Supporting Information

Computational Study on the Acidic Constants of Chiral Brønsted Acids in Dimethyl Sulfoxide

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B3LYP/6-31+G(d) Calculated Cartesian Cooradinates.

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.613121	3.113640	0.396059
2	6	0	-3.864119	2.116514	-0.519008
3	6	0	-2.885956	1.124837	-0.806913
4	6	0	-1.626425	1.158111	-0.123453
5	6	0	-1.400943	2.205738	0.815857
6	6	0	-2.364699	3.158458	1.065127
7	1	0	-4.091105	0.070246	-2.266944
8	1	0	-4.366200	3.868826	0.604520
9	1	0	-4.816613	2.073330	-1.041881
10	6	0	-3.130256	0.103059	-1.759341
11	6	0	-0.634645	0.156024	-0.408645
12	1	0	-0.450013	2.259350	1.335398
13	1	0	-2.164803	3.953675	1.778654
14	6	0	-0.918721	-0.796184	-1.380004
15	6	0	-2.168858	-0.833671	-2.047795
16	1	0	-2.349944	-1.616040	-2.775824
17	6	0	2.058348	-0.274296	2.316012
18	6	0	3.084027	0.488888	1.813019
19	6	0	2.954001	1.153219	0.567705
20	6	0	1.732161	1.023332	-0.174784
21	6	0	0.664583	0.218665	0.344877
22	6	0	0.853538	-0.397825	1.579753
23	1	0	4.927757	2.040551	0.613566
24	1	0	2.154710	-0.784164	3.267365
25	1	0	4.010692	0.587633	2.372633
26	6	0	4.005736	1.953670	0.043754
27	6	0	1.620175	1.710762	-1.417539
28	6	0	2.656596	2.479850	-1.895608
29	6	0	3.861671	2.604574	-1.160408
30	1	0	0.712764	1.608530	-2.001187
31	1	0	2.554216	2.987316	-2.850715
32	1	0	4.672627	3.211897	-1.553422
33	16	0	0.289990	-1.993236	-2.021701
34	8	0	-0.473978	-3.070920	-2.648577
35	8	0	1.318712	-1.280253	-2.771556
36	16	0	-0.355285	-1.514165	2.324307

37	8	0	-0.667929	-2.611480	1.401726
38	8	0	0.061536	-1.799972	3.696022
39	8	0	1.050187	-2.562918	-0.711652
40	1	0	0.396139	-2.896676	-0.048724
41	8	0	-1.745807	-0.653641	2.403608
42	1	0	-1.785821	-0.216771	3.276308

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.574511	3.095832	0.813740
2	6	0	-3.869972	2.184214	-0.175297
3	6	0	-2.920865	1.202281	-0.571689
4	6	0	-1.640115	1.162218	0.068224
5	6	0	-1.374683	2.111548	1.094650
6	6	0	-2.312184	3.054717	1.454776
7	1	0	-4.195360	0.272122	-2.058583
8	1	0	-4.309688	3.840775	1.110063
9	1	0	-4.839811	2.197705	-0.669180
10	6	0	-3.215382	0.255119	-1.585955
11	6	0	-0.664659	0.183359	-0.335993
12	1	0	-0.422241	2.074740	1.610598
13	1	0	-2.086060	3.763492	2.247660
14	6	0	-1.004203	-0.700737	-1.350765
15	6	0	-2.282449	-0.676419	-1.965745
16	1	0	-2.501893	-1.412777	-2.730345
17	6	0	2.196453	-0.443611	2.141564
18	6	0	3.180403	0.384131	1.656293
19	6	0	2.962998	1.160690	0.489460
20	6	0	1.699245	1.068675	-0.182327
21	6	0	0.678911	0.201820	0.341024
22	6	0	0.941138	-0.531256	1.491700
23	1	0	4.918470	2.087685	0.496716
24	1	0	2.347298	-1.045625	3.031070
25	1	0	4.141019	0.451580	2.163892
26	6	0	3.964227	2.031079	-0.024110
27	6	0	1.504110	1.857157	-1.352513
28	6	0	2.493091	2.692306	-1.824655
29	6	0	3.738047	2.784683	-1.154532
30	1	0	0.565082	1.780237	-1.889257

31	1	0	2.320705	3.275332	-2.726180
32	1	0	4.513299	3.444159	-1.538481
33	16	0	0.152711	-1.892181	-2.101858
34	8	0	-0.672568	-2.875397	-2.819705
35	8	0	1.156199	-1.146034	-2.871667
36	16	0	-0.281776	-1.673920	2.251040
37	8	0	-0.467911	-2.757426	1.198179
38	8	0	0.378729	-2.187667	3.472772
39	8	0	0.907382	-2.577532	-0.892773
40	1	0	0.304964	-2.721521	-0.040404
41	8	0	-1.512876	-0.883082	2.467997

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.229562	4.452770	0.319621
2	6	0	2.390344	4.324287	-0.764445
3	6	0	1.759085	3.084875	-1.059737
4	6	0	2.026516	1.941880	-0.232910
5	6	0	2.880074	2.118389	0.892011
6	6	0	3.464674	3.338193	1.160146
7	1	0	0.662855	3.836128	-2.773280
8	1	0	3.699449	5.407513	0.540068
9	1	0	2.183343	5.177473	-1.406484
10	6	0	0.850868	2.968532	-2.145879
11	6	0	1.397449	0.683005	-0.541523
12	1	0	3.063170	1.281125	1.555986
13	1	0	4.105727	3.446219	2.031207
14	6	0	0.453374	0.677833	-1.554921
15	6	0	0.175731	1.793833	-2.369646
16	1	0	-0.552909	1.691613	-3.167526
17	6	0	0.856613	-2.443322	1.577939
18	6	0	2.133398	-2.911034	1.771268
19	6	0	3.239062	-2.281532	1.137843
20	6	0	3.025067	-1.113676	0.329361
21	6	0	1.695480	-0.570198	0.209869
22	6	0	0.665604	-1.288444	0.793288
23	1	0	4.699250	-3.688146	1.892083
24	1	0	-0.009490	-2.931563	2.011838
25	1	0	2.306666	-3.792868	2.382881

26	6	0	4.553027	-2.809649	1.267665
27	6	0	4.143661	-0.564414	-0.358188
28	6	0	5.402516	-1.111438	-0.224453
29	6	0	5.616883	-2.236939	0.607030
30	1	0	3.999383	0.292267	-1.006669
31	1	0	6.237384	-0.676061	-0.767336
32	1	0	6.615211	-2.653769	0.709535
33	8	0	-0.248851	-0.497884	-1.859730
34	8	0	-0.662183	-0.858702	0.623683
35	15	0	-1.337616	-1.131088	-0.829213
36	7	0	-2.664967	-0.044778	-0.703116
37	1	0	-3.490300	-0.344002	-1.220413
38	16	0	-2.941787	1.383452	0.145297
39	8	0	-1.684198	2.004508	0.518412
40	8	0	-4.012777	2.078389	-0.558778
41	6	0	-3.733621	0.738432	1.738655
42	9	0	-2.868344	0.005274	2.438952
43	9	0	-4.126730	1.785068	2.469802
44	9	0	-4.799461	-0.012700	1.430077
45	34	0	-1.943219	-3.013499	-1.408905

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.272836	4.568131	0.288169
2	6	0	2.340590	4.442791	-0.718937
3	6	0	1.718691	3.194793	-0.996895
4	6	0	2.087234	2.035852	-0.232150
5	6	0	3.032854	2.210220	0.818786
6	6	0	3.609879	3.437640	1.071077
7	1	0	0.430217	3.966075	-2.561571
8	1	0	3.734038	5.531157	0.494498
9	1	0	2.051188	5.307626	-1.313155
10	6	0	0.711890	3.081524	-1.994282
11	6	0	1.464637	0.769804	-0.518758
12	1	0	3.293082	1.360249	1.439621
13	1	0	4.323103	3.538215	1.886020
14	6	0	0.444377	0.746355	-1.462552
15	6	0	0.059175	1.891043	-2.197284
16	1	0	-0.752062	1.791208	-2.910580

17	6	0	1.039938	-2.365720	1.592840
18	6	0	2.323696	-2.833827	1.725578
19	6	0	3.399535	-2.203207	1.042259
20	6	0	3.143961	-1.030922	0.251557
21	6	0	1.813445	-0.486957	0.204043
22	6	0	0.797923	-1.197197	0.833783
23	1	0	4.894197	-3.615372	1.710463
24	1	0	0.191558	-2.860083	2.053548
25	1	0	2.525543	-3.724263	2.317295
26	6	0	4.718462	-2.730858	1.100797
27	6	0	4.229638	-0.479208	-0.487084
28	6	0	5.496031	-1.022225	-0.417660
29	6	0	5.751573	-2.154264	0.393757
30	1	0	4.049883	0.380895	-1.123018
31	1	0	6.302912	-0.580542	-0.998056
32	1	0	6.753800	-2.573571	0.443813
33	8	0	-0.201840	-0.438682	-1.748820
34	8	0	-0.499622	-0.745694	0.750877
35	15	0	-1.337335	-1.029877	-0.677249
36	7	0	-2.477453	0.108453	-0.704245
37	16	0	-3.875134	0.211661	0.037637
38	8	0	-4.851560	0.910842	-0.810257
39	8	0	-4.310054	-0.970716	0.798674
40	6	0	-3.503614	1.480897	1.388895
41	9	0	-4.639864	1.793559	2.050593
42	9	0	-2.624287	1.003503	2.288801
43	9	0	-3.000442	2.622801	0.880143
44	34	0	-1.612461	-3.063880	-1.057878

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.504612	4.471715	-0.855362
2	6	0	-1.737257	4.381120	0.284433
3	6	0	-1.279120	3.122358	0.761223
4	6	0	-1.652145	1.924858	0.062576
5	6	0	-2.425747	2.059256	-1.124297
6	6	0	-2.838133	3.296943	-1.571245
7	1	0	-0.168444	3.945851	2.432058
8	1	0	-2.841239	5.440394	-1.214905

9	1	0	-1.453273	5.277329	0.831380
10	6	0	-0.436030	3.035607	1.901429
11	6	0	-1.197840	0.648135	0.553234
12	1	0	-2.682481	1.173149	-1.693827
13	1	0	-3.419637	3.370832	-2.486531
14	6	0	-0.300106	0.657599	1.607479
15	6	0	0.069557	1.824960	2.306431
16	1	0	0.744389	1.737353	3.152031
17	6	0	-1.000110	-2.759260	-1.154270
18	6	0	-2.320920	-3.084341	-1.345723
19	6	0	-3.353326	-2.245199	-0.846181
20	6	0	-3.011206	-1.022650	-0.174744
21	6	0	-1.625151	-0.642670	-0.057570
22	6	0	-0.679709	-1.553589	-0.497991
23	1	0	-4.963667	-3.535046	-1.497260
24	1	0	-0.193662	-3.401720	-1.491916
25	1	0	-2.589055	-4.005049	-1.857624
26	6	0	-4.721318	-2.612128	-0.975256
27	6	0	-4.067824	-0.253971	0.389760
28	6	0	-5.383360	-0.647519	0.263215
29	6	0	-5.719542	-1.830593	-0.437798
30	1	0	-3.831553	0.650746	0.938093
31	1	0	-6.169205	-0.045097	0.711315
32	1	0	-6.760787	-2.125303	-0.537143
33	8	0	0.262721	-0.541932	2.071894
34	8	0	0.687801	-1.278011	-0.326497
35	15	0	1.307809	-1.401153	1.169516
36	7	0	2.731500	-0.467413	0.929492
37	1	0	3.514205	-0.752461	1.516262
38	16	0	3.148068	0.808089	-0.087434
39	8	0	1.957199	1.479795	-0.574006
40	8	0	4.264295	1.493161	0.553379
41	6	0	3.907502	-0.091057	-1.568784
42	9	0	4.405506	0.823952	-2.405038
43	9	0	4.895904	-0.890681	-1.146110
44	9	0	2.991111	-0.821831	-2.203243
45	16	0	1.709828	-3.104733	1.963489

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Standard orientation:

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

1	6	0	-2.566703	4.514693	-0.886492
2	6	0	-1.720178	4.416677	0.196295
3	6	0	-1.257274	3.154289	0.658109
4	6	0	-1.704445	1.956071	0.005078
5	6	0	-2.556139	2.098282	-1.127498
6	6	0	-2.975695	3.338865	-1.560881
7	1	0	0.008389	3.971531	2.217846
8	1	0	-2.904268	5.488103	-1.234844
9	1	0	-1.372952	5.312415	0.707917
10	6	0	-0.333675	3.059530	1.733693
11	6	0	-1.248080	0.676598	0.481029
12	1	0	-2.867111	1.210938	-1.667698
13	1	0	-3.617892	3.413453	-2.435567
14	6	0	-0.286311	0.662043	1.483429
15	6	0	0.161256	1.840690	2.123912
16	1	0	0.906284	1.746870	2.907572
17	6	0	-1.154683	-2.744133	-1.188581
18	6	0	-2.482326	-3.068391	-1.316347
19	6	0	-3.488762	-2.217507	-0.783763
20	6	0	-3.105941	-0.988453	-0.146099
21	6	0	-1.716155	-0.613883	-0.097983
22	6	0	-0.780330	-1.529720	-0.565897
23	1	0	-5.134316	-3.505429	-1.340453
24	1	0	-0.364889	-3.397225	-1.544718
25	1	0	-2.777897	-3.997875	-1.798528
26	6	0	-4.863597	-2.575613	-0.843244
27	6	0	-4.134044	-0.208059	0.456805
28	6	0	-5.457804	-0.591807	0.397431
29	6	0	-5.834241	-1.781854	-0.271335
30	1	0	-3.863510	0.701182	0.981841
31	1	0	-6.217456	0.023381	0.874300
32	1	0	-6.881178	-2.072639	-0.318719
33	8	0	0.235593	-0.534571	1.932796
34	8	0	0.565675	-1.257467	-0.478684
35	15	0	1.338911	-1.383335	1.000064
36	7	0	2.714493	-0.564935	0.868700
37	16	0	3.183847	0.691918	0.025301
38	8	0	2.163183	1.369196	-0.792847
39	8	0	4.113523	1.524849	0.804434
40	6	0	4.311024	-0.121243	-1.252572
41	9	0	4.842001	0.819620	-2.064169
42	9	0	5.329834	-0.782753	-0.673310
43	9	0	3.633684	-0.993431	-2.024075

44	16	0	1.459456	-3.195640	1.707640

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.426451	1.910058	0.142018
2	1	0	0.066821	3.728767	2.614708
3	6	0	-0.239683	2.856813	2.040985
4	6	0	-1.078839	0.608199	0.588483
5	6	0	-0.209539	0.500182	1.679266
6	6	0	0.197643	1.596787	2.429654
7	1	0	0.852390	1.453409	3.283551
8	6	0	-0.978738	-2.681346	-1.313131
9	6	0	-2.331669	-2.952523	-1.476906
10	6	0	-0.620900	-1.539431	-0.607356
11	1	0	-0.207771	-3.339075	-1.700771
12	1	0	-2.635422	-3.839274	-2.028978
13	8	0	0.289825	-0.762938	2.050563
14	8	0	0.751992	-1.295759	-0.404806
15	15	0	1.344471	-1.540472	1.086414
16	6	0	-2.116279	2.098386	-1.203831
17	6	0	-1.403831	4.449250	0.483636
18	6	0	-1.773142	4.585556	-0.996945
19	6	0	-2.754623	3.479782	-1.392829
20	1	0	-1.349092	1.951979	-1.980451
21	1	0	-2.857975	1.316155	-1.382171
22	1	0	-2.263488	4.766280	1.095184
23	1	0	-0.584890	5.133679	0.737725
24	1	0	-2.202705	5.577693	-1.183843
25	1	0	-0.867202	4.507428	-1.614749
26	1	0	-3.662360	3.560169	-0.775923
27	1	0	-3.071886	3.592949	-2.437092
28	6	0	-5.416640	-0.412899	0.114256
29	6	0	-5.709110	-1.907999	-0.032618
30	6	0	-4.775497	-2.520545	-1.081625
31	1	0	-6.111833	0.054639	0.822717
32	1	0	-5.559851	-2.406307	0.936259
33	1	0	-6.754239	-2.077625	-0.320002
34	1	0	-4.864086	-3.614215	-1.081556
35	1	0	-5.101184	-2.192040	-2.081320

36	1	0	-5.570499	0.084630	-0.855056
37	6	0	-1.557725	-0.637958	-0.090316
38	6	0	-3.314448	-2.134649	-0.899765
39	6	0	-2.932793	-0.982506	-0.182795
40	6	0	-3.977380	-0.187676	0.592746
41	1	0	-3.744715	0.879385	0.588738
42	1	0	-3.903026	-0.494587	1.648282
43	6	0	-1.017520	3.033764	0.887646
44	7	0	2.764761	-0.576133	0.945272
45	1	0	3.527645	-0.877994	1.549455
46	16	0	3.223837	0.719487	-0.023280
47	8	0	2.061480	1.409278	-0.551952
48	8	0	4.312704	1.388053	0.679894
49	6	0	4.047445	-0.146438	-1.489850
50	9	0	4.574921	0.787311	-2.287802
51	9	0	5.022371	-0.950528	-1.044848
52	9	0	3.161695	-0.868086	-2.176780
53	16	0	1.746437	-3.303376	1.742223

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.532757	1.996701	0.007365
2	1	0	-0.769578	3.611679	-1.924212
3	6	0	-0.226438	2.783544	-1.471613
4	6	0	1.178076	0.659998	-0.308205
5	6	0	0.058361	0.434056	-1.123315
6	6	0	-0.644318	1.481290	-1.716282
7	1	0	-1.522990	1.256476	-2.312579
8	6	0	1.747445	-2.550833	1.621919
9	6	0	3.109781	-2.756115	1.441201
10	6	0	1.144504	-1.451877	1.011288
11	1	0	1.132928	-3.236198	2.196269
12	1	0	3.588866	-3.614450	1.910036
13	8	0	-0.359795	-0.867602	-1.345059
14	8	0	-0.216097	-1.266221	1.166693
15	15	0	-1.211711	-1.640546	-0.126762
16	6	0	2.553915	2.281443	1.103826
17	6	0	1.216130	4.514356	-0.349504
18	6	0	1.978421	4.731120	0.962511

19	6	0	3.112556	3.709532	1.080921
20	1	0	2.054102	2.114092	2.071583
21	1	0	3.373993	1.559553	1.079138
22	1	0	1.843799	4.872124	-1.182592
23	1	0	0.309649	5.133593	-0.369663
24	1	0	2.366826	5.757948	1.006551
25	1	0	1.292572	4.611443	1.814165
26	1	0	3.798077	3.829450	0.227440
27	1	0	3.705118	3.886024	1.988972
28	6	0	5.539163	-0.156753	-0.980027
29	6	0	5.925734	-1.634430	-0.873804
30	6	0	5.346485	-2.231135	0.413150
31	1	0	5.994506	0.304717	-1.866723
32	1	0	5.529985	-2.176461	-1.745246
33	1	0	7.017313	-1.758232	-0.888133
34	1	0	5.490560	-3.319621	0.426778
35	1	0	5.920056	-1.840463	1.269993
36	1	0	5.933120	0.383035	-0.104915
37	6	0	1.888637	-0.530293	0.255664
38	6	0	3.871001	-1.915254	0.615816
39	6	0	3.256276	-0.806940	0.000316
40	6	0	4.015000	0.001628	-1.047323
41	1	0	3.747432	1.059916	-0.999646
42	1	0	3.666669	-0.335770	-2.036650
43	6	0	0.840059	3.060665	-0.602486
44	7	0	-2.480131	-0.741248	0.298194
45	16	0	-3.910431	-0.627337	-0.366906
46	8	0	-3.912030	-0.073138	-1.737119
47	8	0	-4.847215	-1.725935	-0.080917
48	6	0	-4.554988	0.793592	0.692058
49	9	0	-5.821694	1.083232	0.319156
50	9	0	-4.577030	0.482484	2.001420
51	9	0	-3.822055	1.913796	0.541919
52	16	0	-1.314547	-3.537672	-0.566756

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.323822	4.346023	-1.267674
2	6	0	-1.569715	4.346580	-0.115411

3	6	0	−1.151176	3.128549	0.487153
4	6	0	−1.552043	1.879007	−0.094713
5	6	0	−2.311202	1.917547	−1.297843
6	6	0	−2.683739	3.116220	−1.869013
7	1	0	−0.031134	4.080239	2.082124
8	1	0	−2.629637	5.283594	−1.724109
9	1	0	−1.265462	5.283935	0.344791
10	6	0	−0.320142	3.130415	1.639480
11	6	0	−1.139263	0.643749	0.523681
12	1	0	−2.588049	0.987500	−1.781431
13	1	0	−3.254560	3.115515	−2.793957
14	6	0	−0.245980	0.732003	1.578464
15	6	0	0.149192	1.951885	2.164303
16	1	0	0.817582	1.928693	3.019157
17	6	0	−1.062360	−2.926448	−0.827011
18	6	0	−2.393361	−3.219131	−0.997173
19	6	0	−3.395343	−2.295365	−0.593960
20	6	0	−3.010375	−1.024898	−0.046442
21	6	0	−1.610751	−0.685777	0.042285
22	6	0	−0.700912	−1.672605	−0.294810
23	1	0	−5.049462	−3.585389	−1.122911
24	1	0	−0.278918	−3.630679	−1.086880
25	1	0	−2.693823	−4.176964	−1.414156
26	6	0	−4.775307	−2.623670	−0.695230
27	6	0	−4.039772	−0.165576	0.430447
28	6	0	−5.368571	−0.522271	0.335538
29	6	0	−5.745935	−1.756507	−0.245711
30	1	0	−3.772533	0.780657	0.886635
31	1	0	−6.133027	0.150141	0.715944
32	1	0	−6.796941	−2.021999	−0.321726
33	8	0	0.284196	−0.428084	2.163521
34	8	0	0.678830	−1.437050	−0.135862
35	15	0	1.269046	−1.427934	1.363348
36	8	0	1.489765	−2.683605	2.102344
37	7	0	2.778145	−0.667797	1.093322
38	1	0	3.519311	−1.017789	1.699156
39	16	0	3.320041	0.526184	0.048513
40	8	0	2.192173	1.278640	−0.470926
41	8	0	4.485451	1.134859	0.677336
42	6	0	4.009761	−0.482949	−1.394485
43	9	0	4.592646	0.356485	−2.254396
44	9	0	4.920793	−1.352107	−0.936170
45	9	0	3.037102	−1.151221	−2.014422

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.423028	4.378665	-1.227277
2	6	0	-1.590451	4.356814	-0.129388
3	6	0	-1.154316	3.129831	0.440918
4	6	0	-1.614435	1.888744	-0.115784
5	6	0	-2.451419	1.950686	-1.266440
6	6	0	-2.844790	3.157618	-1.806579
7	1	0	0.106219	4.052202	1.945301
8	1	0	-2.739583	5.325194	-1.659421
9	1	0	-1.233528	5.286151	0.310766
10	6	0	-0.244919	3.109049	1.532469
11	6	0	-1.185652	0.645454	0.469769
12	1	0	-2.771549	1.026846	-1.735440
13	1	0	-3.476093	3.169431	-2.692274
14	6	0	-0.230207	0.697099	1.478247
15	6	0	0.226212	1.918913	2.025831
16	1	0	0.961685	1.878509	2.823062
17	6	0	-1.163708	-2.905603	-0.906152
18	6	0	-2.497709	-3.208660	-1.017038
19	6	0	-3.486661	-2.292703	-0.565385
20	6	0	-3.077774	-1.023955	-0.029991
21	6	0	-1.679297	-0.678536	-0.003002
22	6	0	-0.763183	-1.652519	-0.384406
23	1	0	-5.158549	-3.584707	-1.025215
24	1	0	-0.387614	-3.604727	-1.200567
25	1	0	-2.812568	-4.168115	-1.422310
26	6	0	-4.869090	-2.622775	-0.605664
27	6	0	-4.090943	-0.171957	0.496516
28	6	0	-5.423212	-0.528474	0.458684
29	6	0	-5.824191	-1.761339	-0.110624
30	1	0	-3.802718	0.772217	0.944874
31	1	0	-6.170785	0.142598	0.875564
32	1	0	-6.877506	-2.030452	-0.142099
33	8	0	0.269480	-0.461471	2.029443
34	8	0	0.588547	-1.407222	-0.306536
35	15	0	1.323989	-1.443488	1.187038
36	8	0	1.307462	-2.777837	1.833911

37	7	0	2.756994	-0.735275	1.022451
38	16	0	3.294793	0.456589	0.137338
39	8	0	2.305576	1.178025	-0.683641
40	8	0	4.293355	1.250969	0.871183
41	6	0	4.343817	-0.461424	-1.136787
42	9	0	4.919546	0.418645	-1.985566
43	9	0	5.329974	-1.171755	-0.556385
44	9	0	3.599532	-1.311402	-1.871907

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.601841	-3.414139	-1.437432
2	6	0	2.714101	-3.856318	-0.481154
3	6	0	1.752928	-2.976170	0.086167
4	6	0	1.716509	-1.607790	-0.343628
5	6	0	2.646041	-1.184824	-1.334634
6	6	0	3.563356	-2.065567	-1.867591
7	1	0	0.865103	-4.458046	1.397296
8	1	0	4.329945	-4.097715	-1.865770
9	1	0	2.732483	-4.891408	-0.147896
10	6	0	0.828935	-3.422190	1.069741
11	6	0	0.746453	-0.715963	0.226255
12	1	0	2.625596	-0.155100	-1.676854
13	1	0	4.261584	-1.722542	-2.626478
14	6	0	-0.132324	-1.223652	1.162389
15	6	0	-0.099862	-2.564387	1.605994
16	1	0	-0.811111	-2.893843	2.354756
17	6	0	-0.243959	2.473169	-1.630340
18	6	0	0.632802	3.397998	-1.113241
19	6	0	1.571029	3.037689	-0.108461
20	6	0	1.611823	1.681947	0.360633
21	6	0	0.697953	0.720401	-0.185062
22	6	0	-0.206859	1.148424	-1.138250
23	1	0	2.436430	5.013198	0.076520
24	1	0	-0.959490	2.736537	-2.400615
25	1	0	0.618506	4.421684	-1.479116
26	6	0	2.475017	3.988573	0.439223
27	6	0	2.558809	1.340416	1.366100
28	6	0	3.418593	2.288271	1.879024

29	6	0	3.379955	3.625077	1.412256
30	1	0	2.595584	0.319789	1.733254
31	1	0	4.131767	2.008176	2.649671
32	1	0	4.064339	4.361433	1.824852
33	8	0	-1.028456	-0.330984	1.784779
34	8	0	-1.061566	0.170637	-1.684871
35	16	0	-2.692839	0.308552	-1.501180
36	16	0	-2.650970	-0.423860	1.498812
37	7	0	-2.912174	0.591345	0.161118
38	1	0	-2.933086	1.580519	0.405486
39	8	0	-3.237073	0.305957	2.604122
40	8	0	-3.149715	1.550675	-2.104475
41	8	0	-3.200834	-0.990295	-1.862876
42	8	0	-3.006146	-1.773860	1.120449

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.629962	-3.446983	-1.401361
2	6	0	2.688033	-3.889069	-0.496550
3	6	0	1.719368	-3.003325	0.048855
4	6	0	1.730773	-1.622498	-0.343228
5	6	0	2.711771	-1.202211	-1.286528
6	6	0	3.635498	-2.088056	-1.801331
7	1	0	0.725001	-4.496748	1.266610
8	1	0	4.362633	-4.137692	-1.812782
9	1	0	2.667078	-4.933154	-0.188712
10	6	0	0.734048	-3.449461	0.970957
11	6	0	0.761164	-0.721143	0.206933
12	1	0	2.721310	-0.164614	-1.604980
13	1	0	4.371187	-1.740940	-2.523410
14	6	0	-0.184338	-1.215162	1.094617
15	6	0	-0.196665	-2.579835	1.483495
16	1	0	-0.960372	-2.909846	2.178111
17	6	0	-0.303357	2.534779	-1.460488
18	6	0	0.611656	3.436187	-0.973222
19	6	0	1.626811	3.032336	-0.064239
20	6	0	1.687986	1.657278	0.343439
21	6	0	0.735105	0.722712	-0.177020
22	6	0	-0.241925	1.177865	-1.050567

23	1	0	2.517533	4.993394	0.136048
24	1	0	-1.091673	2.832735	-2.142267
25	1	0	0.565765	4.479104	-1.281006
26	6	0	2.576359	3.954016	0.454757
27	6	0	2.697871	1.277796	1.273269
28	6	0	3.601440	2.198083	1.762674
29	6	0	3.546323	3.551805	1.348458
30	1	0	2.744800	0.244383	1.602077
31	1	0	4.359826	1.882512	2.475689
32	1	0	4.263575	4.269659	1.740060
33	8	0	-1.055838	-0.332946	1.692353
34	8	0	-1.107079	0.243754	-1.581205
35	16	0	-2.810122	0.413697	-1.358638
36	16	0	-2.759035	-0.396672	1.381225
37	7	0	-2.995616	0.704154	0.220066
38	8	0	-3.287714	0.167157	2.618696
39	8	0	-3.195211	1.645737	-2.054283
40	8	0	-3.277777	-0.865372	-1.881481
41	8	0	-3.048648	-1.792199	1.037818

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.322131	1.859976	0.007131
2	1	0	0.212819	3.835092	2.329308
3	6	0	-0.117406	2.927560	1.828629
4	6	0	-1.018961	0.590298	0.565448
5	6	0	-0.158596	0.548786	1.668234
6	6	0	0.278484	1.692236	2.325576
7	1	0	0.925327	1.601728	3.192650
8	6	0	-1.037618	-2.860966	-1.030583
9	6	0	-2.399111	-3.093575	-1.179971
10	6	0	-0.639678	-1.672926	-0.431159
11	1	0	-0.290876	-3.581868	-1.347054
12	1	0	-2.734486	-4.015484	-1.649852
13	8	0	0.300402	-0.691525	2.150026
14	8	0	0.744678	-1.469668	-0.238448
15	15	0	1.307058	-1.595018	1.265280
16	8	0	1.541953	-2.911596	1.885428
17	6	0	-1.999045	1.956427	-1.355066

18	6	0	-1.228238	4.417613	0.137068
19	6	0	-1.596897	4.442650	-1.349909
20	6	0	-2.605134	3.332432	-1.656027
21	1	0	-1.230532	1.734772	-2.112451
22	1	0	-2.755848	1.178078	-1.478365
23	1	0	-2.076990	4.808710	0.720264
24	1	0	-0.389542	5.096949	0.334090
25	1	0	-2.003020	5.426536	-1.615989
26	1	0	-0.694614	4.293695	-1.960120
27	1	0	-3.509991	3.483909	-1.048376
28	1	0	-2.920498	3.368297	-2.706348
29	6	0	-5.390380	-0.304989	0.152985
30	6	0	-5.740102	-1.794888	0.136848
31	6	0	-4.825770	-2.533987	-0.845482
32	1	0	-6.069174	0.249647	0.812827
33	1	0	-5.616344	-2.210431	1.147401
34	1	0	-6.789477	-1.948944	-0.143748
35	1	0	-4.955972	-3.619066	-0.747700
36	1	0	-5.134127	-2.285339	-1.873292
37	1	0	-5.522120	0.110562	-0.857336
38	6	0	-1.541066	-0.692194	-0.005037
39	6	0	-3.351723	-2.188663	-0.688192
40	6	0	-2.928645	-0.991935	-0.075693
41	6	0	-3.944926	-0.092310	0.618789
42	1	0	-3.672446	0.960735	0.521345
43	1	0	-3.884707	-0.306185	1.697843
44	6	0	-0.883279	3.029954	0.658493
45	7	0	2.802713	-0.775017	1.091637
46	1	0	3.528360	-1.123548	1.716661
47	16	0	3.368382	0.443422	0.091181
48	8	0	2.258825	1.181702	-0.484427
49	8	0	4.486619	1.069345	0.786312
50	6	0	4.156840	-0.532736	-1.323238
51	9	0	4.755490	0.330031	-2.149817
52	9	0	5.070954	-1.378163	-0.827919
53	9	0	3.236420	-1.225295	-1.995098

