.480224	1.444433	1.600320
6	6	0	-1.711247	0.283262	1.009232
7	6	0	-1.461406	0.322947	-0.432309
8	15	0	2.663494	-1.595347	-0.497629
9	8	0	3.628141	-0.641969	-1.351724
10	8	0	2.665849	-3.034070	-1.174690
11	8	0	3.458195	-1.899427	0.865884
12	1	0	-1.118170	1.928315	-2.697122
13	1	0	-0.598873	4.405077	-2.491972
14	7	0	-2.277996	-0.323125	-1.383208
15	6	0	-1.745587	-1.127464	-2.486360
16	1	0	-0.948465	-0.596695	-3.015913
17	1	0	-1.350632	-2.078091	-2.113380

18	1	0	-2.547046	-1.320624	-3.200561
19	16	0	-3.898562	0.183259	-1.460398
20	8	0	-4.222845	0.378898	-2.860956
21	8	0	-3.997445	1.261399	-0.491730
22	6	0	-4.820705	-1.217254	-0.864034
23	1	0	-4.581517	-2.082543	-1.483797
24	1	0	-4.553943	-1.388636	0.179174
25	1	0	-5.876707	-0.961525	-0.964888
26	6	0	-2.188451	-0.890567	1.748440
27	6	0	-2.796975	-0.690573	2.993364
28	6	0	-2.098634	-2.186015	1.219081
29	6	0	-3.311720	-1.773149	3.696405
30	1	0	-2.870817	0.318376	3.384353
31	6	0	-2.614073	-3.264323	1.927651
32	1	0	-1.620396	-2.348975	0.256324
33	6	0	-3.223103	-3.058418	3.165346
34	1	0	-3.787469	-1.614178	4.658009
35	1	0	-2.537673	-4.265871	1.518057
36	1	0	-3.626983	-3.901764	3.715793
37	6	0	3.548626	-0.861206	1.856882
38	1	0	2.554948	-0.636054	2.255118
39	1	0	4.188350	-1.249287	2.647173
40	1	0	3.986891	0.045052	1.427386
41	6	0	3.564988	-4.104854	-0.816716
42	1	0	3.266832	-4.953605	-1.428301
43	1	0	4.598917	-3.832040	-1.036628
44	1	0	3.461076	-4.340169	0.242431
45	6	0	4.964781	-1.060432	-1.688603
46	1	0	5.469381	-0.184720	-2.092191
47	1	0	5.490236	-1.414037	-0.797259
48	1	0	4.922516	-1.845080	-2.447419
49	79	0	0.610823	-0.562022	-0.338239
50	6	0	1.683931	2.215071	2.035377
51	6	0	2.544144	2.354649	-0.087671
52	6	0	2.507252	3.238959	2.490502
53	1	0	0.965674	1.735800	2.697923
54	6	0	3.399975	3.391922	0.272600
55	1	0	2.541013	1.964299	-1.103791
56	6	0	3.379544	3.842105	1.588185
57	1	0	2.457222	3.558495	3.525267
58	1	0	4.061585	3.833294	-0.463921
59	1	0	4.030076	4.650447	1.905516
60	7	0	1.696591	1.776023	0.769649
61	6	0	-0.894406	3.696264	0.671518

62	1	0	-0.844004	4.181417	1.642161
63	7	0	-0.670070	4.403276	-0.408601

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.352747	-2.042476	0.208136
2	7	0	1.823092	-0.744163	0.035171
3	6	0	3.132962	-0.524174	-0.318351
4	6	0	3.944677	-1.606946	-0.455830
5	6	0	-1.849115	0.728051	1.790933
6	6	0	0.756862	0.102386	0.217963
7	16	0	-2.783699	-0.647253	-0.330691
8	6	0	0.815651	1.558480	0.038012
9	6	0	-0.127411	2.180455	-0.789902
10	6	0	-0.101836	3.561584	-0.953043
11	6	0	0.868074	4.328291	-0.310559
12	6	0	1.811497	3.712679	0.508146
13	6	0	1.782174	2.333642	0.689392
14	8	0	-2.207417	-0.390346	-1.644396
15	8	0	-3.967546	0.073868	0.109234
16	6	0	-3.073711	-2.396968	-0.196580
17	7	0	-1.617672	-0.377396	0.852466
18	6	0	-0.299543	-0.750925	0.525028
19	1	0	3.437699	0.501537	-0.479744
20	1	0	4.982328	-1.464379	-0.734904
21	1	0	-1.740279	1.713193	1.328277
22	1	0	-2.853902	0.633899	2.200134
23	1	0	-1.117065	0.623140	2.593051
24	1	0	-0.866101	1.569389	-1.303876
25	1	0	-0.836695	4.038363	-1.593414
26	1	0	0.888010	5.404712	-0.446518
27	1	0	2.563035	4.307183	1.017407
28	1	0	2.495415	1.856974	1.357027
29	1	0	-2.114590	-2.905188	-0.297100
30	1	0	-3.516780	-2.586873	0.780115
31	1	0	-3.759397	-2.665170	-1.001127
32	7	0	0.064807	-2.054167	0.517401
33	6	0	2.285438	-3.099121	0.046003
34	1	0	1.934909	-4.118065	0.189352
35	7	0	3.537129	-2.900075	-0.266812

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.392980	-2.073036	-0.070407
2	7	0	-1.672426	-0.752689	0.236585
3	6	0	-2.965215	-0.305328	0.327414
4	6	0	-3.958310	-1.217488	0.143526
5	7	0	-0.088524	-2.296169	-0.144126
6	6	0	0.502897	-1.104746	0.126154
7	6	0	-0.453998	-0.117448	0.365971
8	1	0	-3.114933	0.752183	0.500042
9	1	0	-4.993283	-0.902679	0.206643
10	7	0	-0.329230	1.231168	0.709551
11	6	0	-0.534951	1.630397	2.108814
12	1	0	-1.563488	1.452442	2.440488
13	1	0	0.146614	1.041611	2.727107
14	1	0	-0.302181	2.689764	2.209283
15	16	0	-0.601054	2.359953	-0.515661
16	8	0	-0.554120	3.664851	0.123144
17	8	0	-1.765377	1.957496	-1.290805
18	6	0	0.837297	2.141068	-1.542512
19	1	0	1.718310	2.429491	-0.970958
20	1	0	0.892586	1.094241	-1.844106
21	1	0	0.698418	2.784654	-2.412036
22	6	0	1.970011	-0.967377	0.116147
23	6	0	2.733016	-1.971185	-0.490894
24	6	0	2.622706	0.128142	0.695034
25	6	0	4.118655	-1.874624	-0.528991
26	1	0	2.218840	-2.821646	-0.925462
27	6	0	4.010014	0.220419	0.653588
28	1	0	2.045038	0.905387	1.184347
29	6	0	4.762081	-0.777562	0.039476
30	1	0	4.698437	-2.658763	-1.005290
31	1	0	4.504899	1.071224	1.111091
32	1	0	5.844292	-0.703017	0.008782
33	6	0	-2.502692	-2.942740	-0.245502
34	1	0	-2.306312	-3.985842	-0.479280
35	7	0	-3.739187	-2.539169	-0.137110