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Standard orientation:

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

1	6	0	−1.360565	1.868372	−0.010608
2	1	0	0.358891	3.772268	2.236708
3	6	0	−0.036379	2.879659	1.754684
4	6	0	−1.062629	0.586666	0.517854
5	6	0	−0.150699	0.493266	1.580770
6	6	0	0.346464	1.628040	2.219079
7	1	0	1.051595	1.509598	3.035675
8	6	0	−1.180445	−2.830655	−1.123956
9	6	0	−2.547885	−3.056806	−1.213824
10	6	0	−0.728142	−1.653821	−0.527661
11	1	0	−0.452208	−3.553497	−1.477649
12	1	0	−2.910173	−3.974197	−1.675711
13	8	0	0.269409	−0.751910	2.011909
14	8	0	0.631610	−1.447441	−0.416674
15	15	0	1.346953	−1.614209	1.075534
16	8	0	1.368810	−3.007074	1.586734
17	6	0	−2.085961	1.992985	−1.345966
18	6	0	−1.179737	4.420291	0.127641
19	6	0	−1.580642	4.462027	−1.350792
20	6	0	−2.641481	3.393980	−1.630319
21	1	0	−1.359788	1.733382	−2.132319
22	1	0	−2.883890	1.251002	−1.436422
23	1	0	−2.005342	4.838105	0.727864
24	1	0	−0.316191	5.074377	0.305202
25	1	0	−1.951104	5.463025	−1.612047
26	1	0	−0.698665	4.270586	−1.978553
27	1	0	−3.521786	3.584183	−0.996250
28	1	0	−2.985491	3.446135	−2.672378
29	6	0	−5.455893	−0.272591	0.302220
30	6	0	−5.809216	−1.762209	0.285796
31	6	0	−4.956678	−2.485056	−0.762416
32	1	0	−6.097556	0.274987	1.005858
33	1	0	−5.618566	−2.191602	1.280513
34	1	0	−6.876436	−1.911944	0.071549
35	1	0	−5.092115	−3.571795	−0.679899
36	1	0	−5.326622	−2.211099	−1.764401
37	1	0	−5.645008	0.153594	−0.695218
38	6	0	−1.621146	−0.678912	−0.053929
39	6	0	−3.473678	−2.152409	−0.671925
40	6	0	−3.011280	−0.966868	−0.068267
41	6	0	−3.985068	−0.066593	0.685550
42	1	0	−3.715613	0.986218	0.574278
43	1	0	−3.865457	−0.279708	1.759951
44	6	0	−0.859351	3.018783	0.628150

45	7	0	2.755768	-0.839718	1.001557
46	16	0	3.323986	0.361090	0.154766
47	8	0	2.388629	1.060043	-0.745625
48	8	0	4.249483	1.182156	0.953917
49	6	0	4.487012	-0.532379	-1.035850
50	9	0	5.109230	0.359533	-1.840261
51	9	0	5.441338	-1.224028	-0.383379
52	9	0	3.819426	-1.396692	-1.827072

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.869581	3.965530	1.389012
2	6	0	3.471715	2.563392	1.514551
3	6	0	2.388195	1.490284	1.347045
4	6	0	2.277343	4.152983	-0.011967
5	6	0	1.455189	1.736258	0.170206
6	6	0	1.388436	2.999681	-0.450902
7	6	0	0.742264	-3.220470	1.489879
8	6	0	-0.174434	-2.287550	1.957522
9	6	0	2.593913	-3.993829	-0.029112
10	6	0	-0.206153	-1.035912	1.350228
11	6	0	1.620878	-2.922475	0.437761
12	6	0	3.660860	-2.283018	-1.517103
13	6	0	0.666261	-0.679421	0.320656
14	6	0	1.590844	-1.642779	-0.149593
15	6	0	0.609862	0.693948	-0.276669
16	6	0	0.498000	3.199106	-1.516228
17	6	0	2.500572	-1.298643	-1.320732
18	6	0	3.166387	-3.728932	-1.425604
19	6	0	-0.282414	0.953871	-1.319889
20	6	0	-0.341748	2.185473	-1.966655
21	1	0	3.626504	4.736347	1.578761
22	1	0	3.965594	2.433256	2.485194
23	1	0	2.083971	4.096273	2.147221
24	1	0	4.247435	2.433252	0.745427
25	1	0	1.779513	1.445293	2.263110
26	1	0	1.708057	5.089604	-0.067314
27	1	0	2.850035	0.500590	1.255991
28	1	0	3.100463	4.257471	-0.736119

29	1	0	3.424534	-4.054197	0.691649
30	1	0	4.427596	-2.114238	-0.746336
31	1	0	0.772391	-4.208964	1.942918
32	1	0	-0.865705	-2.522283	2.758994
33	1	0	2.890099	-0.280513	-1.206682
34	1	0	0.460427	4.172573	-2.000648
35	1	0	2.096140	-4.971247	0.003341
36	1	0	4.140068	-2.091917	-2.485196
37	1	0	3.978844	-4.435536	-1.634938
38	1	0	1.888080	-1.276431	-2.235208
39	1	0	2.390309	-3.899965	-2.185411
40	1	0	-1.035741	2.341656	-2.784851
41	7	0	-2.949953	0.580768	0.034277
42	8	0	-1.092993	-0.050101	1.838551
43	8	0	-3.293875	0.776715	2.482644
44	8	0	-3.095103	-1.553164	1.429474
45	8	0	-1.100989	-0.120867	-1.730524
46	8	0	-3.231940	1.090545	-2.368312
47	8	0	-3.207001	-1.360339	-1.655435
48	16	0	-2.711690	-0.163434	1.545804
49	16	0	-2.733150	-0.002935	-1.548606
50	1	0	-2.959613	1.598188	0.089379

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.003308	3.888696	1.386098
2	6	0	3.582409	2.474172	1.484514
3	6	0	2.479493	1.421268	1.313393
4	6	0	2.399975	4.104344	-0.006406
5	6	0	1.530752	1.702606	0.156087
6	6	0	1.472131	2.977924	-0.437196
7	6	0	0.634337	-3.245485	1.438460
8	6	0	-0.268670	-2.291238	1.889272
9	6	0	2.513948	-4.051368	-0.034717
10	6	0	-0.255185	-1.017375	1.314383
11	6	0	1.556809	-2.959831	0.421255
12	6	0	3.642601	-2.360598	-1.498374
13	6	0	0.669443	-0.688352	0.313204
14	6	0	1.576279	-1.671904	-0.145938

15	6	0	0.648429	0.688130	-0.278514
16	6	0	0.538488	3.216114	-1.456536
17	6	0	2.510084	-1.344005	-1.303633
18	6	0	3.105975	-3.793022	-1.424655
19	6	0	-0.289108	0.972090	-1.280463
20	6	0	-0.341253	2.229695	-1.886541
21	1	0	3.775460	4.645165	1.583505
22	1	0	4.088781	2.322835	2.447472
23	1	0	2.224079	4.016700	2.151620
24	1	0	4.346448	2.345615	0.701953
25	1	0	1.884050	1.368117	2.237776
26	1	0	1.855588	5.057650	-0.042686
27	1	0	2.926932	0.426813	1.200943
28	1	0	3.222460	4.198707	-0.735077
29	1	0	3.341333	-4.136491	0.689527
30	1	0	4.405713	-2.224136	-0.716220
31	1	0	0.616521	-4.244558	1.872292
32	1	0	-1.002874	-2.518602	2.653733
33	1	0	2.929449	-0.339209	-1.177766
34	1	0	0.491547	4.205562	-1.910044
35	1	0	1.996263	-5.019887	-0.014672
36	1	0	4.140427	-2.176308	-2.460090
37	1	0	3.899322	-4.522785	-1.637871
38	1	0	1.908410	-1.292834	-2.224165
39	1	0	2.328301	-3.929978	-2.190184
40	1	0	-1.088979	2.421042	-2.648205
41	7	0	-2.976616	0.732958	0.053079
42	8	0	-1.103039	-0.032008	1.783883
43	8	0	-3.317503	0.758367	2.503965
44	8	0	-3.150040	-1.511717	1.402499
45	8	0	-1.125868	-0.056718	-1.675821
46	8	0	-3.260265	1.156230	-2.361732
47	8	0	-3.269543	-1.262002	-1.654465
48	16	0	-2.795832	-0.089212	1.435167
49	16	0	-2.823188	0.110305	-1.430304

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.490911	1.374439	0.666876

2	6	0	0.859115	1.560787	-0.099243
3	6	0	-1.727529	0.861840	-0.121116
4	6	0	-1.988357	-0.681854	-0.039164
5	1	0	-0.271177	0.697109	1.501346
6	1	0	-1.631308	1.116077	-1.182824
7	15	0	0.465937	-0.889575	-1.262799
8	6	0	-2.951081	-1.168525	-1.131089
9	6	0	-3.001201	-2.541754	-1.416706
10	6	0	-3.808307	-0.304528	-1.821807
11	6	0	-3.874270	-3.036820	-2.383681
12	1	0	-2.349154	-3.224460	-0.879612
13	6	0	-4.689718	-0.802662	-2.788171
14	1	0	-3.811593	0.758894	-1.606625
15	6	0	-4.723785	-2.166867	-3.075677
16	1	0	-3.892677	-4.102743	-2.596312
17	1	0	-5.346043	-0.115747	-3.316514
18	1	0	-5.404917	-2.551551	-3.830409
19	6	0	-2.452534	-1.148404	1.346267
20	6	0	-3.809133	-1.051484	1.692207
21	6	0	-1.551689	-1.669348	2.285957
22	6	0	-4.252790	-1.453203	2.952403
23	1	0	-4.522660	-0.664562	0.972396
24	6	0	-1.999389	-2.072855	3.548595
25	1	0	-0.504930	-1.786161	2.030640
26	6	0	-3.348715	-1.964099	3.888631
27	1	0	-5.308528	-1.372893	3.199313
28	1	0	-1.286175	-2.481314	4.260067
29	1	0	-3.695428	-2.282930	4.868367
30	6	0	0.847416	2.398922	-1.384763
31	6	0	-0.142134	3.339379	-1.694898
32	6	0	1.928475	2.252167	-2.269687
33	6	0	-0.064952	4.097130	-2.868701
34	1	0	-0.967818	3.504003	-1.016743
35	6	0	2.007737	3.008392	-3.437253
36	1	0	2.710130	1.533936	-2.044247
37	6	0	1.006867	3.934797	-3.745543
38	1	0	-0.849199	4.816790	-3.090359
39	1	0	2.851117	2.870405	-4.108871
40	1	0	1.064860	4.522930	-4.657795
41	6	0	1.898244	2.073111	0.911088
42	6	0	2.455334	1.194537	1.852441
43	6	0	2.250112	3.427712	0.957188
44	6	0	3.353946	1.663443	2.812863
45	1	0	2.203180	0.139791	1.827413

46	6	0	3.144086	3.896267	1.923226
47	1	0	1.826621	4.122855	0.240194
48	6	0	3.701333	3.016318	2.853277
49	1	0	3.783686	0.966518	3.528048
50	1	0	3.406087	4.951110	1.942759
51	1	0	4.401307	3.380145	3.601247
52	8	0	1.321757	0.200711	-0.455135
53	8	0	-0.692409	-1.345994	-0.252033
54	8	0	0.089949	-0.626809	-2.667774
55	6	0	-2.329146	2.560791	1.395814
56	8	0	-2.813884	1.604840	0.424221
57	8	0	-0.923518	2.636209	1.159546
58	6	0	-2.620621	2.088180	2.819911
59	1	0	-2.256549	2.835463	3.533082
60	1	0	-3.697972	1.959489	2.961160
61	1	0	-2.134818	1.133698	3.032992
62	6	0	-2.952025	3.919365	1.104071
63	1	0	-4.033766	3.874421	1.264941
64	1	0	-2.530220	4.676582	1.772720
65	1	0	-2.765431	4.215418	0.068442
66	7	0	1.537359	-2.225515	-1.204342
67	1	0	1.519867	-2.795101	-2.049364
68	16	0	2.283756	-2.993422	0.075385
69	8	0	1.854266	-2.392581	1.330745
70	8	0	2.262328	-4.427936	-0.180127
71	6	0	4.083520	-2.476099	-0.174307
72	9	0	4.834521	-3.094849	0.741929
73	9	0	4.219195	-1.156678	-0.042255
74	9	0	4.487125	-2.842156	-1.398434

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534038	1.396732	-0.598008
2	6	0	-0.841033	1.567419	0.128865
3	6	0	1.729404	0.815420	0.197829
4	6	0	1.921218	-0.737072	0.054132
5	1	0	0.323966	0.765051	-1.469191
6	1	0	1.624977	1.034784	1.264345
7	15	0	-0.584524	-0.971564	1.190022

8	6	0	2.838697	-1.300861	1.154838
9	6	0	2.707745	-2.649157	1.517588
10	6	0	3.829720	-0.530751	1.776150
11	6	0	3.546714	-3.212819	2.478422
12	1	0	1.928670	-3.249328	1.058358
13	6	0	4.672706	-1.096631	2.739155
14	1	0	3.953422	0.515076	1.512550
15	6	0	4.536204	-2.439330	3.094230
16	1	0	3.418422	-4.256954	2.754364
17	1	0	5.431090	-0.478667	3.215565
18	1	0	5.186277	-2.877481	3.848500
19	6	0	2.453838	-1.144398	-1.334935
20	6	0	3.820035	-1.044672	-1.639481
21	6	0	1.580043	-1.634830	-2.317263
22	6	0	4.301265	-1.409953	-2.897689
23	1	0	4.514030	-0.685197	-0.887283
24	6	0	2.064412	-1.998383	-3.578905
25	1	0	0.526111	-1.755887	-2.090073
26	6	0	3.423768	-1.886018	-3.877120
27	1	0	5.365345	-1.327511	-3.109782
28	1	0	1.369104	-2.381382	-4.322226
29	1	0	3.798472	-2.175705	-4.856631
30	6	0	-0.856414	2.375705	1.439674
31	6	0	0.096473	3.343746	1.778447
32	6	0	-1.931294	2.166568	2.318432
33	6	0	-0.011848	4.071879	2.969270
34	1	0	0.923329	3.542784	1.110282
35	6	0	-2.044561	2.894668	3.501073
36	1	0	-2.671119	1.410979	2.076956
37	6	0	-1.082070	3.852754	3.836084
38	1	0	0.748717	4.810816	3.213646
39	1	0	-2.881049	2.702819	4.169048
40	1	0	-1.164486	4.415723	4.763313
41	6	0	-1.819179	2.176492	-0.901188
42	6	0	-2.499484	1.332290	-1.791718
43	6	0	-2.003661	3.561328	-1.004468
44	6	0	-3.348338	1.870144	-2.763327
45	1	0	-2.378144	0.256566	-1.712210
46	6	0	-2.850358	4.096279	-1.978622
47	1	0	-1.486929	4.227742	-0.321407
48	6	0	-3.527676	3.252281	-2.863013
49	1	0	-3.874569	1.198929	-3.438220
50	1	0	-2.982606	5.174540	-2.040701
51	1	0	-4.192131	3.667586	-3.618008

52	8	0	-1.350565	0.244132	0.381593
53	8	0	0.630456	-1.359234	0.149740
54	8	0	-0.093085	-0.570048	2.535254
55	6	0	2.425362	2.554991	-1.232205
56	8	0	2.860527	1.544218	-0.305391
57	8	0	1.022787	2.671131	-1.029088
58	6	0	2.735795	2.145296	-2.674753
59	1	0	2.408565	2.937042	-3.358309
60	1	0	3.811651	1.987112	-2.800940
61	1	0	2.224672	1.217754	-2.940810
62	6	0	3.087002	3.879575	-0.863382
63	1	0	4.170699	3.806933	-1.004366
64	1	0	2.702846	4.683193	-1.500899
65	1	0	2.886804	4.126869	0.182768
66	7	0	-1.598556	-2.227312	1.110404
67	16	0	-2.251932	-2.877952	-0.172023
68	8	0	-2.003328	-2.198975	-1.465128
69	8	0	-2.172171	-4.347251	-0.151591
70	6	0	-4.088406	-2.563819	0.139890
71	9	0	-4.825539	-3.079670	-0.868987
72	9	0	-4.364602	-1.246659	0.213572
73	9	0	-4.504874	-3.138486	1.284243

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.065547	2.351685	1.221470
2	6	0	2.752780	2.647396	1.664325
3	6	0	1.678233	1.912732	1.213176
4	6	0	1.857140	0.839686	0.294074
5	6	0	3.192540	0.522000	-0.127094
6	6	0	4.277485	1.309302	0.347672
7	6	0	0.760211	0.051942	-0.193716
8	6	0	1.052120	-1.037727	-1.003766
9	6	0	2.365587	-1.370532	-1.405934
10	6	0	3.412007	-0.583194	-0.990301
11	6	0	-0.648871	0.388649	0.195068
12	6	0	-1.260188	1.597849	-0.282670
13	6	0	-2.599090	1.918673	0.124535
14	6	0	-3.311241	1.024002	0.965462

15	6	0	-2.745177	-0.158974	1.372525
16	6	0	-1.419139	-0.457861	0.983177
17	6	0	-0.599811	2.483290	-1.181743
18	6	0	-1.215405	3.632583	-1.626682
19	6	0	-2.524199	3.962288	-1.196697
20	6	0	-3.199365	3.120219	-0.342300
21	16	0	-0.255781	-2.165138	-1.511619
22	16	0	-0.789243	-2.056915	1.502416
23	8	0	0.331887	-3.290803	-2.243081
24	8	0	-1.370876	-1.404185	-2.063635
25	7	0	-0.798155	-2.883747	-0.028105
26	8	0	-1.790577	-2.749768	2.313358
27	8	0	0.584442	-1.942733	2.000059
28	1	0	4.903427	2.942127	1.582277
29	1	0	2.592678	3.457398	2.370728
30	1	0	0.681821	2.146781	1.570956
31	1	0	5.282918	1.063105	0.014716
32	1	0	2.522742	-2.237329	-2.038264
33	1	0	4.426520	-0.815113	-1.304461
34	1	0	-4.325102	1.275065	1.266403
35	1	0	-3.288704	-0.868812	1.985907
36	1	0	0.398090	2.241934	-1.529703
37	1	0	-0.694635	4.289000	-2.318498
38	1	0	-2.996168	4.874279	-1.552167
39	1	0	-4.210897	3.354900	-0.019810
40	1	0	-0.371204	-3.808418	0.078811

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.300589	3.341930	-1.214014
2	6	0	3.266723	1.990678	-1.637660
3	6	0	2.274979	1.142203	-1.193070
4	6	0	1.259032	1.591056	-0.301082
5	6	0	1.274552	2.971194	0.092613
6	6	0	2.320495	3.817063	-0.370614
7	6	0	0.210322	0.729218	0.176406
8	6	0	-0.809611	1.292021	0.932152
9	6	0	-0.804440	2.655793	1.302479
10	6	0	0.231244	3.471396	0.915151

11	6	0	0.210533	-0.729162	-0.176444
12	6	0	1.259444	-1.590730	0.301090
13	6	0	1.275368	-2.970850	-0.092641
14	6	0	0.232231	-3.471331	-0.915224
15	6	0	-0.803655	-2.656007	-1.302605
16	6	0	-0.809189	-1.292233	-0.932281
17	6	0	2.275244	-1.141604	1.193112
18	6	0	3.267203	-1.989813	1.637727
19	6	0	3.301456	-3.341050	1.214062
20	6	0	2.321528	-3.816438	0.370612
21	16	0	-2.280107	0.314656	1.388832
22	16	0	-2.279996	-0.315284	-1.388823
23	8	0	-3.140971	1.197080	2.202583
24	8	0	-1.766800	-0.904328	2.053750
25	7	0	-3.064023	-0.000714	0.000050
26	8	0	-3.140567	-1.197797	-2.202766
27	8	0	-1.767123	0.904051	-2.053450
28	1	0	4.089417	4.002691	-1.566768
29	1	0	4.023695	1.620990	-2.325528
30	1	0	2.254847	0.115040	-1.539507
31	1	0	2.321309	4.858826	-0.054831
32	1	0	-1.635180	3.026906	1.893608
33	1	0	0.248065	4.518963	1.210091
34	1	0	0.249358	-4.518892	-1.210171
35	1	0	-1.634257	-3.027334	-1.893791
36	1	0	2.254812	-0.114450	1.539558
37	1	0	4.024047	-1.619937	2.325635
38	1	0	4.090452	-4.001600	1.566838
39	1	0	2.322650	-4.858193	0.054803

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.765382	0.999630	-0.373524
2	6	0	4.888464	1.962986	-0.879826
3	6	0	5.257838	-0.193871	0.136147
4	6	0	3.510091	1.730382	-0.875117
5	6	0	3.872918	-0.421155	0.140142
6	6	0	2.971603	0.538186	-0.368092
7	6	0	-2.946944	3.754081	-0.987458

8	6	0	3.306659	-1.675756	0.686261
9	6	0	-2.418176	2.461185	-0.921256
10	6	0	-0.671138	-0.005589	-1.319890
11	6	0	-2.549920	-1.369599	-2.292052
12	6	0	-2.443209	4.762206	-0.163866
13	6	0	-1.382806	-1.326307	-1.519476
14	6	0	-3.233104	-2.572329	-2.493537
15	6	0	-0.890788	-2.517398	-0.966850
16	6	0	-1.380093	2.150882	-0.031388
17	6	0	-2.743341	-3.752374	-1.930387
18	6	0	-1.568351	-3.720033	-1.172081
19	6	0	-0.810260	0.730114	0.106240
20	6	0	-1.409760	4.463299	0.728624
21	6	0	-0.886253	3.170865	0.796272
22	6	0	-1.586547	-0.062048	1.170377
23	6	0	-2.989015	-0.072234	1.185468
24	6	0	-0.902489	-0.799077	2.145852
25	6	0	-3.689947	-0.806549	2.143373
26	6	0	-1.604215	-1.527789	3.110712
27	6	0	-3.000019	-1.537493	3.114166
28	1	0	6.837413	1.177249	-0.376085
29	1	0	5.277307	2.896300	-1.279522
30	1	0	5.926311	-0.950415	0.532935
31	1	0	-3.751158	3.969044	-1.686869
32	1	0	2.844304	2.491546	-1.275297
33	1	0	-2.833217	1.697093	-1.572536
34	1	0	-1.005459	0.685505	-2.096964
35	1	0	-2.927370	-0.457793	-2.751863
36	1	0	-2.850267	5.768723	-0.216891
37	1	0	-4.137113	-2.586940	-3.097413
38	1	0	0.025446	-2.503800	-0.385699
39	1	0	-3.267488	-4.691909	-2.087191
40	1	0	-1.176519	-4.636652	-0.737849
41	1	0	-3.548225	0.500114	0.452377
42	1	0	-1.008213	5.238373	1.376912
43	1	0	-0.084055	2.945782	1.490822
44	1	0	0.180647	-0.807170	2.147946
45	1	0	-4.777135	-0.800515	2.132750
46	1	0	-1.052230	-2.090079	3.860198
47	1	0	-3.545114	-2.104660	3.864644
48	5	0	1.406591	0.341215	-0.412462
49	8	0	0.751170	-0.159347	-1.501918
50	8	0	2.111150	-1.914724	0.762253
51	8	0	0.565395	0.854577	0.539263

52	8	0	4.234037	-2.566781	1.113551
53	1	0	3.745685	-3.340955	1.449708

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.746863	-0.284891	0.019073
2	6	0	5.061023	0.826925	-0.496445
3	6	0	5.033334	-1.406580	0.452185
4	6	0	3.662247	0.831547	-0.582205
5	6	0	3.641335	-1.376313	0.356435
6	6	0	2.931576	-0.280759	-0.149155
7	6	0	-0.646776	4.281573	-1.438914
8	6	0	2.689092	-2.466130	0.749379
9	6	0	-0.925329	2.926788	-1.227679
10	6	0	-0.645366	-0.145151	-1.254199
11	6	0	-2.969674	-0.947155	-1.867816
12	6	0	0.268467	4.947429	-0.620934
13	6	0	-1.707311	-1.238858	-1.331284
14	6	0	-3.956534	-1.930350	-1.974499
15	6	0	-1.443561	-2.552477	-0.918586
16	6	0	-0.298470	2.205439	-0.199826
17	6	0	-3.688035	-3.235362	-1.550847
18	6	0	-2.427933	-3.539153	-1.025991
19	6	0	-0.592777	0.716096	0.104109
20	6	0	0.901271	4.240503	0.406537
21	6	0	0.620961	2.887831	0.611294
22	6	0	-1.850071	0.587919	0.988196
23	6	0	-2.975525	1.412575	0.848409
24	6	0	-1.881858	-0.411527	1.973268
25	6	0	-4.103121	1.239820	1.657333
26	6	0	-3.005798	-0.585306	2.783356
27	6	0	-4.125268	0.238276	2.630366
28	1	0	6.834016	-0.271373	0.077563
29	1	0	5.627160	1.694263	-0.834530
30	1	0	5.537212	-2.283890	0.851718
31	1	0	-1.144103	4.812003	-2.248833
32	1	0	3.150662	1.703226	-0.987321
33	1	0	-1.639502	2.436930	-1.884622
34	1	0	-0.835312	0.533351	-2.094638

35	1	0	-3.185542	0.064618	-2.208855
36	1	0	0.490614	5.999749	-0.785823
37	1	0	-4.930108	-1.678609	-2.391250
38	1	0	-0.464502	-2.794691	-0.517602
39	1	0	-4.450873	-4.007226	-1.633588
40	1	0	-2.205120	-4.552354	-0.697240
41	1	0	-2.978233	2.210900	0.113077
42	1	0	1.623544	4.741588	1.048092
43	1	0	1.124600	2.330650	1.393969
44	1	0	-1.008647	-1.042874	2.095356
45	1	0	-4.961777	1.896106	1.527371
46	1	0	-3.004630	-1.369615	3.537681
47	1	0	-5.000594	0.103557	3.262734
48	5	0	1.348816	-0.647971	-0.089667
49	8	0	0.660177	-0.645040	-1.377678
50	8	0	1.441253	-2.076202	0.510527
51	8	0	0.497616	0.158931	0.795271
52	8	0	3.001014	-3.555527	1.218844

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.662148	1.096406	0.145419
2	1	0	-4.295460	0.077873	-1.776922
3	6	0	-3.293028	0.089125	-1.354878
4	6	0	-0.705172	0.142464	-0.274017
5	6	0	-1.104378	-0.854040	-1.179861
6	6	0	-2.387086	-0.896399	-1.724183
7	1	0	-2.660556	-1.692465	-2.408261
8	6	0	2.439226	-0.840000	1.678815
9	6	0	3.301604	0.186303	1.320126
10	6	0	1.147708	-0.834988	1.152476
11	1	0	2.751323	-1.641281	2.339608
12	1	0	4.310702	0.202303	1.725453
13	6	0	-1.326421	2.067326	1.269731
14	6	0	-4.016926	2.086801	-0.016449
15	6	0	-3.752323	2.752709	1.337428
16	6	0	-2.303875	3.242223	1.398017
17	1	0	-1.327834	1.491520	2.208002
18	1	0	-0.305310	2.444789	1.162564

19	1	0	-4.058826	2.864481	-0.795408
20	1	0	-5.000910	1.601863	-0.022940
21	1	0	-4.453876	3.582618	1.486055
22	1	0	-3.931385	2.032789	2.148512
23	1	0	-2.130696	3.963555	0.585400
24	1	0	-2.108476	3.773818	2.337367
25	6	0	2.155241	3.361267	-1.345346
26	6	0	3.621639	2.925723	-1.314607
27	6	0	3.928647	2.240162	0.020276
28	1	0	1.926934	3.905391	-2.270002
29	1	0	3.816632	2.231219	-2.143930
30	1	0	4.289815	3.784427	-1.452889
31	1	0	4.930074	1.792683	0.004263
32	1	0	3.950622	3.000697	0.816749
33	1	0	1.966321	4.057685	-0.514730
34	6	0	0.696076	0.164355	0.273949
35	6	0	2.914354	1.175569	0.405631
36	6	0	1.611096	1.164647	-0.133826
37	6	0	1.224055	2.147892	-1.230766
38	1	0	0.191820	2.485289	-1.101143
39	1	0	1.232932	1.593863	-2.181937
40	6	0	-2.957870	1.070394	-0.411941
41	16	0	0.122953	-2.252224	1.530882
42	16	0	-0.011703	-2.231079	-1.540249
43	7	0	0.147540	-3.054855	-0.017106
44	1	0	-0.507325	-3.841985	0.003180
45	8	0	0.827858	-3.159038	2.437723
46	8	0	-1.248369	-1.842290	1.853838
47	8	0	-0.712781	-3.205895	-2.381088
48	8	0	1.310566	-1.733020	-1.907393

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.623806	1.136740	-0.147359
2	1	0	4.321279	0.162094	1.701001
3	6	0	3.309973	0.150635	1.296127
4	6	0	0.706042	0.136676	0.261459
5	6	0	1.150148	-0.880922	1.120327
6	6	0	2.442647	-0.878497	1.641204

7	1	0	2.749554	-1.694090	2.287870
8	6	0	-2.442874	-0.877767	-1.641274
9	6	0	-3.309889	0.151631	-1.296201
10	6	0	-1.150382	-0.880574	-1.120377
11	1	0	-2.750017	-1.693264	-2.287945
12	1	0	-4.321186	0.163413	-1.701092
13	6	0	1.242175	2.106820	-1.258943
14	6	0	3.944236	2.208210	-0.003092
15	6	0	3.649291	2.862516	-1.356586
16	6	0	2.185605	3.307996	-1.402072
17	1	0	1.237008	1.534600	-2.199487
18	1	0	0.214909	2.460493	-1.132087
19	1	0	3.960054	2.992837	0.771618
20	1	0	4.948715	1.764638	-0.002794
21	1	0	4.325816	3.713093	-1.518944
22	1	0	3.836756	2.141684	-2.165460
23	1	0	2.004530	4.025659	-0.586445
24	1	0	1.964998	3.835656	-2.339980
25	6	0	-2.184630	3.308573	1.402129
26	6	0	-3.648449	2.863544	1.356566
27	6	0	-3.943543	2.209389	0.003035
28	1	0	-1.963905	3.836139	2.340062
29	1	0	-3.836175	2.142742	2.165407
30	1	0	-4.324714	3.714327	1.518928
31	1	0	-4.948173	1.766157	0.002668
32	1	0	-3.959060	2.994057	-0.771641
33	1	0	-2.003303	4.026206	0.586531
34	6	0	-0.705978	0.136883	-0.261471
35	6	0	-2.926501	1.146363	-0.386498
36	6	0	-1.623464	1.137183	0.147367
37	6	0	-1.241569	2.107118	1.259002
38	1	0	-0.214181	2.460458	1.132195
39	1	0	-1.236621	1.534856	2.199521
40	6	0	2.926864	1.145503	0.386452
41	16	0	-0.111977	-2.342144	-1.424457
42	16	0	0.111259	-2.342138	1.424476
43	7	0	-0.000548	-3.120728	0.000027
44	8	0	-0.856228	-3.215132	-2.356183
45	8	0	1.192030	-1.827304	-1.907714
46	8	0	0.855239	-3.215302	2.356267
47	8	0	-1.192542	-1.826795	1.907734

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.672053	-1.839656	-2.011268
2	6	0	-3.938584	-1.526873	-0.696442
3	6	0	-2.957719	-0.901976	0.121449
4	6	0	-1.673552	-0.586854	-0.436466
5	6	0	-1.429790	-0.935093	-1.796684
6	6	0	-2.402576	-1.541458	-2.563150
7	1	0	-4.183810	-0.852349	1.908239
8	1	0	-4.430687	-2.317812	-2.625315
9	1	0	-4.908331	-1.756590	-0.260480
10	6	0	-3.214900	-0.598251	1.484709
11	6	0	-0.687658	0.059393	0.386833
12	1	0	-0.461880	-0.718061	-2.236306
13	1	0	-2.192426	-1.794485	-3.599113
14	6	0	-0.992142	0.350641	1.710055
15	6	0	-2.253455	-0.000816	2.261386
16	1	0	-2.439730	0.216720	3.308749
17	6	0	2.230508	1.534073	-1.641853
18	6	0	3.194947	0.570727	-1.486521
19	6	0	2.954198	-0.571743	-0.678727
20	6	0	1.679469	-0.720611	-0.033848
21	6	0	0.680716	0.297679	-0.193252
22	6	0	0.977365	1.412645	-0.977926
23	1	0	4.906152	-1.450159	-0.997294
24	1	0	2.417362	2.408223	-2.256404
25	1	0	4.157593	0.674400	-1.981234
26	6	0	3.943742	-1.577188	-0.506981
27	6	0	1.454584	-1.888726	0.751280
28	6	0	2.435983	-2.844142	0.899097
29	6	0	3.693302	-2.689692	0.265396
30	1	0	0.501622	-2.015724	1.252681
31	1	0	2.246007	-3.720586	1.512494
32	1	0	4.459138	-3.450322	0.392256
33	6	0	-0.022978	1.027365	2.648073
34	8	0	0.321948	0.524786	3.696307
35	8	0	0.402904	2.249307	2.282900
36	1	0	-0.040050	2.540871	1.449353
37	6	0	0.020359	2.541660	-1.091188
38	8	0	-0.680718	2.969259	-0.181836
39	8	0	0.012054	3.122466	-2.308676

40	1	0	-0.599065	3.882698	-2.261005

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.600334	-2.529834	1.223547
2	6	0	3.912340	-1.711050	0.159664
3	6	0	2.962759	-0.788761	-0.359618
4	6	0	1.658602	-0.711943	0.233769
5	6	0	1.372615	-1.572634	1.332176
6	6	0	2.315829	-2.455163	1.815445
7	1	0	4.254361	-0.009039	-1.917616
8	1	0	4.338335	-3.227748	1.613272
9	1	0	4.898029	-1.755385	-0.300732
10	6	0	3.268524	0.054905	-1.460259
11	6	0	0.692195	0.221490	-0.281241
12	1	0	0.398221	-1.512574	1.804943
13	1	0	2.073999	-3.091182	2.663762
14	6	0	1.046300	1.041712	-1.344954
15	6	0	2.332471	0.936565	-1.940916
16	1	0	2.554525	1.573930	-2.791822
17	6	0	-2.336723	0.893866	1.961354
18	6	0	-3.275877	0.031795	1.451626
19	6	0	-2.968009	-0.792712	0.335879
20	6	0	-1.657805	-0.712152	-0.244805
21	6	0	-0.696859	0.210965	0.298576
22	6	0	-1.042934	1.009347	1.382019
23	1	0	-4.908181	-1.744589	0.243105
24	1	0	-2.556867	1.508385	2.829612
25	1	0	-4.266639	-0.035785	1.898776
26	6	0	-3.918418	-1.698655	-0.208660
27	6	0	-1.368301	-1.558610	-1.353795
28	6	0	-2.312878	-2.427139	-1.861055
29	6	0	-3.603845	-2.502236	-1.284169
30	1	0	-0.387501	-1.504047	-1.814787
31	1	0	-2.065402	-3.053122	-2.715478
32	1	0	-4.343008	-3.188492	-1.692006
33	6	0	0.114936	2.066276	-1.963217
34	8	0	-0.082329	2.055063	-3.174247
35	8	0	-0.405932	2.967013	-1.159536

36	1	0	-0.058068	2.901803	-0.154148
37	6	0	-0.090828	2.029221	2.011268
38	8	0	0.421559	2.884255	1.207425
39	8	0	0.071906	1.959461	3.241023

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.096375	1.690378	-0.148319
2	6	0	2.703029	0.344728	0.300003
3	6	0	0.468804	-0.134825	0.075268
4	1	0	2.226699	2.504848	0.573642
5	1	0	2.481505	2.051642	-1.108511
6	6	0	1.841262	-0.696942	-0.487604
7	6	0	2.260595	0.126511	1.764475
8	1	0	2.777941	-0.722491	2.221402
9	1	0	2.476305	1.002464	2.385408
10	6	0	0.730953	-0.137215	1.628327
11	1	0	0.440206	-1.110507	2.036319
12	1	0	0.112339	0.603443	2.138563
13	1	0	3.781393	0.263110	0.131910
14	6	0	2.128639	-2.158015	-0.101186
15	1	0	1.480414	-2.844909	-0.658069
16	1	0	3.164361	-2.410198	-0.361304
17	1	0	1.996897	-2.368676	0.962548
18	6	0	1.976703	-0.587971	-2.019755
19	1	0	3.014588	-0.780224	-2.318363
20	1	0	1.353958	-1.338130	-2.520829
21	1	0	1.693411	0.388389	-2.425857
22	6	0	-0.773817	-0.884286	-0.394875
23	1	0	-0.831481	-0.951611	-1.485387
24	1	0	-0.766017	-1.903315	0.005686
25	6	0	0.617540	1.342544	-0.298363
26	8	0	-0.254398	2.128344	-0.640752
27	16	0	-2.416713	-0.254301	0.114925
28	8	0	-3.399388	-1.278258	-0.221784
29	8	0	-2.318805	0.272135	1.478621
30	8	0	-2.667771	0.959490	-0.928413
31	1	0	-1.912723	1.601842	-0.825162

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.966317	0.544221	-0.274093
2	6	0	2.443269	-0.837015	0.153426
3	6	0	0.527011	0.434426	0.141102
4	1	0	3.721079	0.973079	0.397071
5	1	0	3.385200	0.559267	-1.287565
6	6	0	1.030536	-0.911619	-0.520730
7	6	0	2.095965	-0.728985	1.660059
8	1	0	1.897698	-1.712096	2.099351
9	1	0	2.922312	-0.282947	2.229054
10	6	0	0.817023	0.164828	1.661287
11	1	0	-0.057224	-0.336264	2.084247
12	1	0	0.955079	1.104472	2.210117
13	1	0	3.108148	-1.671419	-0.100646
14	6	0	0.281344	-2.197648	-0.124120
15	1	0	-0.696263	-2.235736	-0.609621
16	1	0	0.879330	-3.064789	-0.445519
17	1	0	0.102858	-2.286275	0.948952
18	6	0	1.045667	-0.848847	-2.060466
19	1	0	1.575576	-1.719144	-2.473079
20	1	0	0.015016	-0.873580	-2.430012
21	1	0	1.521986	0.052563	-2.463827
22	6	0	-0.826954	1.068408	-0.174261
23	1	0	-0.954314	1.954712	0.454939
24	1	0	-0.860953	1.408586	-1.213954
25	6	0	1.678851	1.381245	-0.244289
26	8	0	1.615284	2.578052	-0.459770
27	16	0	-2.377651	0.093394	0.050214
28	8	0	-2.410138	-0.857166	-1.107700
29	8	0	-2.244671	-0.582516	1.379974
30	8	0	-3.438884	1.139278	-0.001305

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Standard orientation:

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

1	6	0	2.673673	-1.909598	0.227871
2	6	0	1.342680	-1.560374	0.131162
3	6	0	0.945032	-0.197384	0.023243
4	6	0	1.972744	0.805471	-0.003545
5	6	0	3.335073	0.411039	0.100715
6	6	0	3.682655	-0.916621	0.217533
7	1	0	2.950774	-2.957790	0.304975
8	1	0	0.593200	-2.343879	0.108209
9	6	0	-0.427230	0.217943	-0.067464
10	6	0	1.612547	2.174282	-0.140142
11	1	0	4.102147	1.182225	0.082921
12	1	0	4.727658	-1.205124	0.295017
13	6	0	0.292609	2.543928	-0.248156
14	6	0	-0.725055	1.559977	-0.209519
15	1	0	2.400464	2.923898	-0.161505
16	1	0	0.020032	3.589978	-0.359050
17	1	0	-1.758703	1.884203	-0.295624
18	6	0	-1.524854	-0.844556	-0.037450
19	1	0	-1.308748	-1.566948	0.754519
20	8	0	-1.592470	-1.597040	-1.241895
21	1	0	-2.100466	-1.073445	-1.887093
22	6	0	-2.898122	-0.247997	0.260713
23	8	0	-3.109025	-0.056925	1.578871
24	1	0	-3.994054	0.342878	1.683019
25	8	0	-3.713857	0.029883	-0.593869

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.600961	-1.933637	0.267478
2	6	0	1.278145	-1.541017	0.235726
3	6	0	0.913947	-0.172186	0.070987
4	6	0	1.972067	0.790044	-0.078657
5	6	0	3.325541	0.350582	-0.047870
6	6	0	3.639706	-0.980337	0.124938
7	1	0	2.848593	-2.985895	0.392623
8	1	0	0.491006	-2.282938	0.304644
9	6	0	-0.455698	0.267468	0.062908
10	6	0	1.645336	2.162492	-0.251734

11	1	0	4.114717	1.092734	-0.163071
12	1	0	4.679791	-1.300460	0.147356
13	6	0	0.327497	2.560649	-0.261429
14	6	0	-0.715635	1.616701	-0.096209
15	1	0	2.450724	2.886274	-0.369947
16	1	0	0.075282	3.611981	-0.387943
17	1	0	-1.744583	1.958243	-0.060169
18	6	0	-1.579512	-0.755266	0.235851
19	1	0	-1.447017	-1.244708	1.213900
20	8	0	-1.501650	-1.749852	-0.790397
21	1	0	-2.398654	-1.642039	-1.204102
22	6	0	-3.032829	-0.148829	0.233062
23	8	0	-3.319974	0.645278	1.155700
24	8	0	-3.751753	-0.569574	-0.720753

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.754571	-2.988329	4.730874
2	6	0	-1.850490	-2.785243	3.921661
3	6	0	-1.817008	-1.818137	2.880100
4	6	0	-0.625962	-1.049445	2.673622
5	6	0	0.482904	-1.275161	3.535000
6	6	0	0.420434	-2.222857	4.534888
7	1	0	-3.865018	-2.128614	2.269550
8	1	0	-0.788854	-3.733102	5.521162
9	1	0	-2.759289	-3.364382	4.066684
10	6	0	-2.950433	-1.578516	2.062733
11	6	0	-0.596622	-0.089808	1.606725
12	1	0	1.390362	-0.696253	3.398756
13	1	0	1.280986	-2.384411	5.178367
14	6	0	-1.721327	0.061418	0.819810
15	6	0	-2.941340	-0.644246	1.045828
16	6	0	2.962635	0.997946	0.661349
17	6	0	3.029130	2.223566	1.300052
18	6	0	1.928887	2.776428	2.001839
19	6	0	0.711870	2.026653	2.100479
20	6	0	0.620693	0.766008	1.425414
21	6	0	1.708705	0.314219	0.699136
22	1	0	2.952772	4.598484	2.569950

23	1	0	3.971854	2.764905	1.307833
24	6	0	2.024386	4.038190	2.650981
25	6	0	-0.359323	2.568764	2.863309
26	6	0	-0.236585	3.796515	3.478614
27	6	0	0.963527	4.541433	3.370819
28	1	0	-1.283751	2.008030	2.955024
29	1	0	-1.067845	4.197176	4.052298
30	1	0	1.044945	5.507644	3.860949
31	8	0	-1.672758	1.008470	-0.220261
32	8	0	1.554924	-0.916333	0.039872
33	16	0	1.308380	-0.955361	-1.604801
34	16	0	-1.433600	0.472383	-1.770020
35	7	0	0.250375	0.337789	-1.891236
36	1	0	0.709201	1.179595	-2.234659
37	8	0	-1.760236	1.620955	-2.587805
38	8	0	2.521483	-0.532304	-2.282270
39	8	0	0.662025	-2.223885	-1.826511
40	8	0	-2.009021	-0.845417	-1.916521
41	6	0	4.189866	0.421757	0.045844
42	6	0	4.588776	-0.892984	0.320349
43	6	0	5.008982	1.215179	-0.769860
44	6	0	5.778991	-1.396835	-0.209062
45	1	0	3.973174	-1.526155	0.950853
46	6	0	6.193817	0.703523	-1.299502
47	1	0	4.705124	2.227945	-1.014881
48	6	0	6.590981	-0.606353	-1.022233
49	1	0	7.509293	-1.003962	-1.437220
50	6	0	-4.181300	-0.381217	0.264824
51	6	0	-4.909025	-1.453872	-0.277694
52	6	0	-4.675676	0.917704	0.102449
53	6	0	-6.103441	-1.224821	-0.956188
54	1	0	-4.521388	-2.462761	-0.190324
55	6	0	-5.878669	1.139090	-0.577461
56	1	0	-4.130888	1.761484	0.513134
57	6	0	-6.600181	0.074325	-1.110454
58	1	0	-7.529902	0.248554	-1.640413
59	6	0	7.072658	1.597394	-2.138041
60	6	0	6.173442	-2.812611	0.132528
61	6	0	-6.385649	2.554849	-0.698108
62	6	0	-6.897390	-2.370307	-1.533290
63	9	0	5.206152	-3.699628	-0.208298
64	9	0	7.310595	-3.199808	-0.487490
65	9	0	6.377807	-2.961865	1.469430
66	9	0	7.880221	0.897045	-2.966186

67	9	0	7.881903	2.369701	-1.360965
68	9	0	6.348568	2.450036	-2.903859
69	9	0	-7.524740	2.639353	-1.421473
70	9	0	-6.649162	3.092839	0.523969
71	9	0	-5.473612	3.368231	-1.285170
72	9	0	-8.104664	-2.496748	-0.918731
73	9	0	-7.156212	-2.188630	-2.852160
74	9	0	-6.264118	-3.558107	-1.407657

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.020906	-3.417887	4.626962
2	6	0	-2.047863	-3.123917	3.756185
3	6	0	-1.925544	-2.067416	2.812564
4	6	0	-0.717213	-1.300650	2.770541
5	6	0	0.321674	-1.626935	3.685836
6	6	0	0.174615	-2.658644	4.589329
7	1	0	-3.911859	-2.298523	2.000692
8	1	0	-1.123804	-4.232084	5.340263
9	1	0	-2.970140	-3.701247	3.775000
10	6	0	-2.982428	-1.737958	1.927308
11	6	0	-0.598726	-0.242225	1.814400
12	1	0	1.243795	-1.055032	3.658764
13	1	0	0.984581	-2.894902	5.275246
14	6	0	-1.651925	0.025766	0.952697
15	6	0	-2.881729	-0.707698	1.013012
16	6	0	2.936687	0.896404	0.898259
17	6	0	3.021214	2.091191	1.586515
18	6	0	1.951905	2.581684	2.377764
19	6	0	0.744008	1.816999	2.467913
20	6	0	0.646941	0.584756	1.747500
21	6	0	1.718956	0.146414	0.986195
22	1	0	2.979114	4.377986	3.013256
23	1	0	3.943860	2.666377	1.548497
24	6	0	2.056886	3.805845	3.093344
25	6	0	-0.312387	2.318032	3.278592
26	6	0	-0.181472	3.509958	3.960127
27	6	0	1.013963	4.264818	3.868640
28	1	0	-1.234504	1.749739	3.349964

29	1	0	−1.004206	3.876068	4.569564
30	1	0	1.103978	5.204968	4.407377
31	8	0	−1.530233	1.073118	0.069140
32	8	0	1.631527	−1.065684	0.352340
33	16	0	1.010943	−1.176797	−1.285895
34	16	0	−1.075155	0.765449	−1.587751
35	7	0	0.475490	0.322013	−1.553240
36	8	0	−1.136902	2.119774	−2.119776
37	8	0	2.218425	−1.386197	−2.083017
38	8	0	0.033616	−2.256097	−1.175021
39	8	0	−2.011684	−0.253741	−2.063632
40	6	0	4.098872	0.417224	0.103684
41	6	0	4.568089	−0.903801	0.214311
42	6	0	4.781313	1.300360	−0.741015
43	6	0	5.700591	−1.309689	−0.486322
44	1	0	4.037990	−1.608935	0.841703
45	6	0	5.914975	0.882215	−1.447355
46	1	0	4.407089	2.310729	−0.872256
47	6	0	6.385475	−0.422193	−1.323509
48	1	0	7.260174	−0.749273	−1.874621
49	6	0	−4.051664	−0.369094	0.159851
50	6	0	−4.751285	−1.387506	−0.504110
51	6	0	−4.513403	0.949952	0.043460
52	6	0	−5.889313	−1.093846	−1.256016
53	1	0	−4.377784	−2.404495	−0.461658
54	6	0	−5.656341	1.234686	−0.707033
55	1	0	−3.973089	1.753360	0.529922
56	6	0	−6.353516	0.218748	−1.362287
57	1	0	−7.233649	0.446568	−1.954180
58	6	0	6.652329	1.873290	−2.306001
59	6	0	6.239425	−2.707500	−0.340231
60	6	0	−6.191541	2.640687	−0.763172
61	6	0	−6.658932	−2.187037	−1.946312
62	9	0	5.431535	−3.517663	0.377138
63	9	0	6.446584	−3.306255	−1.541930
64	9	0	7.454225	−2.711098	0.290629
65	9	0	7.466898	1.277155	−3.212430
66	9	0	7.450949	2.694042	−1.557895
67	9	0	5.817876	2.688416	−2.994674
68	9	0	−6.757266	2.930554	−1.963873
69	9	0	−7.172219	2.841333	0.170838
70	9	0	−5.246237	3.576054	−0.528890
71	9	0	−7.856198	−2.427315	−1.329520
72	9	0	−6.962453	−1.871158	−3.232504

73	9	0	-5.998246	-3.366667	-1.970954

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.246602	4.455095	-4.042486
2	6	0	3.063204	3.667383	-3.262325
3	6	0	2.540154	2.951313	-2.150219
4	6	0	1.152486	3.079338	-1.818242
5	6	0	0.334589	3.887474	-2.655412
6	6	0	0.866942	4.553150	-3.739795
7	1	0	4.426483	2.047874	-1.613915
8	1	0	2.653600	4.990305	-4.895977
9	1	0	4.120751	3.567164	-3.494973
10	6	0	3.367557	2.102374	-1.374117
11	6	0	0.638478	2.357321	-0.684670
12	1	0	-0.726049	3.969577	-2.445342
13	1	0	0.218997	5.155502	-4.370964
14	6	0	1.480923	1.464414	-0.044385
15	6	0	2.868628	1.337376	-0.338580
16	6	0	-2.985180	1.549084	0.272160
17	6	0	-3.462408	2.802110	0.604436
18	6	0	-2.630047	3.949555	0.602775
19	6	0	-1.257910	3.828807	0.206138
20	6	0	-0.766367	2.542078	-0.214395
21	6	0	-1.619653	1.457778	-0.117486
22	1	0	-4.178433	5.292121	1.300300
23	1	0	-4.506426	2.916251	0.885365
24	6	0	-3.132309	5.215623	1.013446
25	6	0	-0.431745	4.983612	0.293930
26	6	0	-0.943677	6.193043	0.714834
27	6	0	-2.309454	6.318127	1.066264
28	1	0	0.618319	4.908844	0.036017
29	1	0	-0.289627	7.058334	0.781253
30	1	0	-2.700302	7.279100	1.389173
31	8	0	0.976656	0.646163	0.974778
32	8	0	-1.108568	0.173869	-0.396098
33	15	0	-0.172886	-0.471528	0.753849
34	8	0	-0.756394	-0.910775	2.032744
35	7	0	0.461641	-1.829071	-0.061678

36	1	0	0.537508	-2.652540	0.535164
37	16	0	1.111388	-2.075875	-1.589311
38	8	0	1.400237	-0.788214	-2.200283
39	8	0	2.082420	-3.154424	-1.471966
40	6	0	-0.349237	-2.814427	-2.535208
41	9	0	0.078372	-3.179461	-3.745010
42	9	0	-0.808376	-3.883632	-1.878783
43	9	0	-1.325005	-1.913403	-2.660135
44	6	0	3.761725	0.416458	0.415759
45	6	0	3.776853	0.387772	1.817862
46	6	0	4.649895	-0.417121	-0.284351
47	6	0	4.666928	-0.446466	2.499250
48	1	0	3.105709	1.026778	2.380228
49	6	0	5.534394	-1.247612	0.403473
50	1	0	4.632967	-0.428603	-1.368449
51	6	0	5.549869	-1.269769	1.800237
52	1	0	6.240911	-1.914644	2.332635
53	6	0	-3.877962	0.359947	0.337958
54	6	0	-4.020121	-0.511833	-0.751164
55	6	0	-4.633332	0.121970	1.495137
56	6	0	-4.908548	-1.586902	-0.683693
57	1	0	-3.450197	-0.341983	-1.657621
58	6	0	-5.515947	-0.958137	1.556874
59	1	0	-4.511504	0.768710	2.357655
60	6	0	-5.661573	-1.819868	0.469003
61	1	0	-6.348155	-2.657533	0.518661
62	6	0	-5.022349	-2.536726	-1.850033
63	6	0	-6.360363	-1.169029	2.789122
64	6	0	6.495230	-2.141167	-0.341406
65	6	0	4.638588	-0.489566	4.007431
66	9	0	-6.248736	-3.105799	-1.928160
67	9	0	-4.125992	-3.555824	-1.755509
68	9	0	-4.787540	-1.921919	-3.034587
69	9	0	-7.565562	-0.544433	2.678429
70	9	0	-6.622775	-2.479024	3.009308
71	9	0	-5.771399	-0.680520	3.904996
72	9	0	4.303618	0.708088	4.545369
73	9	0	3.730030	-1.391242	4.464025
74	9	0	5.836944	-0.843990	4.530711
75	9	0	7.786819	-1.852104	-0.027734
76	9	0	6.309256	-3.448588	-0.030748
77	9	0	6.378241	-2.026290	-1.683098

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.169539	4.520392	-4.059323
2	6	0	2.989470	3.723006	-3.290848
3	6	0	2.476188	2.998108	-2.180577
4	6	0	1.091706	3.121993	-1.834339
5	6	0	0.269876	3.938019	-2.661911
6	6	0	0.792474	4.615895	-3.744095
7	1	0	4.362852	2.078908	-1.669275
8	1	0	2.571273	5.061011	-4.912852
9	1	0	4.045133	3.619777	-3.533749
10	6	0	3.306757	2.140734	-1.416784
11	6	0	0.586029	2.394240	-0.702351
12	1	0	-0.789904	4.014001	-2.444375
13	1	0	0.137594	5.222815	-4.364867
14	6	0	1.423813	1.490077	-0.061089
15	6	0	2.811415	1.374263	-0.383077
16	6	0	-3.017812	1.531760	0.235783
17	6	0	-3.522371	2.771246	0.575690
18	6	0	-2.709927	3.933026	0.586780
19	6	0	-1.335042	3.833712	0.193326
20	6	0	-0.820864	2.560511	-0.234484
21	6	0	-1.645987	1.448247	-0.150073
22	1	0	-4.280002	5.246499	1.288914
23	1	0	-4.570330	2.866511	0.851377
24	6	0	-3.231404	5.189231	1.003644
25	6	0	-0.528768	5.002977	0.292212
26	6	0	-1.058524	6.203320	0.718025
27	6	0	-2.427314	6.305960	1.066717
28	1	0	0.523181	4.941678	0.037114
29	1	0	-0.416332	7.077726	0.791261
30	1	0	-2.834927	7.258738	1.395668
31	8	0	0.944631	0.705660	0.959572
32	8	0	-1.124468	0.205617	-0.439165
33	15	0	-0.204460	-0.498994	0.767598
34	8	0	-0.934114	-0.625802	2.051242
35	7	0	0.426365	-1.840366	0.155689
36	16	0	1.211627	-2.138506	-1.185309
37	8	0	1.569831	-0.960896	-2.002768
38	8	0	2.238924	-3.168027	-0.978578

39	6	0	-0.089603	-3.029673	-2.221430
40	9	0	0.432744	-3.372737	-3.416158
41	9	0	-0.518215	-4.150280	-1.617699
42	9	0	-1.158942	-2.241095	-2.449216
43	6	0	3.713285	0.451698	0.356541
44	6	0	3.757937	0.435786	1.760253
45	6	0	4.576352	-0.393423	-0.355235
46	6	0	4.664702	-0.388548	2.426421
47	1	0	3.085776	1.068340	2.327031
48	6	0	5.480732	-1.216320	0.320709
49	1	0	4.508591	-0.434161	-1.436485
50	6	0	5.533096	-1.219902	1.713528
51	1	0	6.232284	-1.863880	2.236856
52	6	0	-3.892014	0.329830	0.282618
53	6	0	-3.975602	-0.560905	-0.800304
54	6	0	-4.691091	0.095605	1.409221
55	6	0	-4.863080	-1.636472	-0.759825
56	1	0	-3.352183	-0.408385	-1.673115
57	6	0	-5.568257	-0.991720	1.446910
58	1	0	-4.602324	0.748476	2.270831
59	6	0	-5.664285	-1.862803	0.362863
60	1	0	-6.347107	-2.704959	0.390612
61	6	0	-4.968558	-2.592986	-1.920016
62	6	0	-6.463457	-1.193291	2.639529
63	6	0	6.453933	-2.069952	-0.447887
64	6	0	4.733025	-0.408350	3.930106
65	9	0	-6.272127	-2.882601	-2.208073
66	9	0	-4.368919	-3.781973	-1.662021
67	9	0	-4.418385	-2.104986	-3.053746
68	9	0	-7.670829	-0.571277	2.474490
69	9	0	-6.743802	-2.501900	2.863006
70	9	0	-5.935116	-0.695940	3.782108
71	9	0	3.959296	0.538573	4.508144
72	9	0	4.350725	-1.605008	4.447238
73	9	0	6.007346	-0.198606	4.377027
74	9	0	7.685280	-1.470781	-0.522847
75	9	0	6.664446	-3.274102	0.141129
76	9	0	6.067171	-2.302144	-1.718892

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Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-1.511031	4.062009	3.489413
2	6	0	-2.444411	3.519294	2.634967
3	6	0	-2.044686	2.734035	1.518053
4	6	0	-0.649102	2.535884	1.259568
5	6	0	0.286810	3.092416	2.175089
6	6	0	-0.132773	3.832230	3.260744
7	1	0	-4.060334	2.325648	0.857290
8	1	0	-1.827989	4.652619	4.344821
9	1	0	-3.507319	3.669195	2.810179
10	6	0	-3.007069	2.134200	0.668158
11	6	0	-0.259987	1.749285	0.118449
12	1	0	1.346419	2.920206	2.024096
13	1	0	0.602816	4.237955	3.950395
14	6	0	-1.258136	1.115816	-0.601373
15	6	0	-2.651627	1.306685	-0.379404
16	6	0	3.138289	0.093840	-0.545329
17	6	0	3.939418	1.206718	-0.716296
18	6	0	3.409959	2.521175	-0.760045
19	6	0	2.008244	2.724853	-0.545345
20	6	0	1.174938	1.585225	-0.261856
21	6	0	1.746075	0.326454	-0.357183
22	1	0	5.308522	3.469145	-1.186914
23	1	0	5.007481	1.067687	-0.863698
24	6	0	4.245348	3.639931	-1.033767
25	6	0	1.496999	4.047922	-0.660087
26	6	0	2.329983	5.110002	-0.942852
27	6	0	3.720657	4.910066	-1.120526
28	1	0	0.434051	4.220283	-0.533998
29	1	0	1.913404	6.109625	-1.034747
30	1	0	4.366786	5.756657	-1.336954
31	8	0	-0.894695	0.236696	-1.632275
32	8	0	0.924436	-0.804103	-0.186769
33	15	0	-0.149784	-1.162843	-1.332062
34	8	0	0.267481	-1.818021	-2.586258
35	7	0	-1.174572	-2.213115	-0.458143
36	1	0	-1.607311	-2.933247	-1.035145
37	16	0	-1.660579	-2.309880	1.144450
38	8	0	-1.467795	-1.029611	1.802782
39	8	0	-2.918839	-3.045420	1.153298
40	6	0	-0.388364	-3.498457	1.884768
41	9	0	-0.749333	-3.761263	3.144705
42	9	0	-0.380038	-4.637457	1.179659

43	9	0	0.829376	-2.961842	1.872721
44	6	0	-3.693221	0.652019	-1.217987
45	6	0	-3.643948	0.693873	-2.622757
46	6	0	-4.783698	0.012116	-0.603835
47	6	0	-4.660505	0.119915	-3.387213
48	1	0	-2.811780	1.184540	-3.117944
49	6	0	-5.798102	-0.566312	-1.369976
50	1	0	-4.824242	-0.052958	0.480316
51	6	0	-5.741234	-0.512782	-2.764731
52	1	0	-4.607666	0.168161	-4.471950
53	1	0	-6.626667	-1.065959	-0.874596
54	1	0	-6.529635	-0.962986	-3.362511
55	6	0	3.749096	-1.267100	-0.501471
56	6	0	4.751178	-1.533014	0.447228
57	6	0	3.390895	-2.278542	-1.407516
58	6	0	5.379467	-2.779713	0.493206
59	1	0	5.027478	-0.761344	1.161672
60	6	0	4.022865	-3.523218	-1.361507
61	1	0	2.626878	-2.093959	-2.156107
62	6	0	5.016546	-3.779754	-0.412373
63	1	0	6.147577	-2.968905	1.238988
64	1	0	3.737707	-4.292576	-2.074662
65	1	0	5.503873	-4.750942	-0.379069

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.111196	4.137768	3.539768
2	6	0	-2.076918	3.688508	2.665740
3	6	0	-1.735412	2.884014	1.543666
4	6	0	-0.360354	2.561054	1.301452
5	6	0	0.607981	3.023103	2.236227
6	6	0	0.244223	3.788463	3.324754
7	1	0	-3.767243	2.679034	0.836491
8	1	0	-1.387408	4.742608	4.400418
9	1	0	-3.125692	3.927886	2.830773
10	6	0	-2.732433	2.391721	0.664575
11	6	0	-0.027411	1.752814	0.160970
12	1	0	1.648347	2.750779	2.096507
13	1	0	1.004920	4.117146	4.029163

14	6	0	-1.059336	1.217894	-0.596207
15	6	0	-2.432116	1.556307	-0.393173
16	6	0	3.197560	-0.216829	-0.479148
17	6	0	4.100874	0.813638	-0.657718
18	6	0	3.701129	2.172253	-0.703424
19	6	0	2.324208	2.502445	-0.485444
20	6	0	1.388607	1.448009	-0.201053
21	6	0	1.819801	0.127974	-0.293665
22	1	0	5.678083	2.936755	-1.137926
23	1	0	5.150503	0.574880	-0.813808
24	6	0	4.635646	3.208204	-0.981474
25	6	0	1.942165	3.869635	-0.600506
26	6	0	2.868792	4.851449	-0.885389
27	6	0	4.234754	4.523728	-1.068052
28	1	0	0.899424	4.138421	-0.472262
29	1	0	2.544821	5.885778	-0.975336
30	1	0	4.957813	5.305940	-1.287531
31	8	0	-0.750064	0.332962	-1.607792
32	8	0	0.920262	-0.893370	-0.108445
33	15	0	-0.276274	-1.215160	-1.221174
34	8	0	0.233881	-1.837308	-2.470125
35	7	0	-1.443195	-1.988820	-0.437584
36	16	0	-1.931472	-2.011062	1.064816
37	8	0	-1.328754	-1.021027	1.974641
38	8	0	-3.386373	-2.219472	1.141422
39	6	0	-1.238719	-3.657919	1.675138
40	9	0	-1.566886	-3.845161	2.972441
41	9	0	-1.733183	-4.696788	0.975006
42	9	0	0.103411	-3.694737	1.580667
43	6	0	-3.511553	1.056934	-1.288497
44	6	0	-3.406409	1.162119	-2.686242
45	6	0	-4.685194	0.511688	-0.742869
46	6	0	-4.454694	0.754206	-3.511699
47	1	0	-2.497199	1.560496	-3.125611
48	6	0	-5.731653	0.098592	-1.570045
49	1	0	-4.755154	0.363347	0.330663
50	6	0	-5.623826	0.223480	-2.957240
51	1	0	-4.352787	0.841671	-4.591148
52	1	0	-6.621034	-0.343739	-1.127457
53	1	0	-6.435162	-0.106475	-3.602449
54	6	0	3.692456	-1.622785	-0.435425
55	6	0	4.779015	-1.937259	0.400512
56	6	0	3.142729	-2.639283	-1.235242
57	6	0	5.309389	-3.228811	0.435907

58	1	0	5.195349	-1.165799	1.044214
59	6	0	3.676873	-3.929317	-1.198432
60	1	0	2.298772	-2.424539	-1.884363
61	6	0	4.759452	-4.231576	-0.367170
62	1	0	6.142459	-3.451995	1.099235
63	1	0	3.234752	-4.702556	-1.822254
64	1	0	5.164209	-5.240953	-0.337898

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.031587	4.247785	3.603763
2	6	0	-2.883170	3.462681	2.858874
3	6	0	-2.403171	2.707548	1.752681
4	6	0	-1.019367	2.793656	1.391343
5	6	0	-0.164317	3.600562	2.192346
6	6	0	-0.656340	4.305304	3.271014
7	1	0	-4.325294	1.850485	1.268477
8	1	0	-2.408122	4.813056	4.452214
9	1	0	-3.938185	3.395377	3.114801
10	6	0	-3.269669	1.868044	1.009292
11	6	0	-0.549120	2.031660	0.265969
12	1	0	0.893111	3.651018	1.957045
13	1	0	0.019244	4.906974	3.873482
14	6	0	-1.431851	1.153656	-0.339495
15	6	0	-2.818104	1.065373	-0.021467
16	6	0	3.042778	1.073269	-0.695447
17	6	0	3.549024	2.303576	-1.072478
18	6	0	2.750517	3.474030	-1.109809
19	6	0	1.380438	3.411022	-0.694053
20	6	0	0.854440	2.154247	-0.229324
21	6	0	1.673686	1.040974	-0.303818
22	1	0	4.329820	4.745963	-1.867223
23	1	0	4.595670	2.377725	-1.356908
24	6	0	3.285068	4.711200	-1.566698
25	6	0	0.589551	4.588530	-0.807325
26	6	0	1.132399	5.768066	-1.272114
27	6	0	2.496803	5.837462	-1.644724
28	1	0	-0.458724	4.553560	-0.533309
29	1	0	0.505020	6.651536	-1.356590

30	1	0	2.914110	6.775032	-2.002442
31	8	0	-0.959123	0.303893	-1.350626
32	8	0	1.119289	-0.218301	0.012515
33	15	0	0.123921	-0.862791	-1.079930
34	8	0	0.629995	-1.430833	-2.341550
35	7	0	-0.577517	-2.124541	-0.156625
36	1	0	-0.806168	-2.944243	-0.717806
37	16	0	-1.096758	-2.276082	1.425268
38	8	0	-1.198810	-0.965969	2.044404
39	8	0	-2.166101	-3.266486	1.435186
40	6	0	0.365499	-3.144252	2.248744
41	9	0	0.026040	-3.439128	3.507524
42	9	0	0.647133	-4.276623	1.590299
43	9	0	1.445450	-2.360321	2.255494
44	6	0	-3.746412	0.153206	-0.739906
45	6	0	-3.784772	0.079609	-2.147503
46	6	0	-4.655481	-0.635442	-0.021499
47	6	0	-4.697842	-0.737701	-2.799989
48	1	0	-3.097930	0.677625	-2.737975
49	6	0	-5.577190	-1.467863	-0.664533
50	1	0	-4.631847	-0.624260	1.064965
51	6	0	-5.601965	-1.519830	-2.062998
52	1	0	-4.729641	-0.785807	-3.884454
53	1	0	-6.249979	-2.071830	-0.066141
54	6	0	3.903067	-0.138461	-0.711542
55	6	0	4.001229	-0.990535	0.395777
56	6	0	4.692916	-0.432832	-1.839380
57	6	0	4.857651	-2.094936	0.395000
58	1	0	3.412215	-0.788275	1.284831
59	6	0	5.544968	-1.529920	-1.857713
60	1	0	4.616608	0.194199	-2.723824
61	6	0	5.634870	-2.369818	-0.737648
62	1	0	4.909374	-2.722926	1.277424
63	1	0	6.141606	-1.762334	-2.734776
64	8	0	6.498998	-3.421883	-0.849116
65	8	0	-6.454873	-2.293895	-2.796857
66	6	0	6.622677	-4.321550	0.244950
67	1	0	7.349123	-5.072438	-0.070387
68	1	0	6.993284	-3.809794	1.142868
69	1	0	5.665701	-4.810532	0.469276
70	6	0	-7.396204	-3.108758	-2.109525
71	1	0	-7.961538	-3.626735	-2.886090
72	1	0	-6.893754	-3.845941	-1.469863
73	1	0	-8.080494	-2.501393	-1.502643

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861787	4.396468	3.588566
2	6	0	-2.738637	3.623269	2.858554
3	6	0	-2.289484	2.839431	1.760383
4	6	0	-0.906594	2.877125	1.386501
5	6	0	-0.025658	3.670548	2.174540
6	6	0	-0.488073	4.407825	3.245509
7	1	0	-4.237536	2.023021	1.300980
8	1	0	-2.217167	4.982554	4.433078
9	1	0	-3.793744	3.585764	3.123244
10	6	0	-3.183420	2.014676	1.032447
11	6	0	-0.464211	2.086049	0.270360
12	1	0	1.032125	3.681385	1.935139
13	1	0	0.211466	4.995746	3.835481
14	6	0	-1.367229	1.215047	-0.325886
15	6	0	-2.756446	1.191637	0.010809
16	6	0	3.095899	0.994482	-0.636524
17	6	0	3.656519	2.203663	-1.004746
18	6	0	2.901009	3.400579	-1.074077
19	6	0	1.520264	3.383704	-0.690317
20	6	0	0.943986	2.152619	-0.221295
21	6	0	1.710839	0.995867	-0.273338
22	1	0	4.538073	4.613336	-1.803784
23	1	0	4.713919	2.244818	-1.256062
24	6	0	3.485202	4.616258	-1.527380
25	6	0	0.773133	4.586919	-0.833798
26	6	0	1.362909	5.746099	-1.294880
27	6	0	2.737600	5.768909	-1.635195
28	1	0	-0.282187	4.584107	-0.584403
29	1	0	0.764710	6.648096	-1.401609
30	1	0	3.194894	6.689170	-1.991547
31	8	0	-0.940318	0.365532	-1.320369
32	8	0	1.119748	-0.203856	0.061050
33	15	0	0.098228	-0.912034	-1.050476
34	8	0	0.741090	-1.236957	-2.345392
35	7	0	-0.627393	-2.130223	-0.287452
36	16	0	-1.243026	-2.296180	1.154461

37	8	0	-1.361259	-1.072660	1.971550
38	8	0	-2.382528	-3.226959	1.142245
39	6	0	0.081135	-3.299784	2.057045
40	9	0	-0.327500	-3.581886	3.313488
41	9	0	0.334524	-4.468895	1.438576
42	9	0	1.246731	-2.624848	2.151875
43	6	0	-3.718832	0.306956	-0.697667
44	6	0	-3.819750	0.292399	-2.102203
45	6	0	-4.579231	-0.523927	0.029155
46	6	0	-4.756912	-0.505218	-2.746837
47	1	0	-3.149474	0.907940	-2.694139
48	6	0	-5.520338	-1.340815	-0.606560
49	1	0	-4.481644	-0.575744	1.109676
50	6	0	-5.611355	-1.330343	-2.001050
51	1	0	-4.829427	-0.519263	-3.830670
52	1	0	-6.139417	-1.996063	-0.004038
53	6	0	3.921449	-0.240610	-0.621707
54	6	0	3.840858	-1.178584	0.416860
55	6	0	4.852549	-0.485926	-1.649492
56	6	0	4.656827	-2.312695	0.443695
57	1	0	3.125298	-1.035867	1.218034
58	6	0	5.671095	-1.609606	-1.636884
59	1	0	4.909641	0.197704	-2.492438
60	6	0	5.576939	-2.532772	-0.586796
61	1	0	4.548296	-3.013759	1.263744
62	1	0	6.370639	-1.803170	-2.445271
63	8	0	6.416098	-3.617828	-0.661615
64	8	0	-6.492362	-2.095010	-2.728748
65	6	0	6.287364	-4.631421	0.323476
66	1	0	7.007773	-5.405661	0.049957
67	1	0	6.526288	-4.250815	1.326157
68	1	0	5.275676	-5.057773	0.329185
69	6	0	-7.293942	-3.034055	-2.031262
70	1	0	-7.872311	-3.558675	-2.795391
71	1	0	-6.676606	-3.755267	-1.479463
72	1	0	-7.982163	-2.536696	-1.333164

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Standard orientation:

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

1	6	0	-0.365603	2.457492	1.280164
2	1	0	-3.677251	2.799928	0.563296
3	6	0	-2.650796	2.453864	0.463537
4	6	0	0.006015	1.669569	0.162957
5	6	0	-0.997552	1.200952	-0.691793
6	6	0	-2.339582	1.596661	-0.596737
7	6	0	3.124725	-0.487876	-0.307725
8	6	0	4.078979	0.513418	-0.514338
9	6	0	1.805089	-0.050599	-0.129960
10	1	0	5.118211	0.215683	-0.635903
11	8	0	-0.647259	0.266669	-1.683578
12	8	0	0.784012	-1.021492	-0.010111
13	15	0	-0.173822	-1.229007	-1.290465
14	8	0	0.280834	-1.973175	-2.478389
15	6	0	0.641516	2.764520	2.381149
16	6	0	-2.169905	3.746368	2.561100
17	6	0	-1.230271	3.720302	3.771175
18	6	0	0.217323	3.908278	3.310395
19	1	0	0.760668	1.846834	2.978741
20	1	0	1.631941	2.966614	1.965441
21	1	0	-2.246909	4.781760	2.193295
22	1	0	-3.185271	3.455964	2.858600
23	1	0	-1.520085	4.502191	4.484202
24	1	0	-1.324499	2.758518	4.295386
25	1	0	0.309230	4.870708	2.784801
26	1	0	0.899437	3.951392	4.168801
27	6	0	3.189481	4.715573	-0.585122
28	6	0	4.370729	4.209422	-1.417047
29	6	0	4.865893	2.871708	-0.857753
30	1	0	2.854989	5.699437	-0.937177
31	1	0	4.054103	4.083264	-2.462633
32	1	0	5.190675	4.938343	-1.418842
33	1	0	5.604507	2.423148	-1.533864
34	1	0	5.397692	3.057602	0.088631
35	1	0	3.510826	4.845920	0.459127
36	6	0	1.433290	1.298164	-0.109902
37	6	0	3.749883	1.870931	-0.595308
38	6	0	2.415010	2.277359	-0.408945
39	6	0	2.016774	3.728758	-0.648021
40	1	0	1.230040	4.041235	0.042429
41	1	0	1.559097	3.783481	-1.648691
42	6	0	-1.708434	2.857312	1.415104
43	7	0	-1.471177	-2.076784	-0.556239
44	1	0	-1.952330	-2.705087	-1.198760

45	16	0	-2.188038	-2.057574	0.954830
46	8	0	-1.813563	-0.855281	1.679054
47	8	0	-3.565698	-2.500345	0.778727
48	6	0	-1.327302	-3.495740	1.827844
49	9	0	-1.912670	-3.678520	3.016112
50	9	0	-1.454897	-4.610092	1.096475
51	9	0	-0.031346	-3.235345	2.010168
52	6	0	-3.396808	1.135067	-1.536843
53	6	0	-3.200005	1.147094	-2.929389
54	6	0	-4.643588	0.713773	-1.042126
55	6	0	-4.220579	0.756064	-3.797108
56	1	0	-2.246344	1.471539	-3.333843
57	6	0	-5.662997	0.318397	-1.910729
58	1	0	-4.807528	0.671203	0.031306
59	6	0	-5.456402	0.339780	-3.292207
60	1	0	-4.049244	0.778017	-4.870472
61	1	0	-6.614493	-0.015689	-1.504784
62	6	0	3.522674	-1.921535	-0.300559
63	6	0	3.147957	-2.779694	0.746542
64	6	0	4.329971	-2.431713	-1.330789
65	6	0	3.572524	-4.109052	0.763581
66	1	0	2.530916	-2.400767	1.555357
67	6	0	4.751275	-3.762745	-1.315841
68	1	0	4.607015	-1.786991	-2.160841
69	6	0	4.375233	-4.606201	-0.267391
70	1	0	3.277229	-4.756743	1.585358
71	1	0	5.365450	-4.141907	-2.128764
72	1	0	4.701484	-5.643047	-0.255206
73	1	0	-6.248880	0.031778	-3.969547

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.119386	-2.429335	1.333789
2	1	0	3.391222	-3.051595	0.625875
3	6	0	2.390705	-2.637991	0.512976
4	6	0	-0.193907	-1.656206	0.190319
5	6	0	0.832705	-1.289659	-0.691217
6	6	0	2.135704	-1.806798	-0.581460
7	6	0	-3.113678	0.749307	-0.303128

8	6	0	-4.151927	-0.169040	-0.491221
9	6	0	-1.820256	0.216604	-0.135010
10	1	0	-5.166191	0.210243	-0.601875
11	8	0	0.547895	-0.361572	-1.676796
12	8	0	-0.750685	1.072253	0.002534
13	15	0	0.372249	1.233274	-1.214714
14	8	0	-0.109044	1.984295	-2.398418
15	6	0	-0.903171	-2.594794	2.449984
16	6	0	1.828728	-3.775581	2.681765
17	6	0	0.912880	-3.582109	3.895193
18	6	0	-0.552016	-3.692720	3.462583
19	1	0	-0.965349	-1.629919	2.976931
20	1	0	-1.904757	-2.767525	2.045473
21	1	0	1.811624	-4.839254	2.391279
22	1	0	2.868986	-3.552079	2.951389
23	1	0	1.151690	-4.325121	4.668571
24	1	0	1.088058	-2.590023	4.334848
25	1	0	-0.722124	-4.684456	3.014497
26	1	0	-1.223204	-3.618648	4.328971
27	6	0	-3.620146	-4.431515	-0.523658
28	6	0	-4.745305	-3.830689	-1.370577
29	6	0	-5.137030	-2.458651	-0.812117
30	1	0	-3.367028	-5.443311	-0.868031
31	1	0	-4.401555	-3.724812	-2.410261
32	1	0	-5.621267	-4.493578	-1.389046
33	1	0	-5.839264	-1.956644	-1.490861
34	1	0	-5.685157	-2.607316	0.132713
35	1	0	-3.966858	-4.529533	0.516646
36	6	0	-1.583856	-1.166725	-0.088358
37	6	0	-3.941696	-1.550374	-0.557940
38	6	0	-2.645684	-2.062902	-0.365739
39	6	0	-2.367420	-3.547323	-0.572329
40	1	0	-1.628270	-3.912045	0.145312
41	1	0	-1.888380	-3.661006	-1.558084
42	6	0	1.426967	-2.923620	1.486290
43	7	0	1.724887	1.734284	-0.497863
44	16	0	2.259762	1.736849	0.982506
45	8	0	1.453096	1.036117	1.999509
46	8	0	3.719782	1.544488	1.023001
47	6	0	2.071222	3.554780	1.458809
48	9	0	2.501373	3.755557	2.725210
49	9	0	2.785595	4.362659	0.653737
50	9	0	0.781352	3.948857	1.401060
51	6	0	3.209425	-1.500143	-1.564903

52	6	0	2.987430	-1.635299	-2.946197
53	6	0	4.485898	-1.110765	-1.126733
54	6	0	4.016903	-1.408173	-3.860563
55	1	0	1.999603	-1.912286	-3.301996
56	6	0	5.515031	-0.880581	-2.042282
57	1	0	4.654404	-0.933008	-0.068768
58	6	0	5.287732	-1.033889	-3.412449
59	1	0	3.822428	-1.514211	-4.925722
60	1	0	6.488867	-0.556433	-1.682312
61	6	0	-3.396948	2.209426	-0.288588
62	6	0	-2.810090	3.064189	0.661662
63	6	0	-4.304795	2.763112	-1.208470
64	6	0	-3.132066	4.421554	0.695092
65	1	0	-2.091353	2.664870	1.368847
66	6	0	-4.626077	4.121476	-1.175824
67	1	0	-4.738828	2.127675	-1.976272
68	6	0	-4.042842	4.957639	-0.220245
69	1	0	-2.659002	5.063083	1.434774
70	1	0	-5.319837	4.528277	-1.908670
71	1	0	-4.283814	6.018164	-0.197973
72	1	0	6.087165	-0.845745	-4.126028

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.498507	4.862305	-3.011835
2	6	0	-0.225714	4.780369	-2.394755
3	6	0	0.054591	3.776579	-1.493588
4	6	0	-0.924944	2.797727	-1.163761
5	6	0	-2.203129	2.874574	-1.801489
6	6	0	-2.466093	3.927781	-2.719891
7	6	0	-0.671677	1.721885	-0.250937
8	6	0	-1.662578	0.769648	-0.028286
9	6	0	-2.957642	0.854540	-0.630316
10	6	0	-3.188329	1.904720	-1.498253
11	6	0	0.668026	1.674106	0.437462
12	6	0	0.910153	2.604712	1.501769
13	6	0	2.184055	2.593285	2.152377
14	6	0	3.175756	1.679966	1.720463
15	6	0	2.956595	0.766516	0.708320

16	6	0	1.668408	0.771040	0.085321
17	6	0	-0.076967	3.519495	1.965733
18	6	0	0.192289	4.380845	3.006756
19	6	0	1.460803	4.377230	3.637544
20	6	0	2.435514	3.500597	3.217549
21	16	0	-1.169185	-0.693760	0.919839
22	16	0	1.195428	-0.537056	-1.066815
23	8	0	-2.198122	-1.731961	0.891313
24	8	0	-0.588591	-0.249751	2.182535
25	7	0	0.096501	-1.387156	-0.036741
26	8	0	2.264370	-1.502968	-1.303949
27	8	0	0.499613	0.049841	-2.214120
28	1	0	-1.704991	5.660574	-3.719389
29	1	0	0.538008	5.513777	-2.638297
30	1	0	1.036857	3.726182	-1.037523
31	1	0	-3.443788	3.976395	-3.192849
32	1	0	-4.171742	2.002695	-1.951324
33	1	0	4.152373	1.707784	2.197232
34	1	0	-1.056146	3.531868	1.500770
35	1	0	-0.577329	5.066185	3.350890
36	1	0	1.658319	5.062868	4.456912
37	1	0	3.409775	3.482775	3.699573
38	1	0	-0.241356	-2.234559	-0.501408
39	6	0	-4.102957	-0.063823	-0.343480
40	6	0	-4.659135	-0.827960	-1.370871
41	6	0	-4.697367	-0.096009	0.928280
42	6	0	-5.782774	-1.628679	-1.129568
43	1	0	-4.208901	-0.811930	-2.359184
44	6	0	-5.818091	-0.888015	1.158650
45	1	0	-4.284367	0.501560	1.733863
46	6	0	-6.367681	-1.665842	0.132108
47	1	0	-7.239774	-2.282955	0.316970
48	6	0	4.101931	-0.114814	0.319007
49	6	0	4.592855	-1.057378	1.224181
50	6	0	4.757638	0.057886	-0.909822
51	6	0	5.714953	-1.830697	0.900930
52	1	0	4.091377	-1.202188	2.176605
53	6	0	5.874101	-0.712125	-1.222800
54	1	0	4.391373	0.791273	-1.620213
55	6	0	6.360405	-1.665871	-0.320541
56	1	0	7.227660	-2.266607	-0.570295
57	6	0	6.209064	-2.837867	1.908664
58	6	0	6.607713	-0.510541	-2.524866
59	6	0	-6.465636	-0.935311	2.520145

60	6	0	-6.340415	-2.447837	-2.266051
61	9	0	-5.438425	-3.355154	-2.720756
62	9	0	-7.453481	-3.131111	-1.918154
63	9	0	-6.666920	-1.666146	-3.330160
64	9	0	-7.794735	-0.658329	2.449468
65	9	0	-6.359534	-2.164832	3.083579
66	9	0	-5.920941	-0.050498	3.386273
67	9	0	7.297637	-3.514073	1.477927
68	9	0	6.549629	-2.239188	3.082045
69	9	0	5.258093	-3.757311	2.210258
70	9	0	6.861449	-1.687380	-3.147802
71	9	0	5.921470	0.266164	-3.393681
72	9	0	7.814403	0.088739	-2.328406

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.616374	4.725641	3.224030
2	6	0	0.323639	4.679434	2.646054
3	6	0	0.009771	3.722661	1.704650
4	6	0	0.969345	2.756513	1.288164
5	6	0	2.264179	2.792530	1.893052
6	6	0	2.564285	3.798150	2.853411
7	6	0	0.679456	1.731459	0.325960
8	6	0	1.639701	0.769317	0.028861
9	6	0	2.943027	0.817248	0.613238
10	6	0	3.223879	1.821848	1.520182
11	6	0	-0.679477	1.731508	-0.325719
12	6	0	-0.969377	2.756747	-1.287739
13	6	0	-2.264206	2.792848	-1.892631
14	6	0	-3.223898	1.822079	-1.519936
15	6	0	-2.943041	0.817329	-0.613169
16	6	0	-1.639706	0.769306	-0.028798
17	6	0	-0.009824	3.722984	-1.704043
18	6	0	-0.323704	4.679924	-2.645281
19	6	0	-1.616430	4.726209	-3.223255
20	6	0	-2.564326	3.798628	-2.852808
21	16	0	1.071451	-0.675101	-0.950124
22	16	0	-1.071430	-0.675287	0.949913
23	8	0	2.208839	-1.590123	-1.143941

24	8	0	0.471324	-0.101546	-2.174492
25	7	0	0.000001	-1.436989	-0.000192
26	8	0	-2.208798	-1.590362	1.143587
27	8	0	-0.471274	-0.101958	2.174372
28	1	0	1.852709	5.485680	3.964901
29	1	0	-0.430295	5.400290	2.952817
30	1	0	-0.988330	3.694274	1.282440
31	1	0	3.557139	3.812651	3.298351
32	1	0	4.219036	1.879180	1.956160
33	1	0	-4.219053	1.879486	-1.955908
34	1	0	0.988278	3.694548	-1.281839
35	1	0	0.430224	5.400846	-2.951904
36	1	0	-1.852781	5.486373	-3.963993
37	1	0	-3.557176	3.813193	-3.297756
38	6	0	4.065023	-0.115965	0.281625
39	6	0	4.613027	-0.928649	1.276283
40	6	0	4.657054	-0.109803	-0.991362
41	6	0	5.728417	-1.731885	1.003531
42	1	0	4.150770	-0.955764	2.258047
43	6	0	5.771476	-0.901846	-1.252515
44	1	0	4.233594	0.507659	-1.775094
45	6	0	6.316218	-1.723017	-0.257930
46	1	0	7.178641	-2.345527	-0.469916
47	6	0	-4.065031	-0.115933	-0.281685
48	6	0	-4.613128	-0.928395	-1.276462
49	6	0	-4.656967	-0.110023	0.991357
50	6	0	-5.728522	-1.731665	-1.003787
51	1	0	-4.150957	-0.955322	-2.258272
52	6	0	-5.771378	-0.902096	1.252434
53	1	0	-4.233429	0.507277	1.775175
54	6	0	-6.316219	-1.723052	0.257716
55	1	0	-7.178638	-2.345583	0.469648
56	6	0	-6.327218	-2.560890	-2.106519
57	6	0	-6.437022	-0.878874	2.601246
58	6	0	6.437244	-0.878353	-2.601266
59	6	0	6.327034	-2.561353	2.106123
60	9	0	5.390503	-3.086586	2.931094
61	9	0	7.072111	-3.595089	1.637772
62	9	0	7.160836	-1.822515	2.900339
63	9	0	7.693245	-0.339029	-2.533010
64	9	0	6.600071	-2.125685	-3.116730
65	9	0	5.758112	-0.153524	-3.517264
66	9	0	-7.072612	-3.594474	-1.638353
67	9	0	-7.160716	-1.821776	-2.900786

68	9	0	-5.390705	-3.086299	-2.931416
69	9	0	-6.599890	-2.126322	3.116426
70	9	0	-5.757802	-0.154299	3.517347
71	9	0	-7.693026	-0.339469	2.533201

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.296269	-0.265721	-1.429762
2	6	0	5.108956	-0.563754	-0.098316
3	6	0	4.024782	-0.005097	0.632982
4	6	0	3.130220	0.910469	-0.017631
5	6	0	3.341670	1.176994	-1.400484
6	6	0	4.392682	0.604017	-2.086382
7	1	0	4.481573	-1.048973	2.478290
8	1	0	6.122155	-0.707653	-1.980285
9	1	0	5.779824	-1.250713	0.412257
10	6	0	3.794727	-0.362839	1.989098
11	6	0	2.037167	1.484239	0.726991
12	1	0	2.659625	1.836700	-1.925118
13	1	0	4.525661	0.820916	-3.143166
14	6	0	1.828106	1.021771	2.018421
15	6	0	2.701809	0.121553	2.665291
16	1	0	2.490108	-0.162422	3.691184
17	6	0	-1.185409	3.128436	-0.478601
18	6	0	-0.738740	4.280988	-1.078021
19	6	0	0.638117	4.632061	-1.040283
20	6	0	1.578660	3.748877	-0.409670
21	6	0	1.116427	2.497051	0.135121
22	6	0	-0.249698	2.268397	0.130575
23	1	0	0.371617	6.514358	-2.072830
24	1	0	-2.237026	2.862761	-0.452988
25	1	0	-1.442936	4.954768	-1.559408
26	6	0	1.095060	5.861763	-1.589420
27	6	0	2.932522	4.176418	-0.310074
28	6	0	3.339607	5.384363	-0.836278
29	6	0	2.418017	6.232593	-1.496025
30	1	0	3.652140	3.546295	0.200510
31	1	0	4.377815	5.690340	-0.737570
32	1	0	2.753382	7.178638	-1.912392

33	8	0	0.747347	1.489180	2.767536
34	8	0	-0.755592	1.107852	0.744065
35	15	0	-0.785600	1.101761	2.372342
36	7	0	-0.997834	-0.543662	2.645447
37	1	0	-1.135583	-0.742691	3.637447
38	8	0	-2.040003	-2.922138	2.766741
39	15	0	-1.592605	-1.904621	1.761826
40	8	0	-1.730091	1.993337	3.074960
41	6	0	-2.917278	-1.282216	0.670983
42	6	0	-3.093376	-1.797192	-0.619727
43	6	0	-3.857629	-0.373599	1.185261
44	6	0	-4.181596	-1.397798	-1.399066
45	1	0	-2.385247	-2.511070	-1.028907
46	6	0	-4.943650	0.025181	0.411583
47	1	0	-3.741315	0.033145	2.185442
48	6	0	-5.103056	-0.485172	-0.883005
49	1	0	-4.309136	-1.798097	-2.399090
50	1	0	-5.664763	0.730718	0.813367
51	6	0	-0.243558	-2.548617	0.712726
52	6	0	0.195535	-3.849420	1.004637
53	6	0	0.350188	-1.836539	-0.339034
54	6	0	1.219740	-4.429041	0.256866
55	1	0	-0.274917	-4.398808	1.814390
56	6	0	1.376743	-2.414217	-1.086746
57	1	0	0.020733	-0.830765	-0.576228
58	6	0	1.808314	-3.710405	-0.788849
59	1	0	1.552562	-5.437638	0.482085
60	1	0	1.838392	-1.856182	-1.894436
61	6	0	-6.268124	-0.008027	-1.712567
62	6	0	2.943279	-4.332371	-1.562683
63	9	0	3.129373	-3.749811	-2.770490
64	9	0	4.123369	-4.229324	-0.891637
65	9	0	2.742741	-5.655767	-1.783811
66	9	0	-6.123150	1.297525	-2.069365
67	9	0	-6.418315	-0.713257	-2.857669
68	9	0	-7.439454	-0.091564	-1.033372

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Standard orientation:

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

1	6	0	-6.466486	-1.243906	3.575877
2	6	0	-5.417788	-2.124420	3.419399
3	6	0	-4.468660	-1.962059	2.373183
4	6	0	-4.623307	-0.880294	1.440944
5	6	0	-5.702979	0.024932	1.651048
6	6	0	-6.598028	-0.150343	2.686178
7	1	0	-3.233709	-3.643624	2.965910
8	1	0	-7.179463	-1.376002	4.386379
9	1	0	-5.287861	-2.955465	4.110278
10	6	0	-3.349813	-2.830761	2.252310
11	6	0	-3.671522	-0.723570	0.372532
12	1	0	-5.813008	0.876481	0.988667
13	1	0	-7.406760	0.563739	2.823961
14	6	0	-2.563223	-1.563724	0.354898
15	6	0	-2.403661	-2.622674	1.279847
16	1	0	-1.515630	-3.240954	1.200494
17	6	0	-2.772692	2.276301	-1.785003
18	6	0	-3.900425	2.469755	-2.543686
19	6	0	-4.998526	1.571527	-2.450405
20	6	0	-4.935859	0.478992	-1.519825
21	6	0	-3.786403	0.339503	-0.664601
22	6	0	-2.714791	1.204634	-0.861999
23	1	0	-6.175811	2.556881	-3.973439
24	1	0	-1.904911	2.922459	-1.870248
25	1	0	-3.953866	3.296129	-3.249481
26	6	0	-6.142136	1.716020	-3.282873
27	6	0	-6.012757	-0.453621	-1.520529
28	6	0	-7.100774	-0.295642	-2.353934
29	6	0	-7.177997	0.808017	-3.237769
30	1	0	-5.965404	-1.310992	-0.858203
31	1	0	-7.903108	-1.029683	-2.335249
32	1	0	-8.042782	0.927254	-3.886342
33	8	0	-1.598512	-1.410652	-0.613139
34	8	0	-1.570707	1.069590	-0.112466
35	15	0	-0.495783	-0.161030	-0.488471
36	7	0	0.345660	-0.367990	0.819383
37	8	0	1.988313	-0.550441	2.913173
38	15	0	1.829478	-0.298727	1.435048
39	8	0	0.114664	0.031675	-1.841638
40	6	0	2.914952	-1.494320	0.521544
41	6	0	3.874527	-2.204610	1.257735
42	6	0	2.811637	-1.720346	-0.859963
43	6	0	4.722152	-3.119722	0.632081

44	1	0	3.932780	-2.042133	2.330242
45	6	0	3.658623	-2.631942	-1.492500
46	1	0	2.056867	-1.199909	-1.445181
47	6	0	4.615036	-3.332292	-0.747226
48	1	0	5.455541	-3.670774	1.213530
49	1	0	3.565569	-2.804547	-2.560712
50	6	0	2.575725	1.352488	1.038715
51	6	0	3.281836	2.014321	2.053746
52	6	0	2.464127	1.960485	-0.220961
53	6	0	3.870408	3.257467	1.820246
54	1	0	3.352900	1.541955	3.029379
55	6	0	3.054443	3.202119	-0.463199
56	1	0	1.903606	1.474132	-1.015767
57	6	0	3.761955	3.849773	0.556362
58	1	0	4.415008	3.761881	2.613507
59	1	0	2.965009	3.662327	-1.442558
60	6	0	5.560518	-4.271987	-1.436301
61	6	0	4.360827	5.205276	0.320228
62	9	0	4.620771	5.448609	-0.991418
63	9	0	3.541971	6.218649	0.735353
64	9	0	5.534448	5.382902	0.988821
65	9	0	6.688711	-3.640706	-1.883441
66	9	0	5.994451	-5.273925	-0.623537
67	9	0	5.011458	-4.867806	-2.528394

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.415973	3.915978	-1.260239
2	6	0	-2.791930	4.033772	-0.038089
3	6	0	-2.233383	2.899948	0.613596
4	6	0	-2.351643	1.605335	0.004292
5	6	0	-2.979595	1.526514	-1.271296
6	6	0	-3.496095	2.648408	-1.885759
7	1	0	-1.457019	4.014759	2.304027
8	1	0	-3.835646	4.791020	-1.749487
9	1	0	-2.704448	5.004321	0.445388
10	6	0	-1.537902	3.032268	1.845576

11	6	0	-1.802368	0.453179	0.674243
12	1	0	-3.047208	0.566491	-1.770580
13	1	0	-3.967979	2.557136	-2.860830
14	6	0	-1.069719	0.672327	1.832443
15	6	0	-0.945083	1.942858	2.434791
16	1	0	-0.383011	2.026332	3.359398
17	6	0	-0.872194	-2.994815	-0.662090
18	6	0	-2.088935	-3.535790	-0.998904
19	6	0	-3.295016	-2.836226	-0.722565
20	6	0	-3.237244	-1.530200	-0.128340
21	6	0	-1.953683	-0.930061	0.137213
22	6	0	-0.829638	-1.709557	-0.084291
23	1	0	-4.586891	-4.410452	-1.452702
24	1	0	0.059961	-3.527474	-0.818779
25	1	0	-2.142815	-4.523481	-1.449984
26	6	0	-4.561006	-3.424304	-0.994448
27	6	0	-4.465875	-0.899936	0.216905
28	6	0	-5.677245	-1.505589	-0.043557
29	6	0	-5.730722	-2.774825	-0.668254
30	1	0	-4.446410	0.067874	0.705252
31	1	0	-6.599589	-1.005201	0.239744
32	1	0	-6.691783	-3.238660	-0.873754
33	8	0	-0.464232	-0.393634	2.494337
34	8	0	0.435985	-1.207785	0.255306
35	15	0	0.808762	-1.183075	1.841616
36	7	0	2.117714	-0.138151	1.821591
37	1	0	2.547971	-0.063804	2.744424
38	8	0	4.466044	0.899665	1.470293
39	15	0	3.293358	0.417169	0.668738
40	8	0	1.008325	-2.466383	2.546397
41	6	0	3.640270	-0.988020	-0.437316
42	6	0	3.924995	-0.775283	-1.795137
43	6	0	3.766544	-2.280127	0.099270
44	6	0	4.316369	-1.841990	-2.607733
45	1	0	3.841345	0.219954	-2.221659
46	6	0	4.156731	-3.343292	-0.716019
47	1	0	3.552844	-2.462302	1.148621
48	6	0	4.430591	-3.126580	-2.070136
49	1	0	4.532485	-1.667659	-3.658592
50	1	0	4.246513	-4.340068	-0.292327
51	6	0	2.549108	1.753908	-0.320533
52	6	0	3.103351	3.033350	-0.156623
53	6	0	1.492161	1.566047	-1.225045
54	6	0	2.599553	4.113650	-0.885250

55	1	0	3.929251	3.166608	0.536004
56	6	0	0.991557	2.649192	-1.949585
57	1	0	1.059545	0.580521	-1.362068
58	6	0	1.544080	3.922777	-1.780784
59	1	0	3.034185	5.101463	-0.754996
60	1	0	0.167165	2.498888	-2.641329
61	1	0	4.734824	-3.956355	-2.703223
62	1	0	1.151578	4.763352	-2.347683

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.875197	3.518126	2.145559
2	6	0	3.834773	3.981952	1.369496
3	6	0	3.008195	3.089428	0.633676
4	6	0	3.281176	1.679489	0.671775
5	6	0	4.345984	1.235220	1.507601
6	6	0	5.120389	2.125744	2.222514
7	1	0	1.685937	4.630868	-0.127392
8	1	0	5.493428	4.212784	2.709634
9	1	0	3.615761	5.047174	1.320653
10	6	0	1.894444	3.563150	-0.112319
11	6	0	2.455123	0.776683	-0.086115
12	1	0	4.541326	0.171702	1.590500
13	1	0	5.921283	1.752414	2.856860
14	6	0	1.343028	1.297911	-0.740750
15	6	0	1.065197	2.685831	-0.765194
16	1	0	0.179249	3.018420	-1.295884
17	6	0	1.827201	-2.958818	0.244391
18	6	0	3.032786	-3.515611	-0.103536
19	6	0	4.106824	-2.696750	-0.547857
20	6	0	3.931928	-1.271314	-0.590679
21	6	0	2.694611	-0.692657	-0.137278
22	6	0	1.657106	-1.553095	0.212124
23	1	0	5.453288	-4.345038	-0.930239
24	1	0	0.978145	-3.565267	0.543179
25	1	0	3.169983	-4.594778	-0.074202
26	6	0	5.336751	-3.263736	-0.980668
27	6	0	4.994872	-0.491193	-1.130959

28	6	0	6.170135	-1.073249	-1.559452
29	6	0	6.354244	-2.474622	-1.472682
30	1	0	4.867570	0.582470	-1.215664
31	1	0	6.959078	-0.449369	-1.973535
32	1	0	7.286512	-2.923932	-1.807327
33	8	0	0.499270	0.465674	-1.431971
34	8	0	0.439644	-1.050085	0.591449
35	15	0	-0.610061	-0.472892	-0.592470
36	7	0	-1.588716	0.480689	0.165122
37	8	0	-3.367064	1.902407	1.552815
38	15	0	-3.114826	0.742831	0.619909
39	8	0	-1.040704	-1.568669	-1.516347
40	6	0	-4.143599	0.969737	-0.901300
41	6	0	-5.194646	1.898372	-0.857303
42	6	0	-3.916071	0.254195	-2.087651
43	6	0	-6.007185	2.108993	-1.975572
44	1	0	-5.351217	2.462584	0.058241
45	6	0	-4.730462	0.463758	-3.204962
46	1	0	-3.093480	-0.454860	-2.147183
47	6	0	-5.778748	1.388373	-3.152153
48	1	0	-6.815035	2.837291	-1.929606
49	1	0	-4.540108	-0.093821	-4.119939
50	6	0	-3.786940	-0.799375	1.392175
51	6	0	-4.539294	-0.675212	2.569310
52	6	0	-3.582786	-2.076852	0.846302
53	6	0	-5.080304	-1.804744	3.191812
54	1	0	-4.679733	0.316328	2.991357
55	6	0	-4.127232	-3.205241	1.466172
56	1	0	-2.985908	-2.195634	-0.054981
57	6	0	-4.878801	-3.072923	2.638842
58	1	0	-5.656930	-1.694643	4.108581
59	1	0	-3.959160	-4.189838	1.034068
60	1	0	-6.408867	1.550929	-4.024810
61	1	0	-5.299323	-3.953722	3.120791

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Standard orientation:

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

1	6	0	-1.006724	4.810051	-0.332077
2	6	0	-0.142704	4.373888	0.648088
3	6	0	0.012793	2.987766	0.925416
4	6	0	-0.769098	2.029504	0.195727
5	6	0	-1.634516	2.516018	-0.825080
6	6	0	-1.748057	3.866292	-1.082864
7	1	0	1.528228	3.264586	2.452889
8	1	0	-1.111908	5.871798	-0.538626
9	1	0	0.447995	5.086269	1.219865
10	6	0	0.948955	2.533562	1.894118
11	6	0	-0.621203	0.624842	0.485262
12	1	0	-2.207423	1.810050	-1.415839
13	1	0	-2.411661	4.207792	-1.873106
14	6	0	0.379807	0.254513	1.371872
15	6	0	1.149272	1.190553	2.098063
16	1	0	1.882927	0.820300	2.807093
17	6	0	-1.568884	-2.457923	-1.544081
18	6	0	-2.941734	-2.413275	-1.551870
19	6	0	-3.639555	-1.417491	-0.815729
20	6	0	-2.899623	-0.420261	-0.094741
21	6	0	-1.460294	-0.419512	-0.167091
22	6	0	-0.853165	-1.469873	-0.836445
23	1	0	-5.606044	-2.168408	-1.315068
24	1	0	-1.014512	-3.233964	-2.061157
25	1	0	-3.510492	-3.162518	-2.096853
26	6	0	-5.060404	-1.412543	-0.754605
27	6	0	-3.629590	0.502953	0.705855
28	6	0	-5.007244	0.468533	0.759059
29	6	0	-5.735225	-0.488248	0.011576
30	1	0	-3.090602	1.236797	1.294567
31	1	0	-5.538364	1.179369	1.386784
32	1	0	-6.820968	-0.500426	0.056514
33	8	0	0.631890	-1.090765	1.632811
34	8	0	0.544426	-1.562421	-0.855777
35	15	0	1.286823	-2.099878	0.508253
36	7	0	2.870970	-1.664839	0.184997
37	1	0	3.542743	-2.310557	0.592948
38	16	0	1.106191	-3.940873	1.048272
39	6	0	3.517345	-0.549284	-0.388775
40	6	0	2.864654	0.447062	-1.132275
41	6	0	5.566041	0.446029	-0.695834
42	6	0	3.638541	1.479069	-1.653625
43	1	0	1.797534	0.406422	-1.303551
44	6	0	5.019510	1.492319	-1.436942

45	1	0	6.635853	0.397170	-0.502194
46	1	0	3.161228	2.265885	-2.231953
47	1	0	5.651508	2.281330	-1.832423
48	7	0	4.840262	-0.552522	-0.177899

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.016500	4.344856	-1.080744
2	6	0	-2.062424	4.399395	-0.087079
3	6	0	-1.421404	3.222150	0.386465
4	6	0	-1.798536	1.946094	-0.155646
5	6	0	-2.766783	1.932133	-1.200600
6	6	0	-3.358917	3.094691	-1.650340
7	1	0	-0.097389	4.258866	1.756277
8	1	0	-3.491932	5.255646	-1.437896
9	1	0	-1.768978	5.355403	0.343268
10	6	0	-0.387691	3.287517	1.361018
11	6	0	-1.161686	0.751692	0.334856
12	1	0	-3.032641	0.985561	-1.658249
13	1	0	-4.089309	3.049396	-2.455187
14	6	0	-0.117532	0.892795	1.242663
15	6	0	0.269537	2.151414	1.761672
16	1	0	1.102520	2.179714	2.455633
17	6	0	-0.771068	-2.716720	-1.172390
18	6	0	-2.051678	-3.211288	-1.166665
19	6	0	-3.114860	-2.462315	-0.592272
20	6	0	-2.842866	-1.159714	-0.050134
21	6	0	-1.514947	-0.614068	-0.143511
22	6	0	-0.502923	-1.426591	-0.651095
23	1	0	-4.619859	-3.975846	-0.938569
24	1	0	0.065101	-3.290044	-1.558909
25	1	0	-2.261928	-4.199634	-1.570973
26	6	0	-4.432227	-2.991178	-0.513480
27	6	0	-3.911357	-0.479980	0.603189
28	6	0	-5.175570	-1.027590	0.677957
29	6	0	-5.448515	-2.292355	0.102297
30	1	0	-3.717939	0.484208	1.060491

31	1	0	-5.966866	-0.485074	1.190593
32	1	0	-6.449401	-2.714076	0.161391
33	8	0	0.546385	-0.220720	1.702002
34	8	0	0.787068	-0.972608	-0.704142
35	15	0	1.727550	-0.907369	0.724563
36	7	0	2.785273	0.242664	0.500192
37	16	0	2.114284	-2.714769	1.406159
38	6	0	4.007634	0.237762	-0.098145
39	6	0	4.505074	-0.833755	-0.900146
40	6	0	5.964170	1.420662	-0.496770
41	6	0	5.755439	-0.735825	-1.487974
42	1	0	3.898728	-1.724406	-1.031815
43	6	0	6.524402	0.421258	-1.293668
44	1	0	6.520372	2.342492	-0.311865
45	1	0	6.132385	-1.556610	-2.097109
46	1	0	7.509425	0.542786	-1.737448
47	7	0	4.764110	1.354316	0.086057

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.523619	-3.654274	-2.555300
2	6	0	-4.464741	-3.398636	-1.186337
3	1	0	-3.425073	-3.687052	-4.417191
4	6	0	-3.385366	-3.490474	-3.349811
5	6	0	-3.275499	-2.970129	-0.568547
6	6	0	-2.153315	-2.822161	-1.398474
7	6	0	-2.189155	-3.071896	-2.766307
8	1	0	-1.289106	-2.928165	-3.355963
9	6	0	-2.135219	-2.844599	3.071489
10	6	0	-3.198137	-2.165435	3.667801
11	6	0	-4.274249	-1.735530	2.885473
12	6	0	-4.288779	-1.987456	1.514334
13	6	0	-3.235307	-2.676363	0.884979
14	6	0	-2.169147	-3.083691	1.701822
15	1	0	-1.287317	-3.197393	3.649905
16	1	0	-3.181335	-1.970205	4.736082
17	8	0	-0.948316	-2.314423	-0.867277
18	8	0	-1.121336	-3.846311	1.148895
19	15	0	-0.047765	-3.160254	0.178154

20	8	0	0.998101	-2.279597	0.756027
21	8	0	0.495443	-4.461583	-0.580637
22	1	0	1.462703	-4.445286	-0.684747
23	1	0	-5.457270	-3.985132	-3.000806
24	1	0	-5.348951	-3.543901	-0.572574
25	1	0	-5.115615	-1.628179	0.908706
26	1	0	-5.098647	-1.194602	3.341080
27	6	0	1.056862	1.427535	-0.081018
28	7	0	-0.239115	0.940189	-0.141206
29	1	0	-0.344133	-0.036539	-0.401453
30	7	0	1.950446	0.387595	0.020156
31	1	0	1.565048	-0.512324	0.318211
32	6	0	3.357173	0.401432	-0.038054
33	6	0	4.095048	1.289319	-0.836186
34	6	0	4.031211	-0.586251	0.694045
35	6	0	5.485372	1.184408	-0.875045
36	1	0	3.589179	2.045423	-1.419386
37	6	0	5.422571	-0.680068	0.633668
38	1	0	3.463264	-1.278835	1.307722
39	6	0	6.166313	0.206892	-0.143785
40	1	0	7.246741	0.136472	-0.185174
41	6	0	-1.447192	1.665374	-0.097601
42	6	0	-1.655081	2.722702	0.802634
43	6	0	-2.490346	1.260867	-0.936639
44	6	0	-2.892196	3.361266	0.837563
45	1	0	-0.860670	3.031765	1.467482
46	6	0	-3.730398	1.904833	-0.878343
47	1	0	-2.331788	0.451175	-1.642768
48	6	0	-3.941388	2.964094	0.000672
49	1	0	-4.899381	3.469761	0.038738
50	16	0	1.448329	3.050471	-0.124657
51	6	0	-3.119216	4.520803	1.776152
52	6	0	-4.852272	1.409349	-1.752820
53	6	0	6.280220	2.171097	-1.694860
54	6	0	6.106286	-1.792152	1.386041
55	9	0	-3.109018	5.708466	1.117515
56	9	0	-2.181140	4.596890	2.746186
57	9	0	-4.327428	4.434829	2.393410
58	9	0	-5.825499	2.331955	-1.922255
59	9	0	-5.453151	0.304016	-1.220215
60	9	0	-4.419399	1.047029	-2.985571
61	9	0	6.003698	-2.980436	0.723853
62	9	0	7.426322	-1.561992	1.568230
63	9	0	5.559270	-1.992907	2.610956

64	9	0	7.392743	1.605091	-2.228636
65	9	0	6.703872	3.221942	-0.944577
66	9	0	5.563343	2.685672	-2.721081

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.909376	-5.368940	-2.488707
2	6	0	-4.003672	-5.099089	-1.123484
3	1	0	-2.976257	-4.804715	-4.356216
4	6	0	-3.062770	-4.597728	-3.292260
5	6	0	-3.268374	-4.059235	-0.527297
6	6	0	-2.424457	-3.295718	-1.358958
7	6	0	-2.319311	-3.562959	-2.725666
8	1	0	-1.652954	-2.947864	-3.322273
9	6	0	-2.385836	-3.209701	3.077738
10	6	0	-3.641695	-3.230996	3.683520
11	6	0	-4.778673	-3.515302	2.919617
12	6	0	-4.648643	-3.774870	1.555470
13	6	0	-3.393871	-3.764200	0.920200
14	6	0	-2.263347	-3.475598	1.711778
15	1	0	-1.484864	-2.990754	3.642371
16	1	0	-3.732781	-3.018414	4.746033
17	8	0	-1.759632	-2.203458	-0.846981
18	8	0	-1.000097	-3.547735	1.168755
19	15	0	-0.423555	-2.380665	0.136127
20	8	0	-0.325839	-1.051933	0.867059
21	8	0	0.757679	-2.943806	-0.579469
22	1	0	-4.484212	-6.184479	-2.920736
23	1	0	-4.642823	-5.714388	-0.494954
24	1	0	-5.535509	-3.967587	0.956901
25	1	0	-5.763459	-3.519332	3.380244
26	6	0	1.226358	1.773101	-0.047639
27	7	0	-0.125775	1.615136	0.165589
28	1	0	-0.405507	0.649711	0.407344
29	7	0	1.881362	0.604051	0.258565
30	1	0	1.260094	-0.183988	0.499742
31	6	0	3.238488	0.258510	0.156555
32	6	0	4.292539	1.164004	0.351995
33	6	0	3.527785	-1.099724	-0.081603

34	6	0	5.612842	0.711369	0.288606
35	1	0	4.079754	2.203588	0.555022
36	6	0	4.854920	-1.526531	-0.129136
37	1	0	2.712564	-1.807754	-0.233768
38	6	0	5.912263	-0.628882	0.043717
39	1	0	6.939836	-0.970478	0.004929
40	6	0	-1.205912	2.486276	0.010100
41	6	0	-1.124631	3.889204	-0.007010
42	6	0	-2.476041	1.878754	-0.079390
43	6	0	-2.292210	4.648043	-0.122140
44	1	0	-0.160822	4.371480	0.065734
45	6	0	-3.624542	2.657463	-0.192326
46	1	0	-2.548656	0.794975	-0.066955
47	6	0	-3.550167	4.053249	-0.219180
48	1	0	-4.446499	4.654958	-0.312121
49	16	0	1.961349	3.163564	-0.649734
50	6	0	-2.182437	6.148458	-0.194092
51	6	0	-4.976500	1.995595	-0.234654
52	6	0	6.731993	1.703524	0.455855
53	6	0	5.165633	-2.970335	-0.430468
54	9	0	-2.040213	6.590401	-1.475970
55	9	0	-1.121960	6.630665	0.497201
56	9	0	-3.288636	6.770707	0.297640
57	9	0	-5.860839	2.688549	-1.004092
58	9	0	-5.541533	1.914231	1.004551
59	9	0	-4.930836	0.736289	-0.722053
60	9	0	5.339944	-3.183407	-1.766951
61	9	0	6.326076	-3.374165	0.164284
62	9	0	4.199116	-3.814040	-0.022386
63	9	0	7.872916	1.125552	0.920007
64	9	0	6.420308	2.701847	1.320205
65	9	0	7.066293	2.307005	-0.720023

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.620944	2.426567	0.786658
2	6	0	-4.046544	1.285854	1.345485
3	1	0	-4.582139	3.821687	-0.864708
4	6	0	-4.138942	2.933650	-0.423582

5	6	0	-2.976072	0.619704	0.720856
6	6	0	-2.524377	1.154999	-0.495795
7	6	0	-3.083057	2.291617	-1.071054
8	1	0	-2.681093	2.663008	-2.008506
9	6	0	-1.450548	-2.848421	1.167290
10	6	0	-1.219588	-2.871444	2.543028
11	6	0	-1.547955	-1.757428	3.321359
12	6	0	-2.107445	-0.627948	2.725902
13	6	0	-2.356165	-0.575853	1.341998
14	6	0	-2.006707	-1.710186	0.593365
15	1	0	-1.213217	-3.698231	0.535274
16	1	0	-0.780020	-3.752614	3.001065
17	8	0	-1.402582	0.593181	-1.138843
18	8	0	-2.302517	-1.751830	-0.782855
19	15	0	-1.442478	-0.877661	-1.816975
20	8	0	-0.070481	-1.309099	-2.173001
21	8	0	-2.476373	-0.821040	-3.040023
22	1	0	-2.025155	-0.933610	-3.894596
23	1	0	-5.449249	2.914729	1.292068
24	1	0	-4.439697	0.885010	2.275385
25	1	0	-2.338902	0.242562	3.333019
26	1	0	-1.357943	-1.763543	4.390699
27	6	0	3.180740	-0.373190	-0.636633
28	6	0	2.677576	0.874846	-0.200649
29	6	0	3.958821	1.242544	0.378982
30	6	0	4.495674	-0.080110	-0.077497
31	7	0	2.721857	-1.441340	-1.287101
32	1	0	1.769877	-1.502484	-1.642150
33	7	0	1.524513	1.550868	-0.247814
34	1	0	0.669612	1.179396	-0.642003
35	16	0	4.477805	2.581548	1.180183
36	16	0	5.902059	-0.926694	-0.026941
37	1	0	1.499870	2.462432	0.194881
38	1	0	3.371618	-2.198682	-1.463777

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.556168	3.667233	-0.443806

2	6	0	3.250801	2.619742	0.161752
3	1	0	1.058748	4.197421	-1.911686
4	6	0	1.612385	3.389739	-1.438753
5	6	0	3.030403	1.280117	-0.205376
6	6	0	2.076792	1.024260	-1.213936
7	6	0	1.373299	2.069681	-1.820269
8	1	0	0.648490	1.823002	-2.590065
9	6	0	3.862162	-2.052371	1.431215
10	6	0	5.227265	-1.909140	1.677129
11	6	0	5.882977	-0.730127	1.305815
12	6	0	5.165727	0.294508	0.688152
13	6	0	3.788227	0.176816	0.431421
14	6	0	3.147582	-1.018930	0.818757
15	1	0	3.325387	-2.954956	1.706267
16	1	0	5.778359	-2.717778	2.151684
17	8	0	1.893622	-0.251874	-1.683944
18	8	0	1.786502	-1.142158	0.691785
19	15	0	1.061960	-1.404995	-0.797694
20	8	0	1.398650	-2.734888	-1.372986
21	8	0	-0.364962	-0.936924	-0.589161
22	1	0	2.740435	4.692314	-0.131493
23	1	0	3.965679	2.834087	0.952633
24	1	0	5.680288	1.200254	0.376150
25	1	0	6.949406	-0.614331	1.484055
26	6	0	-3.202775	0.328067	0.481392
27	6	0	-3.634121	-0.813748	-0.252154
28	6	0	-5.027345	-0.513369	0.032999
29	6	0	-4.574999	0.683978	0.801233
30	7	0	-2.018014	0.852695	0.757108
31	1	0	-1.169582	0.392932	0.396663
32	7	0	-3.007570	-1.766901	-0.925947
33	1	0	-1.979062	-1.750159	-0.980825
34	16	0	-6.449388	-1.255080	-0.374959
35	16	0	-5.247163	1.925136	1.665451
36	1	0	-3.551608	-2.495719	-1.369844
37	1	0	-1.969815	1.694412	1.316892

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Standard orientation:

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

1	6	0	2.810896	3.853315	2.110560
2	6	0	2.199852	4.155803	0.913773
3	6	0	1.717183	3.129711	0.056131
4	6	0	1.899592	1.755337	0.427653
5	6	0	2.516308	1.481204	1.681027
6	6	0	2.956535	2.500306	2.499790
7	1	0	0.907748	4.486462	-1.429816
8	1	0	3.168002	4.647270	2.761074
9	1	0	2.061075	5.191389	0.611401
10	6	0	1.033544	3.443753	-1.149349
11	6	0	1.419622	0.714587	-0.447014
12	1	0	2.631403	0.451959	2.002519
13	1	0	3.415504	2.260739	3.455624
14	6	0	0.671645	1.102851	-1.547275
15	6	0	0.495466	2.449549	-1.926896
16	1	0	-0.072562	2.666623	-2.825595
17	6	0	0.760624	-2.989533	0.191595
18	6	0	2.017341	-3.490472	0.428214
19	6	0	3.163341	-2.658893	0.303850
20	6	0	2.999677	-1.270836	-0.025628
21	6	0	1.671082	-0.729894	-0.179537
22	6	0	0.614743	-1.622959	-0.123920
23	1	0	4.578382	-4.239803	0.726798
24	1	0	-0.125827	-3.613988	0.232776
25	1	0	2.150096	-4.539694	0.679869
26	6	0	4.472977	-3.188963	0.466380
27	6	0	4.173240	-0.493280	-0.235140
28	6	0	5.429756	-1.042782	-0.089707
29	6	0	5.586372	-2.400458	0.278993
30	1	0	4.075602	0.545989	-0.527219
31	1	0	6.308203	-0.427406	-0.265704
32	1	0	6.582001	-2.819570	0.397727
33	8	0	0.092409	0.147306	-2.388076
34	8	0	-0.694160	-1.172509	-0.369292
35	15	0	-1.091144	-0.852815	-1.909637
36	8	0	-1.274265	-1.956621	-2.872018
37	7	0	-2.538698	-0.009500	-1.696930
38	1	0	-3.247066	-0.238026	-2.391245
39	16	0	-3.152102	1.008624	-0.469474
40	8	0	-2.031977	1.777984	0.062849
41	8	0	-4.312651	1.638525	-1.103812
42	6	0	-3.748782	-0.091507	0.818772
43	6	0	-5.034066	-0.629025	0.706917

44	6	0	-2.928409	-0.364966	1.915116
45	6	0	-5.497882	-1.477250	1.713589
46	1	0	-5.661514	-0.373992	-0.141189
47	6	0	-3.407912	-1.212248	2.916363
48	1	0	-1.943242	0.082908	1.981033
49	6	0	-4.685919	-1.769653	2.814464
50	1	0	-6.495863	-1.900639	1.642021
51	1	0	-2.782609	-1.431817	3.777330
52	1	0	-5.053470	-2.427332	3.597709

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.912880	3.983403	1.875211
2	6	0	2.219874	4.214768	0.705741
3	6	0	1.698000	3.142923	-0.067483
4	6	0	1.922385	1.789540	0.356194
5	6	0	2.619212	1.590461	1.582549
6	6	0	3.099876	2.653164	2.320874
7	1	0	0.755040	4.411173	-1.553610
8	1	0	3.298264	4.814875	2.461048
9	1	0	2.043197	5.232479	0.361954
10	6	0	0.928191	3.384502	-1.238107
11	6	0	1.408773	0.699588	-0.434940
12	1	0	2.761865	0.579920	1.949652
13	1	0	3.620174	2.464617	3.257449
14	6	0	0.577935	1.008328	-1.508487
15	6	0	0.358519	2.344722	-1.924315
16	1	0	-0.287342	2.508166	-2.780284
17	6	0	0.846656	-2.964293	0.438540
18	6	0	2.118558	-3.439423	0.638399
19	6	0	3.245737	-2.604280	0.407090
20	6	0	3.040193	-1.239378	0.008804
21	6	0	1.698909	-0.723827	-0.104663
22	6	0	0.646438	-1.617782	0.051309
23	1	0	4.704817	-4.139173	0.844349
24	1	0	-0.028676	-3.594861	0.556495
25	1	0	2.279954	-4.472212	0.940630
26	6	0	4.570670	-3.105225	0.530892
27	6	0	4.192277	-0.463034	-0.306130

28	6	0	5.465050	-0.983789	-0.194087
29	6	0	5.663228	-2.315905	0.242859
30	1	0	4.059989	0.555677	-0.652833
31	1	0	6.322714	-0.365933	-0.450456
32	1	0	6.670581	-2.715801	0.334295
33	8	0	0.000836	0.027695	-2.272795
34	8	0	-0.650816	-1.200446	-0.143540
35	15	0	-1.171220	-1.044045	-1.731590
36	8	0	-1.012102	-2.292583	-2.520456
37	7	0	-2.634475	-0.400878	-1.685781
38	16	0	-3.251219	0.781092	-0.795377
39	8	0	-2.262377	1.795573	-0.355611
40	8	0	-4.474084	1.272675	-1.463493
41	6	0	-3.831452	-0.034607	0.721774
42	6	0	-5.014529	-0.777834	0.687859
43	6	0	-3.098060	0.087539	1.902490
44	6	0	-5.462754	-1.410341	1.849187
45	1	0	-5.572746	-0.848107	-0.240672
46	6	0	-3.554231	-0.545706	3.063092
47	1	0	-2.186928	0.676671	1.901658
48	6	0	-4.733808	-1.295462	3.038953
49	1	0	-6.383020	-1.990337	1.827042
50	1	0	-2.985648	-0.451896	3.985877
51	1	0	-5.085907	-1.787539	3.943307

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.520120	4.554383	-0.751860
2	6	0	-0.669205	4.358005	0.312847
3	6	0	-0.342718	3.047392	0.757786
4	6	0	-0.938454	1.912405	0.110875
5	6	0	-1.793710	2.153721	-1.000982
6	6	0	-2.074118	3.436941	-1.421188
7	1	0	1.025013	3.708066	2.306319
8	1	0	-1.755015	5.560449	-1.088688
9	1	0	-0.217313	5.206077	0.822315
10	6	0	0.587063	2.844031	1.812927
11	6	0	-0.617980	0.583866	0.571227
12	1	0	-2.220914	1.312715	-1.535130

13	1	0	-2.722677	3.590471	-2.279719
14	6	0	0.367103	0.467290	1.538760
15	6	0	0.957715	1.574467	2.183236
16	1	0	1.689424	1.393991	2.964420
17	6	0	-1.034114	-2.801218	-1.143792
18	6	0	-2.398269	-2.937719	-1.225860
19	6	0	-3.259940	-1.972991	-0.636844
20	6	0	-2.698171	-0.819145	0.007219
21	6	0	-1.267743	-0.632661	0.005091
22	6	0	-0.498790	-1.660160	-0.514044
23	1	0	-5.080185	-3.024193	-1.148080
24	1	0	-0.354100	-3.545487	-1.544728
25	1	0	-2.832235	-3.806162	-1.714755
26	6	0	-4.670888	-2.150428	-0.646160
27	6	0	-3.587351	0.075038	0.666989
28	6	0	-4.950073	-0.136847	0.657097
29	6	0	-5.503362	-1.251406	-0.017636
30	1	0	-3.184441	0.930148	1.197777
31	1	0	-5.604781	0.557068	1.177744
32	1	0	-6.579459	-1.402352	-0.024687
33	8	0	0.796573	-0.793405	1.968900
34	8	0	0.907784	-1.586563	-0.445185
35	15	0	1.578582	-1.829028	0.998285
36	8	0	1.626053	-3.175419	1.594831
37	7	0	3.174951	-1.266700	0.747132
38	1	0	3.796564	-1.722038	1.416337
39	6	0	3.930049	-0.454785	-0.083314
40	8	0	5.119447	-0.300987	0.096204
41	6	0	3.263035	0.229985	-1.311178
42	9	0	4.125251	1.084312	-1.871682
43	9	0	2.922469	-0.689080	-2.238527
44	9	0	2.158740	0.924054	-0.967401

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.184704	4.011379	1.417904
2	6	0	2.301225	4.229403	0.382592
3	6	0	1.591406	3.155200	-0.220483
4	6	0	1.823669	1.812116	0.233534

5	6	0	2.722666	1.629038	1.323446
6	6	0	3.383636	2.694704	1.898990
7	1	0	0.448223	4.409807	-1.570572
8	1	0	3.713339	4.844737	1.875029
9	1	0	2.117285	5.238590	0.018190
10	6	0	0.627709	3.388975	-1.239570
11	6	0	1.116752	0.722036	-0.386529
12	1	0	2.877955	0.629667	1.714829
13	1	0	4.056691	2.521057	2.735637
14	6	0	0.140907	1.026440	-1.330550
15	6	0	-0.100769	2.351552	-1.765801
16	1	0	-0.882416	2.509907	-2.501099
17	6	0	0.359563	-2.809732	0.804296
18	6	0	1.593517	-3.411173	0.818189
19	6	0	2.744674	-2.713179	0.360697
20	6	0	2.612176	-1.352215	-0.080471
21	6	0	1.329804	-0.703043	-0.007102
22	6	0	0.230603	-1.465624	0.377739
23	1	0	4.097620	-4.375239	0.648573
24	1	0	-0.541422	-3.334980	1.104623
25	1	0	1.699470	-4.442162	1.149786
26	6	0	4.015871	-3.347117	0.299951
27	6	0	3.767531	-0.716868	-0.620257
28	6	0	4.983777	-1.365302	-0.681717
29	6	0	5.118496	-2.691894	-0.204957
30	1	0	3.680727	0.295136	-1.000175
31	1	0	5.844618	-0.853895	-1.106590
32	1	0	6.082666	-3.192990	-0.251955
33	8	0	-0.593435	0.020969	-1.908613
34	8	0	-1.023407	-0.909208	0.400504
35	15	0	-1.846285	-0.681876	-1.051642
36	8	0	-2.190370	-1.956418	-1.735916
37	7	0	-2.865657	0.515258	-0.798811
38	6	0	-4.003388	0.724678	-0.144738
39	8	0	-4.718142	1.726769	-0.220774
40	6	0	-4.530216	-0.330246	0.890139
41	9	0	-5.848665	-0.588506	0.701307
42	9	0	-3.896451	-1.527133	0.862787
43	9	0	-4.401987	0.146753	2.159974

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.711978	4.486263	0.988471
2	6	0	0.819865	4.369187	-0.054290
3	6	0	0.418048	3.093339	-0.536379
4	6	0	0.976927	1.909065	0.050815
5	6	0	1.879346	2.068185	1.139936
6	6	0	2.234497	3.320090	1.597089
7	1	0	-0.958964	3.873762	-2.019089
8	1	0	2.004336	5.467166	1.353695
9	1	0	0.392635	5.255907	-0.517204
10	6	0	-0.547367	2.972490	-1.571917
11	6	0	0.579096	0.615874	-0.446828
12	1	0	2.285250	1.188240	1.626537
13	1	0	2.918209	3.410769	2.437277
14	6	0	-0.443194	0.581231	-1.381353
15	6	0	-0.992121	1.737647	-1.972295
16	1	0	-1.762431	1.621372	-2.727652
17	6	0	0.937382	-2.873325	1.058942
18	6	0	2.297054	-3.066893	1.068604
19	6	0	3.169487	-2.099713	0.499960
20	6	0	2.625323	-0.889396	-0.048746
21	6	0	1.204805	-0.649124	0.031963
22	6	0	0.418761	-1.674948	0.527518
23	1	0	4.967833	-3.245758	0.864847
24	1	0	0.247470	-3.618476	1.441447
25	1	0	2.717157	-3.980555	1.481459
26	6	0	4.571514	-2.329005	0.434020
27	6	0	3.519470	0.008781	-0.696498
28	6	0	4.872000	-0.252592	-0.761115
29	6	0	5.410417	-1.424833	-0.178384
30	1	0	3.127328	0.908115	-1.157255
31	1	0	5.529810	0.447235	-1.269868
32	1	0	6.479180	-1.614915	-0.229205
33	8	0	-0.948451	-0.641704	-1.838286
34	8	0	-0.982539	-1.540433	0.537566
35	15	0	-1.753706	-1.675899	-0.886859
36	8	0	-1.890373	-2.995979	-1.531712
37	7	0	-3.268577	-1.061231	-0.460006
38	1	0	-4.050322	-1.518449	-0.924770
39	16	0	-3.789612	0.101996	0.676394
40	8	0	-2.821088	1.193215	0.705471

41	8	0	-5.197655	0.322121	0.337169
42	6	0	-3.707730	-0.768515	2.252359
43	1	0	-4.027012	-0.054863	3.016156
44	1	0	-4.386878	-1.621985	2.213016
45	1	0	-2.676683	-1.083008	2.418339

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.036528	4.448593	1.001819
2	6	0	1.063869	4.379818	0.026456
3	6	0	0.561117	3.131120	-0.428367
4	6	0	1.095836	1.913587	0.112141
5	6	0	2.080354	2.024307	1.135523
6	6	0	2.537538	3.252768	1.568863
7	1	0	-0.896345	3.985920	-1.789266
8	1	0	2.404683	5.412510	1.346039
9	1	0	0.647667	5.290034	-0.401912
10	6	0	-0.487622	3.061717	-1.386214
11	6	0	0.600625	0.644518	-0.360679
12	1	0	2.468927	1.120881	1.592789
13	1	0	3.283603	3.299771	2.359236
14	6	0	-0.497009	0.649941	-1.217302
15	6	0	-1.023454	1.854231	-1.747641
16	1	0	-1.871618	1.781658	-2.418930
17	6	0	0.893211	-2.848340	1.128145
18	6	0	2.239311	-3.107738	1.061391
19	6	0	3.121623	-2.185160	0.435279
20	6	0	2.596834	-0.953896	-0.086215
21	6	0	1.198132	-0.647255	0.078893
22	6	0	0.380182	-1.629630	0.623189
23	1	0	4.884922	-3.409543	0.696548
24	1	0	0.190553	-3.560803	1.548343
25	1	0	2.641110	-4.040480	1.452083
26	6	0	4.505429	-2.475802	0.284903
27	6	0	3.492434	-0.102037	-0.794239
28	6	0	4.826780	-0.421046	-0.940059
29	6	0	5.348219	-1.613914	-0.383395
30	1	0	3.109374	0.810650	-1.236632
31	1	0	5.481469	0.248171	-1.493779

32	1	0	6.402949	-1.853706	-0.497837
33	8	0	-1.064754	-0.513400	-1.666017
34	8	0	-0.979406	-1.428076	0.707964
35	15	0	-1.863823	-1.640144	-0.713477
36	8	0	-1.631864	-2.971998	-1.330107
37	7	0	-3.373998	-1.246217	-0.380702
38	16	0	-3.984802	0.017422	0.406437
39	8	0	-3.231387	1.281316	0.197529
40	8	0	-5.442465	0.064921	0.160505
41	6	0	-3.792097	-0.392832	2.165290
42	1	0	-4.211363	0.437569	2.739667
43	1	0	-4.342444	-1.315402	2.362185
44	1	0	-2.729370	-0.520134	2.379847

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.436126	4.638374	0.018217
2	6	0	-0.272988	4.099092	-1.032141
3	6	0	-0.252240	2.700446	-1.289401
4	6	0	0.549536	1.842652	-0.463088
5	6	0	1.247724	2.432025	0.628405
6	6	0	1.190727	3.789628	0.863577
7	1	0	-1.630206	2.791460	-2.962585
8	1	0	0.408017	5.708110	0.207892
9	1	0	-0.874341	4.736055	-1.677177
10	6	0	-1.033938	2.135384	-2.333187
11	6	0	0.586688	0.427828	-0.735630
12	1	0	1.823662	1.798069	1.293144
13	1	0	1.728184	4.211028	1.709193
14	6	0	-0.273598	-0.059250	-1.708972
15	6	0	-1.067592	0.775714	-2.525132
16	1	0	-1.686469	0.319320	-3.291087
17	6	0	1.700520	-2.525563	1.404182
18	6	0	3.051683	-2.318380	1.537702
19	6	0	3.690592	-1.243817	0.861467
20	6	0	2.907094	-0.340911	0.066034
21	6	0	1.476059	-0.509338	0.006902
22	6	0	0.941518	-1.625886	0.627979
23	1	0	5.676937	-1.756075	1.548484

24	1	0	1.197402	-3.365318	1.872183
25	1	0	3.652687	-2.997166	2.137551
26	6	0	5.100270	-1.069820	0.932335
27	6	0	3.594285	0.662293	-0.673901
28	6	0	4.965261	0.792147	-0.598981
29	6	0	5.729041	-0.070950	0.222832
30	1	0	3.030239	1.327127	-1.318145
31	1	0	5.464047	1.561568	-1.182544
32	1	0	6.807950	0.046442	0.278700
33	8	0	-0.347376	-1.429285	-1.964600
34	8	0	-0.433460	-1.887802	0.527574
35	15	0	-0.996095	-2.462048	-0.879050
36	8	0	-0.722510	-3.861026	-1.256861
37	7	0	-2.659193	-2.177764	-0.746948
38	1	0	-3.136413	-2.759222	-1.436788
39	6	0	-3.458471	-1.032978	-0.481194
40	8	0	-4.394373	-0.791472	-1.228329
41	6	0	-3.205685	-0.235087	0.751584
42	6	0	-2.776531	-0.827675	1.948265
43	6	0	-3.535432	1.129768	0.731690
44	6	0	-2.664468	-0.057968	3.107054
45	1	0	-2.550751	-1.887456	1.977112
46	6	0	-3.399550	1.900015	1.884736
47	1	0	-3.895181	1.571336	-0.192237
48	6	0	-2.964602	1.306591	3.075008
49	1	0	-2.344174	-0.524943	4.034669
50	1	0	-3.638955	2.959662	1.858828
51	1	0	-2.867294	1.905757	3.976868

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.053674	4.642606	0.971076
2	6	0	1.084237	4.393587	0.022922
3	6	0	0.787203	3.069196	-0.400122
4	6	0	1.534747	1.969870	0.145831
5	6	0	2.508667	2.263298	1.143503
6	6	0	2.761945	3.559101	1.544882
7	1	0	-0.828433	3.645908	-1.727053

8	1	0	2.263222	5.661270	1.289776
9	1	0	0.513085	5.213430	-0.409471
10	6	0	-0.260078	2.808509	-1.326862
11	6	0	1.245622	0.630462	-0.293831
12	1	0	3.052877	1.445402	1.603122
13	1	0	3.507412	3.747652	2.314379
14	6	0	0.166141	0.441092	-1.151910
15	6	0	-0.583093	1.521486	-1.679179
16	1	0	-1.417472	1.282238	-2.331499
17	6	0	1.956164	-2.772721	1.253159
18	6	0	3.323260	-2.874356	1.180757
19	6	0	4.091330	-1.859727	0.547193
20	6	0	3.424159	-0.702832	0.017096
21	6	0	2.000345	-0.564562	0.177968
22	6	0	1.297142	-1.628410	0.739774
23	1	0	5.987230	-2.864220	0.816562
24	1	0	1.343802	-3.555499	1.689356
25	1	0	3.832416	-3.750126	1.578497
26	6	0	5.499927	-1.984586	0.399149
27	6	0	4.214194	0.246514	-0.693733
28	6	0	5.577553	0.088710	-0.834581
29	6	0	6.235991	-1.031680	-0.271821
30	1	0	3.725655	1.104585	-1.142037
31	1	0	6.149489	0.828923	-1.389727
32	1	0	7.312013	-1.144830	-0.383402
33	8	0	-0.175503	-0.824981	-1.551167
34	8	0	-0.065350	-1.573361	0.866331
35	15	0	-1.023351	-1.820402	-0.497824
36	8	0	-0.910579	-3.213987	-1.007669
37	7	0	-2.400938	-1.183214	0.023759
38	6	0	-3.369346	-0.647663	-0.743626
39	8	0	-3.337309	-0.401939	-1.966647
40	6	0	-4.633264	-0.289694	0.026052
41	6	0	-4.751676	-0.512781	1.405387
42	6	0	-5.714054	0.277022	-0.663825
43	6	0	-5.927255	-0.174735	2.081181
44	1	0	-3.908620	-0.952939	1.928172
45	6	0	-6.890830	0.615469	0.008787
46	1	0	-5.605780	0.441009	-1.731833
47	6	0	-7.001715	0.390938	1.385651
48	1	0	-6.005797	-0.352783	3.152243
49	1	0	-7.722582	1.054029	-0.539953
50	1	0	-7.917712	0.653943	1.911864

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.284383	4.549328	-0.869199
2	6	0	-0.301698	4.370796	0.078875
3	6	0	0.086420	3.067527	0.495848
4	6	0	-0.580300	1.921157	-0.055979
5	6	0	-1.573397	2.144338	-1.051646
6	6	0	-1.914041	3.420788	-1.447307
7	1	0	1.634097	3.752954	1.852983
8	1	0	-1.567757	5.549925	-1.184325
9	1	0	0.205832	5.227652	0.516185
10	6	0	1.142231	2.880972	1.429190
11	6	0	-0.196138	0.600379	0.376418
12	1	0	-2.062805	1.293914	-1.512855
13	1	0	-2.670730	3.560712	-2.214859
14	6	0	0.902833	0.496451	1.217099
15	6	0	1.561442	1.617382	1.768370
16	1	0	2.386315	1.450171	2.453788
17	6	0	-0.776411	-2.823558	-1.199099
18	6	0	-2.136561	-2.984412	-1.095786
19	6	0	-2.932983	-2.015533	-0.427034
20	6	0	-2.313828	-0.835358	0.107634
21	6	0	-0.899570	-0.630301	-0.084386
22	6	0	-0.182549	-1.656733	-0.676490
23	1	0	-4.784932	-3.107095	-0.669872
24	1	0	-0.141183	-3.569988	-1.664477
25	1	0	-2.614083	-3.874120	-1.498353
26	6	0	-4.330190	-2.212731	-0.249988
27	6	0	-3.127403	0.066181	0.849832
28	6	0	-4.476849	-0.163173	1.018491
29	6	0	-5.091772	-1.305875	0.452904
30	1	0	-2.674638	0.941894	1.300896
31	1	0	-5.072159	0.538121	1.597353
32	1	0	-6.157267	-1.471542	0.587585
33	8	0	1.385199	-0.754787	1.598191
34	8	0	1.212504	-1.548772	-0.804413
35	15	0	2.108363	-1.758515	0.534809
36	8	0	2.257741	-3.106381	1.113897
37	7	0	3.596157	-1.126374	0.057165

38	1	0	4.366642	-1.613113	0.513163
39	6	0	4.082967	-0.136616	-0.820753
40	8	0	5.288482	0.039632	-0.869609
41	6	0	3.107769	0.637595	-1.674102
42	1	0	2.530841	-0.036404	-2.313589
43	1	0	2.395891	1.197033	-1.060307
44	1	0	3.682447	1.333068	-2.287488

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.633408	4.143903	-1.138603
2	6	0	-1.600609	4.289431	-0.237074
3	6	0	-0.870222	3.165716	0.237035
4	6	0	-1.234862	1.848130	-0.205115
5	6	0	-2.288297	1.739918	-1.158329
6	6	0	-2.968169	2.852052	-1.611510
7	1	0	0.518851	4.326285	1.431625
8	1	0	-3.177341	5.014558	-1.498077
9	1	0	-1.313445	5.278139	0.116892
10	6	0	0.239187	3.324293	1.112462
11	6	0	-0.506267	0.708340	0.287028
12	1	0	-2.551269	0.760545	-1.542793
13	1	0	-3.763225	2.734042	-2.344544
14	6	0	0.605882	0.938124	1.091490
15	6	0	0.977589	2.238371	1.510775
16	1	0	1.864731	2.337445	2.126938
17	6	0	-0.102029	-2.815812	-1.082136
18	6	0	-1.355494	-3.357544	-0.940717
19	6	0	-2.394960	-2.621328	-0.309140
20	6	0	-2.130626	-1.283972	0.144950
21	6	0	-0.839898	-0.693666	-0.091166
22	6	0	0.158362	-1.493000	-0.645332
23	1	0	-3.859933	-4.205533	-0.450062
24	1	0	0.719971	-3.375934	-1.516531
25	1	0	-1.559063	-4.371348	-1.280420
26	6	0	-3.677295	-3.194568	-0.089325
27	6	0	-3.166297	-0.612340	0.856974
28	6	0	-4.395425	-1.202316	1.068931
29	6	0	-4.664713	-2.503898	0.580253

30	1	0	-2.974616	0.380672	1.248603
31	1	0	-5.161440	-0.663929	1.622706
32	1	0	-5.638535	-2.958710	0.747329
33	8	0	1.353570	-0.118130	1.544398
34	8	0	1.420185	-0.997460	-0.829089
35	15	0	2.455475	-0.847286	0.513618
36	8	0	2.781524	-2.189949	1.081553
37	7	0	3.491741	0.296831	0.137703
38	6	0	4.698026	0.191366	-0.485501
39	8	0	5.460848	1.159325	-0.609639
40	6	0	5.122927	-1.158524	-1.082342
41	1	0	5.040988	-1.960676	-0.340527
42	1	0	4.460353	-1.422138	-1.917739
43	1	0	6.150233	-1.088286	-1.451015

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.335638	2.782237	-0.595072
2	6	0	2.154650	2.627920	-1.859670
3	6	0	2.387273	1.101941	-1.924556
4	6	0	2.421142	0.647968	-0.425849
5	6	0	1.385892	1.599308	0.165225
6	6	0	3.849058	0.907139	0.167340
7	6	0	4.678682	-0.323204	-0.261145
8	6	0	3.637717	-1.422584	-0.296708
9	6	0	2.344678	-0.867081	-0.283702
10	6	0	0.561717	1.506301	1.282695
11	6	0	-0.199490	2.593830	1.715625
12	6	0	-0.173663	3.786191	0.990284
13	6	0	0.576248	3.876109	-0.187177
14	6	0	3.833597	-2.801827	-0.296447
15	6	0	2.721893	-3.651126	-0.253203
16	6	0	1.433628	-3.119808	-0.169790
17	6	0	1.263944	-1.735270	-0.174179
18	8	0	0.442587	0.301593	2.001720
19	8	0	-0.044658	-1.225080	-0.013501
20	15	0	-0.513451	-0.898920	1.492867
21	8	0	-0.591882	-1.976474	2.496484

22	1	0	1.629298	3.010826	-2.741914
23	1	0	3.104602	3.176907	-1.791158
24	1	0	3.297938	0.822274	-2.464130
25	1	0	1.538491	0.619657	-2.422964
26	1	0	3.778522	0.943266	1.260958
27	1	0	4.272526	1.857700	-0.171851
28	1	0	5.134312	-0.174317	-1.250433
29	1	0	5.496064	-0.544170	0.434684
30	1	0	-0.816965	2.487559	2.602357
31	1	0	-0.772082	4.629275	1.324197
32	1	0	0.548749	4.782993	-0.786470
33	1	0	4.839071	-3.215780	-0.307794
34	1	0	2.857339	-4.729042	-0.243848
35	1	0	0.563150	-3.759954	-0.070002
36	7	0	-2.073840	-0.264313	1.178178
37	1	0	-2.730778	-0.415532	1.942556
38	16	0	-2.802982	0.478363	-0.135308
39	8	0	-3.929116	1.240399	0.390029
40	8	0	-1.798930	1.027264	-1.028112
41	6	0	-3.584498	-0.986939	-1.040154
42	9	0	-4.300825	-0.517290	-2.065559
43	9	0	-2.647420	-1.818592	-1.497122
44	9	0	-4.392482	-1.650754	-0.202160

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.555678	2.772846	-0.537282
2	6	0	2.461809	2.633979	-1.744181
3	6	0	2.652445	1.103369	-1.841546
4	6	0	2.562562	0.600021	-0.361416
5	6	0	1.521726	1.569837	0.187899
6	6	0	3.953994	0.779053	0.337264
7	6	0	4.762300	-0.473607	-0.069358
8	6	0	3.680537	-1.524748	-0.217914
9	6	0	2.415587	-0.915077	-0.280579
10	6	0	0.615061	1.443636	1.242647
11	6	0	-0.164781	2.538531	1.632431
12	6	0	-0.065846	3.749990	0.946064
13	6	0	0.782580	3.868745	-0.160456

14	6	0	3.819719	-2.911039	-0.247221
15	6	0	2.667774	-3.705195	-0.312401
16	6	0	1.402433	-3.116029	-0.308852
17	6	0	1.276164	-1.722420	-0.277866
18	8	0	0.449105	0.233762	1.895004
19	8	0	0.016122	-1.157353	-0.218055
20	15	0	-0.630785	-0.881476	1.288354
21	8	0	-0.582609	-2.067100	2.180354
22	1	0	2.013332	3.059518	-2.650258
23	1	0	3.422822	3.148554	-1.591295
24	1	0	3.591215	0.808841	-2.325219
25	1	0	1.824649	0.665236	-2.410598
26	1	0	3.803204	0.785324	1.423435
27	1	0	4.440678	1.721149	0.060423
28	1	0	5.298419	-0.311825	-1.016875
29	1	0	5.516291	-0.751343	0.677987
30	1	0	-0.877655	2.406080	2.439740
31	1	0	-0.696351	4.584615	1.242710
32	1	0	0.808692	4.790535	-0.738465
33	1	0	4.804965	-3.371012	-0.195231
34	1	0	2.753351	-4.789520	-0.323396
35	1	0	0.498881	-3.716373	-0.286766
36	7	0	-2.045204	-0.151926	1.060590
37	16	0	-2.789773	0.520259	-0.151784
38	8	0	-3.746721	1.533475	0.322635
39	8	0	-1.983948	0.835155	-1.344605
40	6	0	-3.922285	-0.868930	-0.751639
41	9	0	-4.662074	-0.451823	-1.803887
42	9	0	-3.214601	-1.945341	-1.152901
43	9	0	-4.775353	-1.272789	0.209754

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.434094	-2.442683	-2.338916
2	6	0	-1.084402	-2.556487	-2.096041
3	6	0	-3.307637	-1.875997	-1.383474
4	6	0	-0.528564	-2.058366	-0.895919
5	6	0	-1.393167	-1.480422	0.031654
6	6	0	-2.804345	-1.412004	-0.126113

7	6	0	3.165631	-1.300649	-0.042842
8	6	0	3.699460	-2.614032	-0.255018
9	6	0	2.863964	-3.670600	-0.681312
10	6	0	1.519215	-3.476910	-0.893504
11	6	0	0.929851	-2.214345	-0.653845
12	6	0	1.758114	-1.177855	-0.221579
13	8	0	-0.820203	-0.978862	1.209289
14	8	0	1.146082	0.074160	-0.010538
15	15	0	0.148414	0.310227	1.227613
16	8	0	0.657769	0.573223	2.585042
17	1	0	-2.848030	-2.784442	-3.284160
18	1	0	3.303615	-4.653319	-0.831831
19	6	0	-5.568830	-1.191173	-0.808288
20	6	0	-5.130714	-0.777730	0.492996
21	1	0	-7.110315	-0.172756	1.094588
22	1	0	-6.620263	-1.075880	-1.060714
23	6	0	-6.076596	-0.274514	1.417459
24	6	0	-3.423312	-0.585932	2.214394
25	6	0	-4.374281	-0.112238	3.104992
26	6	0	-5.710818	0.064962	2.705726
27	1	0	-2.416219	-0.733069	2.572944
28	1	0	-4.076556	0.116232	4.125161
29	1	0	-6.448863	0.446852	3.406092
30	6	0	5.464301	-0.555920	0.572078
31	6	0	5.929238	-1.900722	0.401203
32	6	0	3.737924	1.146840	0.437964
33	6	0	6.384299	0.449154	0.953961
34	6	0	5.995924	1.769006	1.075897
35	6	0	4.661655	2.114061	0.800044
36	6	0	5.088056	-2.880717	-0.018124
37	6	0	4.090964	-0.223339	0.329784
38	1	0	5.447724	-3.895014	-0.172156
39	1	0	6.977714	-2.114704	0.594658
40	1	0	7.416036	0.159846	1.140931
41	1	0	6.713295	2.531005	1.368722
42	1	0	4.342818	3.150798	0.868620
43	1	0	2.732309	1.462301	0.218426
44	6	0	-4.700987	-1.745305	-1.694703
45	6	0	-3.755257	-0.910710	0.871622
46	1	0	-5.042849	-2.086546	-2.668662
47	1	0	-0.426432	-2.989699	-2.843417
48	1	0	0.887416	-4.301042	-1.210623
49	7	0	-0.698432	1.688406	0.667077
50	1	0	-1.048399	2.275338	1.423660

51	16	0	-1.233361	2.219624	-0.832658
52	8	0	-1.128839	1.151365	-1.810271
53	8	0	-2.440888	3.001045	-0.602590
54	6	0	0.091268	3.489364	-1.282695
55	9	0	0.187244	4.403774	-0.307934
56	9	0	-0.266900	4.090624	-2.419625
57	9	0	1.277553	2.899157	-1.447474

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.400795	-2.663496	-2.247104
2	6	0	-1.052941	-2.731519	-1.978087
3	6	0	-3.289955	-2.034136	-1.347982
4	6	0	-0.519874	-2.128455	-0.818027
5	6	0	-1.389307	-1.457669	0.049060
6	6	0	-2.804373	-1.433631	-0.142865
7	6	0	3.167945	-1.343101	-0.004993
8	6	0	3.694571	-2.671797	-0.097925
9	6	0	2.851508	-3.758309	-0.421102
10	6	0	1.508471	-3.566180	-0.653457
11	6	0	0.931555	-2.281843	-0.535419
12	6	0	1.756883	-1.205450	-0.188033
13	8	0	-0.842472	-0.887603	1.176166
14	8	0	1.166830	0.035399	-0.101311
15	15	0	0.167760	0.435667	1.165399
16	8	0	0.839968	0.470159	2.486231
17	1	0	-2.800911	-3.094236	-3.162333
18	1	0	3.282143	-4.755727	-0.478542
19	6	0	-5.586191	-1.423646	-0.821076
20	6	0	-5.165741	-0.862136	0.428874
21	1	0	-7.176595	-0.325849	0.990491
22	1	0	-6.644297	-1.391305	-1.073792
23	6	0	-6.135090	-0.322968	1.307462
24	6	0	-3.455905	-0.341306	2.075373
25	6	0	-4.426863	0.171194	2.921066
26	6	0	-5.779470	0.193076	2.538872
27	1	0	-2.430699	-0.340825	2.407416
28	1	0	-4.126430	0.569581	3.886959
29	1	0	-6.534259	0.609174	3.202358

30	6	0	5.480915	-0.551124	0.505078
31	6	0	5.938820	-1.908824	0.458494
32	6	0	3.747143	1.132175	0.243876
33	6	0	6.406721	0.485116	0.773723
34	6	0	6.017212	1.811150	0.777603
35	6	0	4.676497	2.128514	0.497407
36	6	0	5.085648	-2.919980	0.149466
37	6	0	4.103091	-0.241762	0.255718
38	1	0	5.439305	-3.947439	0.090738
39	1	0	6.990131	-2.108798	0.656885
40	1	0	7.442646	0.213667	0.970014
41	1	0	6.738772	2.597932	0.985949
42	1	0	4.352499	3.165888	0.479440
43	1	0	2.732717	1.417955	0.022262
44	6	0	-4.688321	-1.998236	-1.663023
45	6	0	-3.779778	-0.866064	0.796121
46	1	0	-5.011460	-2.438543	-2.604122
47	1	0	-0.377977	-3.219933	-2.675822
48	1	0	0.867565	-4.408831	-0.898390
49	7	0	-0.609406	1.771133	0.720658
50	16	0	-1.220308	2.254070	-0.656874
51	8	0	-1.178586	1.289262	-1.770976
52	8	0	-2.453570	3.025879	-0.448594
53	6	0	0.013105	3.588036	-1.176367
54	9	0	0.105670	4.568690	-0.258267
55	9	0	-0.374536	4.151340	-2.340467
56	9	0	1.251195	3.080935	-1.361672

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.033467	-2.201903	0.789529
2	6	0	3.160787	-1.523554	1.538075
3	6	0	2.829320	-0.023059	1.382806
4	6	0	2.014907	0.093435	0.049908
5	6	0	1.341428	-1.271405	-0.002094
6	6	0	2.958263	0.268205	-1.191428
7	6	0	3.157986	1.788320	-1.354935
8	6	0	1.893563	2.363371	-0.755615
9	6	0	1.218081	1.392684	0.002595

10	6	0	0.281612	-1.724264	-0.786126
11	6	0	-0.076786	-3.074992	-0.816593
12	6	0	0.622730	-3.982003	-0.013938
13	6	0	1.676619	-3.550088	0.797315
14	6	0	1.413914	3.667831	-0.856905
15	6	0	0.248262	4.019547	-0.171488
16	6	0	-0.432141	3.078875	0.604725
17	6	0	0.052320	1.771456	0.668081
18	1	0	3.220769	-1.834628	2.587302
19	1	0	4.127348	-1.772867	1.077163
20	1	0	3.716665	0.618728	1.374383
21	1	0	2.194320	0.299575	2.215294
22	1	0	2.452355	-0.129890	-2.078072
23	1	0	3.895926	-0.284457	-1.069529
24	1	0	4.038824	2.141593	-0.799558
25	1	0	3.304329	2.081354	-2.400890
26	1	0	-0.887589	-3.406458	-1.455873
27	1	0	0.340422	-5.031149	-0.029667
28	1	0	2.213897	-4.259930	1.421548
29	1	0	1.942308	4.404935	-1.456724
30	1	0	-0.138828	5.032698	-0.234320
31	1	0	-1.335045	3.351025	1.135777
32	16	0	-2.158051	0.435933	1.447959
33	8	0	-2.928955	1.599045	1.067427
34	8	0	-2.383664	-0.321442	2.662957
35	16	0	-2.031820	-0.614211	-1.442351
36	8	0	-2.318626	0.728476	-1.884611
37	8	0	-2.653162	-1.798863	-2.009306
38	8	0	-0.557884	0.798562	1.500548
39	8	0	-0.391405	-0.760445	-1.566918
40	7	0	-2.333804	-0.741457	0.224177
41	1	0	-2.207581	-1.685277	0.589937

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143065	-2.168318	0.712652
2	6	0	3.273279	-1.475585	1.446558
3	6	0	2.878953	0.015123	1.350768
4	6	0	2.039336	0.142432	0.035591

5	6	0	1.405907	-1.239959	-0.036647
6	6	0	2.961193	0.388227	-1.207264
7	6	0	3.126191	1.918711	-1.306514
8	6	0	1.844347	2.433391	-0.685655
9	6	0	1.199846	1.415571	0.033998
10	6	0	0.307119	-1.675647	-0.782847
11	6	0	-0.038624	-3.033540	-0.789815
12	6	0	0.707959	-3.944484	-0.039558
13	6	0	1.804989	-3.520755	0.720077
14	6	0	1.314776	3.720453	-0.758656
15	6	0	0.118097	3.991809	-0.087563
16	6	0	-0.535075	2.996779	0.641870
17	6	0	-0.002895	1.700336	0.694511
18	1	0	3.376929	-1.816370	2.484591
19	1	0	4.237516	-1.668474	0.950952
20	1	0	3.738964	0.695760	1.357284
21	1	0	2.236329	0.277450	2.198588
22	1	0	2.444236	0.018919	-2.100082
23	1	0	3.912915	-0.150555	-1.124740
24	1	0	4.002047	2.266036	-0.736512
25	1	0	3.265036	2.260570	-2.340165
26	1	0	-0.907466	-3.351117	-1.355602
27	1	0	0.418348	-4.993173	-0.037745
28	1	0	2.372965	-4.232892	1.316131
29	1	0	1.817759	4.496802	-1.332534
30	1	0	-0.319626	4.986699	-0.134574
31	1	0	-1.471280	3.201144	1.145024
32	16	0	-2.237492	0.252706	1.371515
33	8	0	-2.995214	1.482058	1.115748
34	8	0	-2.405666	-0.425548	2.652529
35	16	0	-2.095545	-0.612539	-1.348972
36	8	0	-2.331750	0.730686	-1.872748
37	8	0	-2.645715	-1.764214	-2.070946
38	8	0	-0.571331	0.697307	1.459902
39	8	0	-0.383627	-0.729501	-1.516008
40	7	0	-2.345779	-0.878145	0.221692

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Standard orientation:

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

1	6	0	-1.522707	3.117287	0.220610
2	6	0	-1.851543	1.815794	-0.155582
3	1	0	-0.382874	4.402468	1.525354
4	6	0	-0.637081	3.386587	1.243593
5	6	0	-1.320837	0.691470	0.469662
6	6	0	-0.388861	0.986607	1.495297
7	6	0	-0.061177	2.277221	1.887129
8	1	0	0.643144	2.413678	2.700810
9	6	0	-1.083096	-3.033576	-0.394031
10	6	0	-2.424442	-3.386691	-0.624650
11	6	0	-3.362261	-2.384632	-0.478504
12	6	0	-3.011695	-1.082774	-0.122612
13	6	0	-1.694819	-0.687184	0.098077
14	6	0	-0.749939	-1.732871	-0.043073
15	1	0	-0.290971	-3.767881	-0.490882
16	1	0	-2.708084	-4.399467	-0.888907
17	8	0	0.191396	-0.069006	2.214052
18	8	0	0.615871	-1.433453	0.107697
19	15	0	1.228859	-1.119438	1.561516
20	8	0	1.563240	-2.206602	2.498147
21	7	0	2.660845	-0.300487	1.104264
22	1	0	3.438600	-0.450476	1.745585
23	16	0	3.075317	0.700810	-0.175058
24	8	0	1.877207	1.217045	-0.812879
25	8	0	4.175914	1.537846	0.285584
26	6	0	3.856883	-0.516276	-1.393163
27	9	0	4.334243	0.174085	-2.432257
28	9	0	4.863073	-1.164710	-0.790940
29	9	0	2.957726	-1.402066	-1.822377
30	8	0	-2.158876	4.009060	-0.612634
31	8	0	-2.687808	1.851204	-1.241534
32	6	0	-3.089499	3.222997	-1.365248
33	1	0	-4.096696	3.343679	-0.942316
34	1	0	-3.049396	3.516628	-2.415280
35	8	0	-4.148451	-0.332625	0.039567
36	8	0	-4.732329	-2.480559	-0.569076
37	6	0	-5.205070	-1.129429	-0.513445
38	1	0	-6.077484	-1.074897	0.139059
39	1	0	-5.427952	-0.777960	-1.530661

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.489083	3.117362	0.224195
2	6	0	-1.881429	1.835849	-0.146737
3	1	0	-0.213500	4.342753	1.459993
4	6	0	-0.534014	3.340511	1.195284
5	6	0	-1.356327	0.686691	0.434616
6	6	0	-0.365113	0.921583	1.423791
7	6	0	0.029929	2.204378	1.798105
8	1	0	0.796739	2.303184	2.558844
9	6	0	-1.219090	-3.017068	-0.501461
10	6	0	-2.572659	-3.349178	-0.677547
11	6	0	-3.489757	-2.336668	-0.475771
12	6	0	-3.101804	-1.051349	-0.112665
13	6	0	-1.771764	-0.677649	0.056874
14	6	0	-0.832354	-1.725003	-0.144580
15	1	0	-0.441366	-3.759773	-0.642040
16	1	0	-2.882558	-4.354466	-0.944394
17	8	0	0.172471	-0.155036	2.096295
18	8	0	0.512207	-1.443264	-0.071670
19	15	0	1.268613	-1.187668	1.385037
20	8	0	1.362035	-2.395854	2.240036
21	7	0	2.642833	-0.416364	1.058214
22	16	0	3.070260	0.617887	-0.055470
23	8	0	2.014517	1.101132	-0.964371
24	8	0	4.025173	1.603684	0.477192
25	6	0	4.155332	-0.451826	-1.172118
26	9	0	4.632502	0.283229	-2.201581
27	9	0	5.213510	-0.956679	-0.508844
28	9	0	3.463780	-1.484545	-1.693858
29	8	0	-2.136391	4.046727	-0.578406
30	8	0	-2.772039	1.919562	-1.199890
31	6	0	-3.153864	3.294250	-1.240066
32	1	0	-4.108476	3.420260	-0.703100
33	1	0	-3.229220	3.618670	-2.279896
34	8	0	-4.230988	-0.287191	0.120160
35	8	0	-4.876714	-2.409469	-0.499254
36	6	0	-5.294862	-1.043126	-0.455015
37	1	0	-6.183641	-0.954414	0.172442
38	1	0	-5.480301	-0.685738	-1.481014

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.709299	4.816312	-0.357291
2	6	0	-1.551164	4.974525	-1.086225
3	6	0	-0.519845	3.997415	-1.041562
4	6	0	-0.696411	2.823887	-0.233379
5	6	0	-1.899428	2.702388	0.520340
6	6	0	-2.879763	3.670120	0.456039
7	1	0	0.826470	5.063675	-2.364482
8	1	0	-3.490990	5.569992	-0.400975
9	1	0	-1.405861	5.854803	-1.708229
10	6	0	0.690826	4.167613	-1.763617
11	6	0	0.337975	1.825929	-0.203277
12	1	0	-2.052411	1.833480	1.150246
13	1	0	-3.791306	3.549502	1.035071
14	6	0	1.502929	2.038097	-0.931896
15	6	0	1.683434	3.222331	-1.696996
16	1	0	2.619248	3.359603	-2.230090
17	6	0	-0.766916	-1.568419	1.238835
18	6	0	-0.187492	-1.548242	2.481529
19	6	0	0.576890	-0.430956	2.906450
20	6	0	0.756809	0.678927	2.012291
21	6	0	0.173981	0.634441	0.701872
22	6	0	-0.591022	-0.478132	0.343794
23	1	0	1.026687	-1.237066	4.863327
24	1	0	-1.333749	-2.435422	0.919661
25	1	0	-0.308734	-2.393360	3.154392
26	6	0	1.166455	-0.387872	4.198644
27	6	0	1.515979	1.795500	2.469650
28	6	0	2.072736	1.806392	3.729555
29	6	0	1.899742	0.705262	4.603655
30	1	0	1.664261	2.643481	1.810435
31	1	0	2.653501	2.665400	4.053850
32	1	0	2.347118	0.726495	5.593757
33	6	0	2.674050	1.089709	-0.941269
34	8	0	3.795123	1.429700	-0.621909
35	6	0	-1.123189	-0.602708	-1.037114
36	8	0	-0.449363	-0.401309	-2.039596
37	7	0	2.356172	-0.196295	-1.401602
38	1	0	1.395011	-0.384376	-1.722497
39	7	0	-2.442415	-1.072453	-1.269698

40	1	0	-2.630935	-1.133208	-2.271551
41	16	0	3.442987	-1.432455	-1.762275
42	8	0	2.636137	-2.463798	-2.406619
43	8	0	4.679679	-0.922887	-2.326662
44	16	0	-3.881354	-0.813092	-0.404107
45	8	0	-3.587250	-0.262556	0.907789
46	8	0	-4.846122	-0.237091	-1.329641
47	6	0	3.870506	-2.114328	-0.049286
48	6	0	-4.455349	-2.598049	-0.149992
49	9	0	4.675787	-3.169086	-0.215149
50	9	0	2.750046	-2.510404	0.571395
51	9	0	4.483863	-1.198062	0.697231
52	9	0	-5.657999	-2.571541	0.423406
53	9	0	-3.603867	-3.265475	0.635067
54	9	0	-4.534606	-3.211029	-1.335629

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.135255	4.521697	-0.318507
2	6	0	-2.042028	4.729730	-1.131338
3	6	0	-0.947626	3.823116	-1.128137
4	6	0	-0.987872	2.675340	-0.267764
5	6	0	-2.129478	2.497227	0.564877
6	6	0	-3.176212	3.393957	0.535895
7	1	0	0.225068	4.906141	-2.595932
8	1	0	-3.971190	5.217111	-0.337530
9	1	0	-2.000817	5.591693	-1.794617
10	6	0	0.192973	4.032772	-1.947751
11	6	0	0.111452	1.747943	-0.265582
12	1	0	-2.191748	1.627276	1.209242
13	1	0	-4.047354	3.218307	1.160980
14	6	0	1.202519	1.995652	-1.091346
15	6	0	1.244148	3.151882	-1.919234
16	1	0	2.126581	3.319256	-2.529341
17	6	0	-0.567438	-1.673904	1.312226
18	6	0	0.065291	-1.564436	2.524410
19	6	0	0.723416	-0.361898	2.893370
20	6	0	0.736707	0.735521	1.969854
21	6	0	0.090025	0.590351	0.694177

22	6	0	-0.567534	-0.594065	0.389072
23	1	0	1.351693	-1.062981	4.840870
24	1	0	-1.077407	-2.593107	1.043567
25	1	0	0.061927	-2.399577	3.221803
26	6	0	1.367884	-0.220076	4.152486
27	6	0	1.397812	1.934535	2.363273
28	6	0	2.012634	2.041544	3.593264
29	6	0	2.000277	0.954118	4.500102
30	1	0	1.422154	2.774635	1.676849
31	1	0	2.514230	2.966991	3.865806
32	1	0	2.490159	1.047775	5.466578
33	6	0	2.450380	1.150730	-1.134430
34	8	0	3.554384	1.643535	-0.974787
35	6	0	-1.148668	-0.828700	-0.994492
36	8	0	-0.313419	-0.874530	-1.928275
37	7	0	2.240245	-0.201323	-1.424205
38	1	0	1.250466	-0.554566	-1.612242
39	7	0	-2.452663	-1.020949	-1.263803
40	16	0	3.454976	-1.306224	-1.728994
41	8	0	2.796811	-2.528323	-2.179131
42	8	0	4.577658	-0.723241	-2.451588
43	16	0	-3.683999	-0.917329	-0.239962
44	8	0	-3.388279	-0.670204	1.187090
45	8	0	-4.794922	-0.172990	-0.848014
46	6	0	4.111078	-1.720148	-0.002064
47	6	0	-4.292618	-2.707032	-0.265965
48	9	0	5.050307	-2.674105	-0.134309
49	9	0	3.123316	-2.193878	0.767212
50	9	0	4.657133	-0.658140	0.593595
51	9	0	-5.360715	-2.835007	0.547604
52	9	0	-3.337394	-3.555343	0.177196
53	9	0	-4.658372	-3.100784	-1.495458

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.781501	0.821306	1.928518
2	1	0	-0.215234	-2.153646	3.274812
3	6	0	-0.120048	-1.348642	2.549489
4	6	0	0.184186	0.695346	0.651848

5	6	0	-0.593752	-0.450468	0.359523
6	6	0	-0.744168	-1.463265	1.317967
7	1	0	-1.305060	-2.359556	1.080381
8	6	0	1.750181	3.034864	-1.921198
9	6	0	0.762450	4.002004	-2.043611
10	6	0	1.543498	1.933793	-1.081872
11	1	0	2.679471	3.117503	-2.477531
12	1	0	0.917206	4.845831	-2.713037
13	6	0	1.589594	2.068464	2.268042
14	6	0	1.281997	-0.146845	4.249272
15	6	0	2.379533	0.915372	4.363474
16	6	0	1.881904	2.233041	3.765099
17	1	0	2.541661	2.031693	1.720061
18	1	0	1.069504	2.955648	1.889661
19	1	0	0.491899	0.071046	4.984949
20	1	0	1.670805	-1.138661	4.513517
21	1	0	2.665043	1.041066	5.414879
22	1	0	3.278917	0.585138	3.824985
23	1	0	0.971672	2.551318	4.294743
24	1	0	2.621772	3.030761	3.901626
25	6	0	-2.673027	4.067093	0.497296
26	6	0	-2.834166	4.684622	-0.893933
27	6	0	-1.456490	5.029328	-1.468751
28	1	0	-3.648683	3.881200	0.962188
29	1	0	-3.347976	3.969957	-1.553046
30	1	0	-3.457769	5.586164	-0.856138
31	1	0	-1.537152	5.296505	-2.530401
32	1	0	-1.072142	5.928221	-0.962027
33	1	0	-2.139818	4.774716	1.149402
34	6	0	0.355874	1.820499	-0.337062
35	6	0	-0.430701	3.916912	-1.313533
36	6	0	-0.630676	2.832898	-0.434967
37	6	0	-1.894713	2.748268	0.410586
38	1	0	-1.645830	2.393773	1.417463
39	1	0	-2.559951	1.979043	-0.004649
40	6	0	0.641260	-0.218580	2.873828
41	6	0	-1.128539	-0.681098	-1.001154
42	8	0	-0.498394	-0.473317	-2.031077
43	6	0	2.669086	0.935107	-1.015009
44	8	0	3.784448	1.211961	-0.620513
45	7	0	-2.406305	-1.287910	-1.185688
46	1	0	-2.577722	-1.446341	-2.180008
47	7	0	2.319244	-0.332660	-1.505921
48	1	0	1.351903	-0.486980	-1.825746

49	16	0	-3.874880	-1.025677	-0.375586
50	8	0	-3.646281	-0.311129	0.868695
51	8	0	-4.851808	-0.614207	-1.375304
52	16	0	3.359184	-1.615318	-1.825687
53	8	0	2.536074	-2.606535	-2.511225
54	8	0	4.641183	-1.158582	-2.331423
55	6	0	3.685953	-2.336179	-0.106487
56	6	0	-4.358576	-2.800337	0.068241
57	9	0	-3.507741	-3.320050	0.958476
58	9	0	-5.584836	-2.778435	0.590406
59	9	0	-4.353373	-3.552492	-1.037272
60	9	0	4.432876	-3.435625	-0.254590
61	9	0	2.523358	-2.669852	0.472471
62	9	0	4.326751	-1.465882	0.673695

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.979183	1.127864	1.762721
2	1	0	0.613894	-1.598370	3.774396
3	6	0	0.501981	-0.956042	2.902224
4	6	0	0.243361	0.667272	0.642832
5	6	0	-0.377803	-0.599606	0.677865
6	6	0	-0.244657	-1.401354	1.819038
7	1	0	-0.716503	-2.378141	1.849049
8	6	0	0.994280	2.565269	-2.588777
9	6	0	-0.143674	3.349996	-2.707697
10	6	0	1.109163	1.662031	-1.524208
11	1	0	1.792730	2.627823	-3.322704
12	1	0	-0.247351	4.024558	-3.556380
13	6	0	1.631749	2.505769	1.725989
14	6	0	1.907574	0.735382	4.119743
15	6	0	2.850634	1.912978	3.852434
16	6	0	2.096325	3.011389	3.098566
17	1	0	2.496612	2.474377	1.047599
18	1	0	0.939926	3.230077	1.280485
19	1	0	1.198329	1.021525	4.913046
20	1	0	2.466826	-0.124194	4.512817
21	1	0	3.256572	2.291145	4.800406
22	1	0	3.705886	1.578012	3.247797

23	1	0	1.227446	3.325820	3.696845
24	1	0	2.726202	3.900625	2.964281
25	6	0	-3.083393	3.564244	0.390423
26	6	0	-3.566932	3.787205	-1.044462
27	6	0	-2.380002	4.190637	-1.924951
28	1	0	-3.925213	3.351568	1.060811
29	1	0	-4.016427	2.858960	-1.424026
30	1	0	-4.343992	4.562246	-1.087114
31	1	0	-2.669211	4.196536	-2.984795
32	1	0	-2.093809	5.227584	-1.684651
33	1	0	-2.608140	4.488439	0.756100
34	6	0	0.098559	1.577784	-0.550590
35	6	0	-1.164158	3.292836	-1.749024
36	6	0	-1.032461	2.428058	-0.644674
37	6	0	-2.090706	2.396218	0.448212
38	1	0	-1.600486	2.375236	1.429321
39	1	0	-2.648317	1.453521	0.396299
40	6	0	1.119965	0.299332	2.893531
41	6	0	-1.062358	-1.179409	-0.543160
42	8	0	-0.399893	-1.206497	-1.609368
43	6	0	2.379390	0.853762	-1.493122
44	8	0	3.481568	1.377085	-1.476628
45	7	0	-2.299385	-1.705795	-0.526781
46	7	0	2.175595	-0.529063	-1.544424
47	1	0	1.168481	-0.896316	-1.563769
48	16	0	-3.340670	-1.710136	0.691899
49	8	0	-3.188872	-2.839998	1.630289
50	8	0	-3.690183	-0.392538	1.265406
51	16	0	3.374767	-1.665674	-1.756500
52	8	0	2.704540	-2.948008	-1.945901
53	8	0	4.429239	-1.206690	-2.651798
54	6	0	4.179475	-1.794300	-0.047377
55	6	0	-4.856323	-2.172087	-0.325335
56	9	0	-4.720149	-3.361269	-0.932382
57	9	0	-5.923285	-2.249224	0.500317
58	9	0	-5.131040	-1.245413	-1.261235
59	9	0	5.115198	-2.759259	-0.100240
60	9	0	3.268448	-2.129704	0.873894
61	9	0	4.765417	-0.649827	0.318428

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.233970	3.757502	-0.651257
2	6	0	0.945599	4.242357	0.161392
3	6	0	1.304864	3.010029	1.015301
4	6	0	-0.026831	2.198927	1.174165
5	6	0	-0.786968	2.595432	-0.093074
6	6	0	-0.820259	2.656949	2.447720
7	6	0	-0.375139	1.718034	3.586166
8	6	0	0.096830	0.481539	2.858101
9	6	0	0.274998	0.727388	1.486801
10	6	0	-1.918370	2.015722	-0.692529
11	6	0	-2.448670	2.593419	-1.858310
12	6	0	-1.891402	3.752757	-2.401117
13	6	0	-0.779732	4.341822	-1.795250
14	6	0	0.385028	-0.760913	3.421795
15	6	0	0.883089	-1.784030	2.613763
16	6	0	1.114715	-1.545387	1.260705
17	6	0	0.819876	-0.296673	0.684731
18	1	0	1.783229	4.582549	-0.458385
19	1	0	0.648501	5.095048	0.788825
20	1	0	1.738664	3.263938	1.988284
21	1	0	2.046149	2.401464	0.488354
22	1	0	-1.889103	2.526389	2.267464
23	1	0	-0.638850	3.714569	2.667310
24	1	0	0.452440	2.146425	4.169734
25	1	0	-1.186449	1.506320	4.291940
26	1	0	-3.317702	2.142681	-2.329718
27	1	0	-2.325173	4.191310	-3.295613
28	1	0	-0.339323	5.243679	-2.214754
29	1	0	0.221551	-0.930479	4.483595
30	1	0	1.097716	-2.763054	3.032974
31	1	0	1.499304	-2.344344	0.634855
32	6	0	1.015904	-0.192778	-0.789748
33	8	0	0.131722	0.021171	-1.600102
34	6	0	-2.609171	0.817580	-0.117047
35	8	0	-2.972561	0.708041	1.036069
36	7	0	-2.845993	-0.186951	-1.084208
37	1	0	-2.214716	-0.236574	-1.881612
38	7	0	2.301479	-0.489929	-1.337458
39	1	0	2.283929	-0.456926	-2.357787
40	16	0	3.852983	-0.121360	-0.762401
41	8	0	4.569960	0.490836	-1.874034

42	8	0	3.779811	0.458095	0.568053
43	16	0	-3.906632	-1.484796	-0.971622
44	8	0	-5.129190	-1.080484	-0.301505
45	8	0	-3.874762	-2.108914	-2.290430
46	6	0	-3.035423	-2.716704	0.173795
47	6	0	4.622388	-1.841098	-0.586278
48	9	0	-2.994233	-2.276345	1.427230
49	9	0	-3.713079	-3.869003	0.127153
50	9	0	-1.784781	-2.925126	-0.266179
51	9	0	4.464173	-2.517264	-1.730191
52	9	0	4.054566	-2.522514	0.411109
53	9	0	5.922890	-1.688365	-0.333874

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.832643	3.379244	0.071612
2	6	0	1.882767	3.348673	1.158415
3	6	0	1.646813	1.988491	1.849001
4	6	0	0.161862	1.583352	1.542507
5	6	0	-0.142702	2.391856	0.282284
6	6	0	-0.803745	2.000028	2.702546
7	6	0	-0.837487	0.800502	3.669985
8	6	0	-0.508345	-0.373648	2.774368
9	6	0	0.026804	0.051680	1.546216
10	6	0	-1.249630	2.330553	-0.574920
11	6	0	-1.328080	3.211136	-1.663748
12	6	0	-0.336618	4.169885	-1.879918
13	6	0	0.746016	4.264483	-1.002273
14	6	0	-0.629105	-1.727224	3.087466
15	6	0	-0.190801	-2.677833	2.164842
16	6	0	0.368377	-2.270028	0.952315
17	6	0	0.489603	-0.909817	0.624605
18	1	0	2.902631	3.439371	0.765224
19	1	0	1.731215	4.192001	1.849683
20	1	0	1.830963	2.019424	2.929219
21	1	0	2.327227	1.240387	1.436699
22	1	0	-1.806022	2.170498	2.297802
23	1	0	-0.474724	2.932480	3.176168
24	1	0	-0.076763	0.897236	4.459310

25	1	0	-1.807050	0.695260	4.172809
26	1	0	-2.173433	3.141658	-2.344075
27	1	0	-0.411475	4.838567	-2.734103
28	1	0	1.518537	5.014861	-1.159583
29	1	0	-1.052054	-2.035795	4.041961
30	1	0	-0.275799	-3.738984	2.386368
31	1	0	0.725365	-3.015437	0.247763
32	6	0	1.051873	-0.585999	-0.748855
33	8	0	0.254565	-0.187381	-1.631305
34	6	0	-2.430612	1.407484	-0.386646
35	8	0	-3.395780	1.697787	0.296260
36	7	0	-2.332182	0.235206	-1.146619
37	1	0	-1.351196	-0.063681	-1.440084
38	7	0	2.346006	-0.766477	-1.063468
39	16	0	3.479754	-1.336266	-0.073688
40	8	0	3.706057	-0.581924	1.177526
41	8	0	3.543397	-2.808344	-0.003647
42	16	0	-3.609200	-0.727825	-1.604466
43	8	0	-4.800284	0.070665	-1.869500
44	8	0	-3.084037	-1.685524	-2.572892
45	6	0	-4.028948	-1.772294	-0.082614
46	6	0	4.953368	-0.867035	-1.148592
47	9	0	-4.441424	-1.022085	0.940986
48	9	0	-5.018395	-2.618246	-0.425067
49	9	0	-2.964276	-2.486053	0.295997
50	9	0	5.032596	0.463201	-1.336619
51	9	0	4.922466	-1.463994	-2.350336
52	9	0	6.083620	-1.260228	-0.521317

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.128621	-1.970673	2.198033
2	6	0	-0.914307	-1.320259	2.162860
3	6	0	-3.211137	-1.544260	1.399089
4	6	0	-0.682657	-0.309948	1.206542
5	6	0	-1.732468	0.080273	0.370299
6	6	0	-3.066504	-0.404496	0.546314
7	6	0	3.076949	0.393409	0.543177
8	6	0	3.224682	1.535627	1.391616

9	6	0	2.141342	1.970576	2.184829
10	6	0	0.924811	1.324205	2.151173
11	6	0	0.690116	0.307861	1.201491
12	6	0	1.741590	-0.087822	0.367327
13	1	0	-2.271066	-2.821357	2.859930
14	1	0	2.284841	2.824909	2.841766
15	6	0	-5.532206	-1.827157	0.722767
16	6	0	-5.492953	-0.572767	0.027102
17	1	0	-7.577412	-0.639595	-0.527008
18	1	0	-6.462404	-2.390220	0.727901
19	6	0	-6.673179	-0.035344	-0.537874
20	6	0	-4.359200	1.522384	-0.467256
21	6	0	-5.535068	2.041966	-0.981216
22	6	0	-6.694910	1.248104	-1.052141
23	1	0	-3.503017	2.179559	-0.384561
24	1	0	-5.559055	3.073240	-1.322145
25	1	0	-7.610816	1.655072	-1.472392
26	6	0	5.503533	0.550766	0.024458
27	6	0	5.546973	1.807465	0.715586
28	6	0	4.361576	-1.542524	-0.460042
29	6	0	6.681622	0.006085	-0.537670
30	6	0	6.698018	-1.279839	-1.046217
31	6	0	5.535215	-2.068983	-0.972056
32	6	0	4.474833	2.241495	1.430491
33	6	0	4.288454	-0.203132	-0.008651
34	1	0	4.533981	3.144690	2.032650
35	1	0	6.479098	2.367303	0.718887
36	1	0	7.588438	0.606443	-0.529139
37	1	0	7.612407	-1.692340	-1.464348
38	1	0	5.555368	-3.101832	-1.308394
39	1	0	3.501918	-2.194637	-0.374518
40	6	0	-4.458734	-2.254675	1.439487
41	6	0	-4.280827	0.185716	-0.008270
42	1	0	-4.515070	-3.155713	2.045204
43	1	0	-0.100130	-1.627530	2.811762
44	1	0	0.110830	1.637839	2.797090
45	16	0	-1.204386	1.057562	-1.063152
46	8	0	-2.171495	1.030491	-2.162172
47	8	0	-0.663346	2.327601	-0.581681
48	16	0	1.195571	-1.020517	-1.083387
49	8	0	2.185196	-1.112078	-2.155781
50	8	0	0.509964	-2.239489	-0.642784
51	7	0	0.088630	0.129421	-1.737876
52	1	0	-0.191488	-0.181025	-2.671080

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.127998	-1.931780	2.242453
2	6	0	-0.913565	-1.286118	2.169429
3	6	0	-3.212480	-1.517516	1.439967
4	6	0	-0.684288	-0.314050	1.171143
5	6	0	-1.721268	0.044149	0.306057
6	6	0	-3.055161	-0.418828	0.536356
7	6	0	3.055212	0.418971	0.536178
8	6	0	3.212667	1.517732	1.439678
9	6	0	2.128239	1.932215	2.242127
10	6	0	0.913746	1.286651	2.169216
11	6	0	0.684358	0.314481	1.171056
12	6	0	1.721265	-0.043888	0.305952
13	1	0	-2.270601	-2.760392	2.933121
14	1	0	2.270942	2.760891	2.932697
15	6	0	-5.559083	-1.772838	0.831176
16	6	0	-5.508958	-0.542032	0.094589
17	1	0	-7.614476	-0.567877	-0.381840
18	1	0	-6.502401	-2.313418	0.880629
19	6	0	-6.694745	0.011110	-0.445814
20	6	0	-4.332645	1.496890	-0.516568
21	6	0	-5.512713	2.033750	-1.004610
22	6	0	-6.699575	1.276866	-1.002971
23	1	0	-3.446532	2.115533	-0.508797
24	1	0	-5.514193	3.049618	-1.391685
25	1	0	-7.618710	1.696357	-1.406417
26	6	0	5.509037	0.541760	0.094478
27	6	0	5.559321	1.772649	0.830916
28	6	0	4.332427	-1.497055	-0.516489
29	6	0	6.694756	-0.011631	-0.445819
30	6	0	6.699409	-1.277456	-1.002825
31	6	0	5.512430	-2.034158	-1.004421
32	6	0	4.473551	2.200520	1.529172
33	6	0	4.276112	-0.175801	-0.009358
34	1	0	4.531520	3.083376	2.162981
35	1	0	6.502721	2.313087	0.880348
36	1	0	7.614576	0.567219	-0.381877

37	1	0	7.618495	-1.697142	-1.406178
38	1	0	5.513770	-3.050074	-1.391370
39	1	0	3.446203	-2.115541	-0.508682
40	6	0	-4.473273	-2.200467	1.529514
41	6	0	-4.276138	0.175707	-0.009277
42	1	0	-4.531132	-3.083261	2.163420
43	1	0	-0.093197	-1.572056	2.821578
44	1	0	0.093424	1.572729	2.821362
45	16	0	-1.146612	0.925979	-1.207853
46	8	0	-2.233131	0.971284	-2.200809
47	8	0	-0.643272	2.230755	-0.715332
48	16	0	1.146503	-0.925904	-1.207815
49	8	0	2.232914	-0.971293	-2.200888
50	8	0	0.643251	-2.230642	-0.715105
51	7	0	-0.000086	-0.000013	-1.857049

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.885060	-2.843831	2.889786
2	6	0	-3.510472	-3.497336	1.736920
3	6	0	-2.937017	-2.788627	0.645836
4	6	0	-2.778108	-1.364738	0.734623
5	6	0	-3.155245	-0.726836	1.949491
6	6	0	-3.690741	-1.445843	2.997456
7	1	0	-2.629406	-4.548617	-0.583551
8	1	0	-4.314290	-3.397898	3.720262
9	1	0	-3.632137	-4.574558	1.648576
10	6	0	-2.495625	-3.471759	-0.519181
11	6	0	-2.209509	-0.644782	-0.377260
12	1	0	-3.005529	0.341658	2.057098
13	1	0	-3.960290	-0.933637	3.917443
14	6	0	-1.711896	-1.394592	-1.430072
15	6	0	-1.868367	-2.791552	-1.532982
16	1	0	-1.483545	-3.296294	-2.413223
17	6	0	-0.719752	2.863426	-0.598822
18	6	0	-1.804685	3.673786	-0.369483
19	6	0	-3.103376	3.117708	-0.215629
20	6	0	-3.274449	1.692472	-0.255470
21	6	0	-2.117588	0.842682	-0.402428

22	6	0	-0.902206	1.466105	-0.626030
23	1	0	-4.093387	5.031298	-0.018410
24	1	0	0.273716	3.266382	-0.766825
25	1	0	-1.684192	4.753617	-0.337016
26	6	0	-4.242345	3.954590	-0.057602
27	6	0	-4.600437	1.178837	-0.193923
28	6	0	-5.685940	2.018951	-0.060700
29	6	0	-5.509079	3.420821	0.023435
30	1	0	-4.759213	0.109001	-0.265291
31	1	0	-6.687945	1.599462	-0.025517
32	1	0	-6.372401	4.071113	0.136113
33	8	0	-1.054641	-0.769453	-2.499903
34	8	0	0.247432	0.691012	-0.877107
35	15	0	0.369519	-0.027670	-2.324220
36	8	0	0.728266	0.757305	-3.519416
37	7	0	1.585474	-1.168643	-1.982460
38	1	0	2.283087	-1.258132	-2.719572
39	16	0	2.088496	-1.886688	-0.538401
40	8	0	0.914236	-2.202521	0.253388
41	8	0	3.067375	-2.892521	-0.935257
42	6	0	3.005620	-0.567022	0.308493
43	6	0	4.101493	0.020241	-0.336218
44	6	0	2.697812	-0.136179	1.604899
45	6	0	4.865627	1.008748	0.272016
46	6	0	3.461157	0.853517	2.226740
47	6	0	4.542231	1.425074	1.562825
48	9	0	4.432288	-0.347442	-1.582943
49	9	0	5.902929	1.558256	-0.368862
50	9	0	5.269202	2.371010	2.159564
51	9	0	3.155174	1.255074	3.465892
52	9	0	1.679839	-0.640743	2.300895

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.691229	3.116259	2.778471
2	6	0	3.240012	3.697424	1.612661
3	6	0	2.693239	2.912822	0.561448
4	6	0	2.639362	1.485169	0.698606
5	6	0	3.090222	0.923009	1.926841

6	6	0	3.600026	1.712864	2.937120
7	1	0	2.204997	4.600155	-0.711463
8	1	0	4.096912	3.730583	3.579014
9	1	0	3.276139	4.777854	1.485050
10	6	0	2.166895	3.517496	-0.612508
11	6	0	2.102181	0.685259	-0.373730
12	1	0	3.014899	-0.148576	2.075427
13	1	0	3.924343	1.251633	3.867257
14	6	0	1.510144	1.347551	-1.443953
15	6	0	1.563650	2.755742	-1.578477
16	1	0	1.097475	3.200313	-2.451167
17	6	0	0.892849	-2.927889	-0.424830
18	6	0	2.036949	-3.645310	-0.179802
19	6	0	3.292660	-2.987045	-0.074545
20	6	0	3.348096	-1.555662	-0.179000
21	6	0	2.128014	-0.804156	-0.338328
22	6	0	0.950427	-1.517738	-0.517884
23	1	0	4.431873	-4.806825	0.184150
24	1	0	-0.069342	-3.409968	-0.564849
25	1	0	2.000806	-4.729872	-0.101762
26	6	0	4.496825	-3.723727	0.096610
27	6	0	4.633377	-0.941778	-0.167888
28	6	0	5.785437	-1.686193	-0.019728
29	6	0	5.721502	-3.092692	0.129208
30	1	0	4.703692	0.133165	-0.290040
31	1	0	6.751576	-1.186748	-0.023438
32	1	0	6.634923	-3.669977	0.252465
33	8	0	0.917806	0.657231	-2.475355
34	8	0	-0.231347	-0.851480	-0.776176
35	15	0	-0.453777	-0.279574	-2.333003
36	8	0	-0.382132	-1.334150	-3.373257
37	7	0	-1.808502	0.588044	-2.290887
38	16	0	-2.355606	1.603778	-1.200616
39	8	0	-1.330841	2.418060	-0.524240
40	8	0	-3.533134	2.308674	-1.727748
41	6	0	-3.062939	0.494485	0.111637
42	6	0	-4.175387	-0.299164	-0.193079
43	6	0	-2.543017	0.390027	1.405129
44	6	0	-4.755019	-1.149512	0.744689
45	6	0	-3.115704	-0.457110	2.356318
46	6	0	-4.222678	-1.228139	2.027330
47	9	0	-4.729336	-0.281593	-1.411514
48	9	0	-5.828447	-1.898520	0.422887
49	9	0	-4.777888	-2.044314	2.942027

50	9	0	-2.598557	-0.534318	3.598690
51	9	0	-1.475259	1.087243	1.810217

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.301145	1.579346	0.699703
2	6	0	1.635303	2.765191	1.359427
3	6	0	0.141777	2.395323	1.288022
4	6	0	0.004517	1.504696	0.006532
5	6	0	1.366922	0.796767	-0.003542
6	6	0	-0.127468	2.408416	-1.266805
7	6	0	-1.619336	2.784294	-1.338503
8	6	0	-2.290622	1.593582	-0.693496
9	6	0	-1.360868	0.802847	0.007406
10	6	0	1.834635	-0.377142	-0.610308
11	6	0	3.184811	-0.746338	-0.547340
12	6	0	4.095756	0.072139	0.118329
13	6	0	3.649487	1.232855	0.755270
14	6	0	-3.638934	1.249662	-0.758881
15	6	0	-4.091851	0.082770	-0.137326
16	6	0	-3.186695	-0.743672	0.524885
17	6	0	-1.837628	-0.374028	0.600649
18	1	0	1.980579	2.915610	2.388547
19	1	0	1.852319	3.692953	0.811040
20	1	0	-0.520414	3.266032	1.249287
21	1	0	-0.130985	1.798558	2.163724
22	1	0	0.145397	1.819068	-2.147431
23	1	0	0.537818	3.276172	-1.217650
24	1	0	-1.834836	3.706600	-0.780372
25	1	0	-1.961230	2.947006	-2.366852
26	1	0	3.503898	-1.670504	-1.016892
27	1	0	5.144070	-0.209648	0.158477
28	1	0	4.348990	1.856977	1.306785
29	1	0	-4.334264	1.880681	-1.307858
30	1	0	-5.139791	-0.197986	-0.189903
31	1	0	-3.506566	-1.675789	0.977872
32	16	0	-0.746270	-1.562181	1.360655
33	16	0	0.725959	-1.560941	-1.366742
34	8	0	-1.505084	-2.637849	2.002368

35	8	0	0.299909	-0.867447	2.117205
36	8	0	1.500828	-2.660929	-1.946850
37	8	0	-0.278585	-0.844786	-2.148679
38	7	0	-0.094353	-2.331498	-0.051831
39	1	0	0.398197	-3.187466	0.214948

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.299832	1.598595	0.672998
2	6	0	1.622021	2.782410	1.327155
3	6	0	0.135252	2.380849	1.276969
4	6	0	0.000006	1.485546	0.000002
5	6	0	1.368521	0.788193	-0.003059
6	6	0	-0.135234	2.380850	-1.276965
7	6	0	-1.622000	2.782421	-1.327152
8	6	0	-2.299819	1.598609	-0.672997
9	6	0	-1.368513	0.788200	0.003061
10	6	0	1.824146	-0.400741	-0.584759
11	6	0	3.179405	-0.744175	-0.526193
12	6	0	4.096736	0.097132	0.104638
13	6	0	3.652565	1.270098	0.722327
14	6	0	-3.652554	1.270119	-0.722328
15	6	0	-4.096733	0.097155	-0.104642
16	6	0	-3.179408	-0.744157	0.526189
17	6	0	-1.824147	-0.400732	0.584758
18	1	0	1.977254	2.950479	2.351791
19	1	0	1.810485	3.711536	0.767175
20	1	0	-0.547642	3.237830	1.253105
21	1	0	-0.108629	1.766945	2.149580
22	1	0	0.108644	1.766946	-2.149576
23	1	0	0.547664	3.237828	-1.253100
24	1	0	-1.810460	3.711547	-0.767169
25	1	0	-1.977232	2.950494	-2.351787
26	1	0	3.490362	-1.683935	-0.970823
27	1	0	5.148479	-0.178673	0.141295
28	1	0	4.352483	1.911673	1.255778
29	1	0	-4.352467	1.911699	-1.255779
30	1	0	-5.148478	-0.178643	-0.141300
31	1	0	-3.490371	-1.683916	0.970819

32	16	0	-0.688659	-1.637724	1.265081
33	16	0	0.688646	-1.637723	-1.265081
34	8	0	-1.517053	-2.647538	1.954955
35	8	0	0.270681	-0.880595	2.107357
36	8	0	1.517029	-2.647541	-1.954964
37	8	0	-0.270693	-0.880585	-2.107349
38	7	0	-0.000007	-2.393831	-0.000001

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.323797	1.122349	-0.446036
2	6	0	-1.868261	2.392525	-1.130821
3	6	0	-0.330242	2.243303	-1.167329
4	6	0	0.035631	1.301799	0.033586
5	6	0	-1.256249	0.512809	0.230951
6	6	0	0.447765	2.126247	1.300662
7	6	0	1.982253	2.285462	1.205617
8	6	0	2.402105	1.055436	0.430556
9	6	0	1.302399	0.490982	-0.233418
10	6	0	-1.473336	-0.667046	0.960275
11	6	0	-2.757479	-1.237365	0.962340
12	6	0	-3.812946	-0.625068	0.282906
13	6	0	-3.602359	0.566402	-0.419230
14	6	0	3.666999	0.476977	0.341355
15	6	0	3.833096	-0.701372	-0.394132
16	6	0	2.742299	-1.288455	-1.035057
17	6	0	1.475230	-0.683970	-0.981845
18	1	0	-2.300352	2.518614	-2.130617
19	1	0	-2.172991	3.269397	-0.541134
20	1	0	0.195145	3.201691	-1.097562
21	1	0	-0.033283	1.770316	-2.107051
22	1	0	0.198201	1.554817	2.198645
23	1	0	-0.083567	3.083190	1.346676
24	1	0	2.262420	3.197391	0.657799
25	1	0	2.456942	2.345609	2.191365
26	1	0	-2.930831	-2.157720	1.514337
27	1	0	-4.800713	-1.078059	0.304791
28	1	0	-4.425552	1.047333	-0.943367
29	1	0	4.513517	0.921435	0.859938

30	1	0	4.808877	-1.175826	-0.451552
31	1	0	2.865359	-2.219827	-1.580681
32	6	0	0.356939	-1.389132	-1.677951
33	8	0	-0.019562	-2.522349	-1.412840
34	8	0	-0.203755	-0.677616	-2.675347
35	1	0	-0.937714	-1.213238	-3.035705
36	6	0	-0.417834	-1.314303	1.827312
37	8	0	-0.022183	-0.808608	2.855928
38	8	0	0.014624	-2.535819	1.453329
39	1	0	-0.181715	-2.715453	0.507123

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.289828	1.141680	0.606372
2	6	0	1.711882	2.395196	1.226198
3	6	0	0.189558	2.163884	1.123119
4	6	0	-0.019306	1.194916	-0.090020
5	6	0	1.312229	0.441732	-0.119575
6	6	0	-0.241318	1.964032	-1.436911
7	6	0	-1.767947	2.154656	-1.568256
8	6	0	-2.327159	1.002430	-0.761093
9	6	0	-1.338530	0.435631	0.059181
10	6	0	1.664660	-0.723064	-0.816327
11	6	0	2.991646	-1.174199	-0.747539
12	6	0	3.952969	-0.483754	-0.006871
13	6	0	3.605808	0.687495	0.672839
14	6	0	-3.638267	0.528450	-0.741138
15	6	0	-3.958319	-0.525841	0.121471
16	6	0	-2.979759	-1.080549	0.950180
17	6	0	-1.657327	-0.608844	0.940282
18	1	0	2.041399	2.545485	2.262115
19	1	0	2.028467	3.283834	0.657365
20	1	0	-0.383511	3.091562	1.002536
21	1	0	-0.162650	1.662995	2.030588
22	1	0	0.118502	1.340811	-2.262480
23	1	0	0.318665	2.907173	-1.462199
24	1	0	-2.091876	3.115831	-1.139170
25	1	0	-2.100586	2.145677	-2.614350
26	1	0	3.266729	-2.083361	-1.276934

27	1	0	4.971388	-0.863844	0.042202
28	1	0	4.349968	1.231968	1.252103
29	1	0	-4.397355	0.965926	-1.388121
30	1	0	-4.972767	-0.920271	0.146188
31	1	0	-3.237681	-1.900108	1.617339
32	6	0	-0.642839	-1.255365	1.886251
33	8	0	0.003639	-2.253488	1.409318
34	8	0	-0.554102	-0.783136	3.033053
35	6	0	0.713495	-1.521798	-1.690509
36	8	0	0.691987	-1.332063	-2.902353
37	8	0	-0.007171	-2.450625	-1.099510
38	1	0	0.008657	-2.389303	-0.037164

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.679562	-0.572684	-0.213237
2	1	0	3.911362	1.024537	-2.244256
3	6	0	2.993234	0.844665	-1.688793
4	6	0	0.639006	0.386436	-0.234549
5	6	0	0.802584	1.570296	-0.985942
6	6	0	1.971000	1.780382	-1.734280
7	1	0	2.080880	2.689645	-2.316122
8	6	0	-1.945089	-0.135034	2.520169
9	6	0	-2.988868	-0.701953	1.801056
10	6	0	-0.782944	0.272318	1.855754
11	1	0	-2.023874	0.008149	3.594098
12	1	0	-3.899211	-0.998922	2.318507
13	6	0	1.512660	-1.852714	0.596892
14	6	0	4.033508	-1.305992	-0.912083
15	6	0	3.958659	-2.330038	0.224389
16	6	0	2.553525	-2.933729	0.278624
17	1	0	1.571954	-1.599270	1.664869
18	1	0	0.503012	-2.252112	0.448585
19	1	0	4.048460	-1.839012	-1.875896
20	1	0	4.975244	-0.743934	-0.866290
21	1	0	4.717638	-3.107585	0.073579
22	1	0	4.185509	-1.842780	1.183136
23	1	0	2.324630	-3.403888	-0.689652
24	1	0	2.494484	-3.725194	1.035431

25	6	0	-2.613763	-1.721378	-2.340051
26	6	0	-4.014126	-1.372270	-1.830192
27	6	0	-4.065589	-1.543882	-0.308891
28	1	0	-2.571598	-1.683097	-3.435711
29	1	0	-4.252986	-0.332594	-2.098326
30	1	0	-4.774893	-2.005503	-2.303341
31	1	0	-5.003962	-1.139944	0.092683
32	1	0	-4.075993	-2.619411	-0.072000
33	1	0	-2.371751	-2.754713	-2.050308
34	6	0	-0.654578	0.070182	0.471169
35	6	0	-2.894102	-0.899602	0.416583
36	6	0	-1.711878	-0.530507	-0.255570
37	6	0	-1.570070	-0.760132	-1.756053
38	1	0	-0.561408	-1.125077	-1.982388
39	1	0	-1.651908	0.207352	-2.274907
40	6	0	2.872684	-0.324794	-0.925436
41	6	0	-0.194014	2.665232	-0.923619
42	8	0	-0.820592	3.001665	0.074734
43	8	0	-0.338859	3.335243	-2.088847
44	1	0	-0.951241	4.076125	-1.916979
45	6	0	0.290519	0.933505	2.681996
46	8	0	0.846694	0.379664	3.607840
47	8	0	0.574130	2.210546	2.364638
48	1	0	0.003154	2.520440	1.620758

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.710768	-0.598907	-0.056386
2	1	0	-3.892103	-0.108028	2.515050
3	6	0	-2.977549	-0.024751	1.927297
4	6	0	-0.645489	0.207836	0.416199
5	6	0	-0.756874	0.895799	1.636118
6	6	0	-1.924792	0.752204	2.395664
7	1	0	-1.995540	1.267845	3.349877
8	6	0	1.948784	1.164063	-2.210457
9	6	0	2.983624	0.293684	-1.892853
10	6	0	0.781781	1.179679	-1.437040
11	1	0	2.038931	1.853926	-3.045146
12	1	0	3.901646	0.308944	-2.479888

13	6	0	-1.581172	-1.311976	-1.397714
14	6	0	-4.075604	-1.538438	0.237799
15	6	0	-4.041563	-1.855729	-1.261133
16	6	0	-2.654768	-2.381130	-1.642833
17	1	0	-1.630921	-0.561897	-2.200624
18	1	0	-0.584707	-1.761582	-1.485167
19	1	0	-4.090016	-2.488253	0.798262
20	1	0	-5.010288	-1.022614	0.498104
21	1	0	-4.823527	-2.587102	-1.509654
22	1	0	-4.256604	-0.945210	-1.839334
23	1	0	-2.435454	-3.278279	-1.042633
24	1	0	-2.628453	-2.691988	-2.696121
25	6	0	2.606306	-2.663212	1.194875
26	6	0	3.998436	-2.086097	0.922778
27	6	0	4.046841	-1.513741	-0.498041
28	1	0	2.568514	-3.149386	2.178885
29	1	0	4.210930	-1.290818	1.651462
30	1	0	4.775877	-2.853185	1.045700
31	1	0	4.987055	-0.968879	-0.659921
32	1	0	4.055434	-2.350255	-1.216535
33	1	0	2.392023	-3.443813	0.447667
34	6	0	0.635863	0.274912	-0.372719
35	6	0	2.875980	-0.594656	-0.813760
36	6	0	1.688160	-0.620791	-0.058949
37	6	0	1.537672	-1.563569	1.128381
38	1	0	0.539520	-2.017188	1.116105
39	1	0	1.571979	-0.964850	2.049919
40	6	0	-2.892995	-0.699854	0.700829
41	6	0	0.337736	1.837098	2.139712
42	8	0	0.633679	2.801736	1.350192
43	8	0	0.822617	1.610140	3.263406
44	6	0	-0.267494	2.213199	-1.787512
45	8	0	-0.727143	2.273880	-2.924600
46	8	0	-0.613396	3.056613	-0.835874
47	1	0	-0.093046	2.919918	0.077466

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.751099	-1.940988	-1.289799

2	6	0	-4.029023	-1.106543	-0.227707
3	6	0	-3.029781	-0.257434	0.318634
4	6	0	-1.710734	-0.268815	-0.245848
5	6	0	-1.457271	-1.142638	-1.339996
6	6	0	-2.449945	-1.955513	-1.847967
7	1	0	-4.300688	0.618164	1.842334
8	1	0	-4.524710	-2.585748	-1.698590
9	1	0	-5.025060	-1.085956	0.210188
10	6	0	-3.300738	0.608717	1.414243
11	6	0	-0.698951	0.583395	0.304544
12	1	0	-0.463161	-1.164300	-1.776610
13	1	0	-2.230917	-2.613968	-2.685058
14	6	0	-1.022353	1.409602	1.371454
15	6	0	-2.324610	1.423161	1.932126
16	1	0	-2.519474	2.088613	2.767805
17	6	0	2.328759	1.541512	-1.818000
18	6	0	3.301998	0.686912	-1.358316
19	6	0	3.024091	-0.249506	-0.327358
20	6	0	1.702965	-0.289400	0.232890
21	6	0	0.690675	0.607024	-0.252032
22	6	0	1.022419	1.500508	-1.264017
23	1	0	5.015117	-1.097479	-0.275963
24	1	0	2.551466	2.254474	-2.610242
25	1	0	4.301418	0.721934	-1.785875
26	6	0	4.018479	-1.141645	0.158366
27	6	0	1.440855	-1.237421	1.262487
28	6	0	2.427745	-2.090105	1.711174
29	6	0	3.731144	-2.045383	1.157985
30	1	0	0.444731	-1.282949	1.691232
31	1	0	2.202517	-2.805760	2.497807
32	1	0	4.498465	-2.723449	1.521843
33	8	0	-0.117028	2.252948	1.954696
34	1	0	0.734895	2.169780	1.490967
35	8	0	0.045421	2.344546	-1.720537
36	1	0	0.400505	2.914048	-2.420282

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.281499	-2.462502	1.086109

2	6	0	3.770380	-1.462326	0.271699
3	6	0	2.955767	-0.368056	-0.127623
4	6	0	1.580131	-0.309398	0.290975
5	6	0	1.121752	-1.349513	1.153475
6	6	0	1.941820	-2.389615	1.541040
7	1	0	4.513266	0.645880	-1.250594
8	1	0	3.919675	-3.290333	1.389030
9	1	0	4.804674	-1.486977	-0.070558
10	6	0	3.478488	0.694135	-0.913755
11	6	0	0.728765	0.779752	-0.124216
12	1	0	0.102177	-1.305758	1.519687
13	1	0	1.554836	-3.158230	2.207412
14	6	0	1.342185	1.861129	-0.779333
15	6	0	2.699540	1.787420	-1.200838
16	1	0	3.092947	2.636440	-1.754563
17	6	0	-2.723712	1.768521	1.221177
18	6	0	-3.488548	0.680465	0.903752
19	6	0	-2.955397	-0.382612	0.117080
20	6	0	-1.568163	-0.321241	-0.271407
21	6	0	-0.739266	0.771136	0.158063
22	6	0	-1.341746	1.891186	0.809832
23	1	0	-4.806753	-1.484749	0.022646
24	1	0	-3.132456	2.604469	1.785067
25	1	0	-4.529922	0.623073	1.222890
26	6	0	-3.765480	-1.467624	-0.299998
27	6	0	-1.103371	-1.368252	-1.127545
28	6	0	-1.921567	-2.405906	-1.530469
29	6	0	-3.270129	-2.475558	-1.106645
30	1	0	-0.079158	-1.336247	-1.483183
31	1	0	-1.521637	-3.175514	-2.188973
32	1	0	-3.907193	-3.299107	-1.422881
33	8	0	0.685550	3.005147	-1.061647
34	1	0	0.065166	3.169288	-0.249909
35	8	0	-0.712213	2.998717	1.042358

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.750972	0.008855	-0.198403
2	1	0	-4.039394	-1.689608	1.663493

3	6	0	-3.091679	-1.227120	1.392365
4	6	0	-0.665453	-0.034341	0.706496
5	6	0	-0.823576	-0.669601	1.948046
6	6	0	-2.034889	-1.273172	2.293255
7	1	0	-2.131528	-1.754607	3.261937
8	6	0	2.079774	2.574939	0.361238
9	6	0	3.129263	1.805055	-0.129792
10	6	0	0.847525	1.967443	0.620054
11	1	0	2.216709	3.638908	0.548509
12	1	0	4.089132	2.280504	-0.323572
13	6	0	-1.584062	0.739346	-1.522906
14	6	0	-4.168298	-0.584164	-0.798125
15	6	0	-4.067143	0.488375	-1.888513
16	6	0	-2.685184	0.430216	-2.546220
17	1	0	-1.574263	1.821282	-1.320631
18	1	0	-0.600324	0.512305	-1.951893
19	1	0	-4.254174	-1.570932	-1.281039
20	1	0	-5.091807	-0.452652	-0.218758
21	1	0	-4.861676	0.343778	-2.631908
22	1	0	-4.219332	1.484361	-1.447020
23	1	0	-2.530632	-0.573934	-2.968856
24	1	0	-2.617040	1.137761	-3.382597
25	6	0	2.621434	-2.301627	-1.239731
26	6	0	4.014148	-1.864083	-0.777488
27	6	0	4.160804	-0.347370	-0.941771
28	1	0	2.520917	-3.393637	-1.206189
29	1	0	4.152736	-2.141739	0.277833
30	1	0	4.797688	-2.378834	-1.347679
31	1	0	5.088793	0.001510	-0.469749
32	1	0	4.263246	-0.117011	-2.014127
33	1	0	2.480108	-2.003561	-2.289259
34	6	0	0.659873	0.593738	0.389003
35	6	0	2.982731	0.434239	-0.378846
36	6	0	1.737323	-0.173929	-0.121119
37	6	0	1.533527	-1.663064	-0.366229
38	1	0	0.545302	-1.828940	-0.809799
39	1	0	1.504670	-2.179806	0.605188
40	6	0	-2.975837	-0.591276	0.146742
41	8	0	0.191813	-0.728626	2.870940
42	1	0	0.945427	-0.209767	2.539428
43	8	0	-0.221722	2.678329	1.108141
44	1	0	0.038864	3.602245	1.245707

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.602181	-0.195284	0.207528
2	1	0	4.377540	0.728840	-1.546186
3	6	0	3.363142	0.772092	-1.147708
4	6	0	0.718410	0.851417	-0.179724
5	6	0	1.249834	1.931377	-0.929626
6	6	0	2.554863	1.862493	-1.442396
7	1	0	2.918235	2.695797	-2.039045
8	6	0	-2.581527	1.840357	1.464625
9	6	0	-3.376556	0.755268	1.138844
10	6	0	-1.250484	1.962892	0.961525
11	1	0	-2.962668	2.658273	2.073147
12	1	0	-4.398347	0.705112	1.521946
13	6	0	1.162482	-1.201830	1.269055
14	6	0	3.874046	-1.385055	0.047008
15	6	0	3.517154	-2.109309	1.349223
16	6	0	2.028236	-2.465913	1.343002
17	1	0	1.201607	-0.687961	2.243483
18	1	0	0.113877	-1.477343	1.140843
19	1	0	3.871467	-2.126449	-0.770990
20	1	0	4.902483	-0.999322	0.096373
21	1	0	4.140155	-3.008122	1.466982
22	1	0	3.729556	-1.455403	2.208687
23	1	0	1.819824	-3.112638	0.475991
24	1	0	1.759199	-3.044042	2.238704
25	6	0	-2.001958	-2.479495	-1.333564
26	6	0	-3.490823	-2.124637	-1.370705
27	6	0	-3.874521	-1.400493	-0.075805
28	1	0	-1.713518	-3.060340	-2.222120
29	1	0	-3.684548	-1.470230	-2.234535
30	1	0	-4.109052	-3.025245	-1.503206
31	1	0	-4.901753	-1.013757	-0.151079
32	1	0	-3.898420	-2.148650	0.737849
33	1	0	-1.811138	-3.123205	-0.460052
34	6	0	-0.732018	0.844928	0.213961
35	6	0	-2.924766	-0.266848	0.283053
36	6	0	-1.597038	-0.208095	-0.186734
37	6	0	-1.139585	-1.213359	-1.244802
38	1	0	-0.093186	-1.494141	-1.102392

39	1	0	-1.164701	-0.702576	-2.221723
40	6	0	2.919340	-0.247702	-0.292440
41	8	0	0.527026	3.052319	-1.160215
42	1	0	0.027939	3.226502	-0.272737
43	8	0	-0.557904	3.047439	1.144484

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.272233	0.760402	3.628369
2	6	0	-2.885025	3.438379	0.853269
3	6	0	-2.547669	4.329773	-0.170520
4	6	0	-2.655774	2.069361	0.702402
5	6	0	-0.003664	-0.290410	2.556296
6	6	0	-1.988574	3.834373	-1.349601
7	6	0	0.306472	-1.668666	3.139036
8	6	0	-2.074000	1.562423	-0.471548
9	6	0	4.305996	2.682844	0.611280
10	6	0	-1.756721	2.462005	-1.497476
11	6	0	3.152400	1.892987	0.539872
12	6	0	0.649131	0.358620	0.394883
13	6	0	-0.682787	-0.444028	0.332044
14	6	0	-3.240542	-1.903158	0.309728
15	6	0	-4.441794	-2.620296	0.344809
16	6	0	5.377231	2.451231	-0.251502
17	6	0	-3.120631	-0.744798	-0.467291
18	6	0	-1.809451	0.050218	-0.635604
19	6	0	-5.541366	-2.195516	-0.401370
20	6	0	-4.233091	-0.329379	-1.216408
21	6	0	-5.430334	-1.044097	-1.186923
22	6	0	3.056838	0.854949	-0.396947
23	6	0	1.796017	-0.003967	-0.600715
24	6	0	2.909547	-2.034279	0.445557
25	6	0	5.291403	1.418925	-1.191986
26	6	0	3.208425	-3.397521	0.481768
27	6	0	2.129951	-1.499235	-0.591673
28	6	0	4.144067	0.630127	-1.261248
29	6	0	2.734259	-4.249934	-0.519846
30	6	0	1.661386	-2.359132	-1.594399

31	6	0	1.961586	-3.724671	-1.557176
32	1	0	-3.339328	3.808256	1.769582
33	1	0	-1.151056	0.481513	4.219736
34	1	0	0.589141	0.842820	4.299336
35	1	0	-2.731972	5.394942	-0.054338
36	1	0	-0.456712	1.732326	3.161848
37	1	0	-2.938394	1.385487	1.495103
38	1	0	1.219543	-1.627707	3.742686
39	1	0	-0.520347	-2.002157	3.775204
40	1	0	4.361713	3.478984	1.349448
41	1	0	-1.739942	4.511896	-2.163276
42	1	0	2.345041	2.079002	1.238022
43	1	0	0.457229	-2.397219	2.337503
44	1	0	0.427329	1.426955	0.262917
45	1	0	-2.409572	-2.252523	0.910600
46	1	0	-4.512099	-3.513737	0.960818
47	1	0	6.271969	3.065723	-0.192307
48	1	0	-1.354417	2.082915	-2.431582
49	1	0	-6.474096	-2.753532	-0.372465
50	1	0	3.288636	-1.379580	1.223340
51	1	0	-4.156958	0.561003	-1.833500
52	1	0	-6.276244	-0.701068	-1.777829
53	1	0	-0.475680	-1.490891	0.075242
54	1	0	3.817788	-3.791544	1.291478
55	1	0	1.494230	1.251243	-2.106977
56	1	0	-0.453896	-0.002519	-2.081268
57	1	0	6.119651	1.224998	-1.868859
58	1	0	4.086733	-0.173425	-1.990309
59	1	0	2.969835	-5.310909	-0.493786
60	1	0	1.064117	-1.967255	-2.409641
61	1	0	1.588513	-4.374486	-2.344803
62	8	0	-1.130697	-0.344369	1.686238
63	8	0	1.098988	0.120358	1.728657
64	8	0	-1.393454	-0.260446	-1.968540
65	8	0	1.285529	0.320121	-1.928155

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.341890	-1.202498	3.398165

2	6	0	3.325051	-3.249981	0.858443
3	6	0	2.812663	-4.238976	0.012139
4	6	0	2.997441	-1.907113	0.651348
5	6	0	0.042952	0.061110	2.585304
6	6	0	1.973124	-3.867672	-1.041931
7	6	0	-0.203166	1.282380	3.474410
8	6	0	2.152549	-1.524611	-0.402290
9	6	0	-4.664185	-2.229566	0.615573
10	6	0	1.649208	-2.522562	-1.247695
11	6	0	-3.518654	-1.422279	0.627148
12	6	0	-0.667648	-0.360819	0.393890
13	6	0	0.665283	0.425712	0.350669
14	6	0	3.282578	1.822899	0.379458
15	6	0	4.447824	2.601329	0.334949
16	6	0	-5.334656	-2.492845	-0.580316
17	6	0	3.041767	0.832465	-0.580599
18	6	0	1.768564	-0.043996	-0.658949
19	6	0	5.396411	2.401608	-0.667656
20	6	0	4.003783	0.645962	-1.589285
21	6	0	5.165832	1.414293	-1.634174
22	6	0	-3.011496	-0.869705	-0.559287
23	6	0	-1.750453	0.044089	-0.671144
24	6	0	-2.982578	1.959550	0.631981
25	6	0	-4.835728	-1.949438	-1.770323
26	6	0	-3.368333	3.297870	0.754964
27	6	0	-2.209252	1.525476	-0.457346
28	6	0	-3.685693	-1.158973	-1.757047
29	6	0	-2.990161	4.234519	-0.213043
30	6	0	-1.843556	2.472573	-1.423253
31	6	0	-2.225154	3.813131	-1.304409
32	1	0	3.984764	-3.523117	1.680371
33	1	0	1.268709	-1.077420	3.970339
34	1	0	-0.478898	-1.406692	4.095802
35	1	0	3.067605	-5.285105	0.171673
36	1	0	0.461600	-2.058423	2.728113
37	1	0	3.404296	-1.147205	1.311436
38	1	0	-1.085673	1.122347	4.104903
39	1	0	0.663693	1.462413	4.121003
40	1	0	-5.028435	-2.654432	1.550095
41	1	0	1.565294	-4.625919	-1.707875
42	1	0	-3.012881	-1.234961	1.567847
43	1	0	-0.376282	2.165162	2.852148
44	1	0	-0.479565	-1.432772	0.254899
45	1	0	2.569481	1.987696	1.178802

46	1	0	4.607107	3.366634	1.092706
47	1	0	-6.225896	-3.118170	-0.588135
48	1	0	1.001676	-2.226626	-2.066819
49	1	0	6.301086	3.005837	-0.700862
50	1	0	-3.291410	1.248284	1.390588
51	1	0	3.817167	-0.102155	-2.353808
52	1	0	5.891623	1.247789	-2.428252
53	1	0	0.458210	1.480895	0.127338
54	1	0	-3.970403	3.608259	1.607888
55	1	0	0.206430	0.021045	-1.962770
56	1	0	-5.339254	-2.152755	-2.714483
57	1	0	-3.262576	-0.763253	-2.674836
58	1	0	-3.292057	5.276324	-0.118596
59	1	0	-1.259792	2.121643	-2.268747
60	1	0	-1.924088	4.528845	-2.067965
61	8	0	1.141877	0.304674	1.705975
62	8	0	-1.094488	-0.127359	1.757326
63	8	0	1.273358	0.131502	-1.959195
64	8	0	-1.183093	-0.133538	-1.905476

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.570119	-2.924340	-0.546260
2	6	0	-2.236903	-3.071229	-1.001732
3	6	0	-3.962176	-1.743988	0.043496
4	6	0	-1.312469	-2.068936	-0.799904
5	6	0	-3.045364	-0.669797	0.222750
6	6	0	-1.662520	-0.853823	-0.140005
7	6	0	-3.495598	0.594968	0.684032
8	6	0	1.297124	1.466393	-0.429777
9	6	0	-0.751078	0.235468	0.082363
10	6	0	2.666175	1.597829	-0.751942
11	6	0	-2.637550	1.673568	0.699014
12	6	0	0.747657	0.216488	-0.103907
13	6	0	-1.270489	1.502548	0.388288
14	6	0	3.497247	0.498233	-0.726063
15	6	0	1.633852	-0.891216	0.131386
16	6	0	3.019042	-0.747114	-0.240532
17	6	0	1.256850	-2.087276	0.811182

18	6	0	3.909810	-1.840934	-0.048599
19	6	0	2.157405	-3.108672	1.025313
20	6	0	3.491735	-3.001689	0.561917
21	1	0	-4.285571	-3.729636	-0.691683
22	1	0	-1.941232	-3.978222	-1.522896
23	1	0	-4.994968	-1.599441	0.353100
24	1	0	-0.305510	-2.195966	-1.177876
25	1	0	-4.541401	0.711610	0.959807
26	1	0	3.062487	2.571013	-1.033041
27	1	0	-3.013564	2.661670	0.954880
28	1	0	4.542453	0.583297	-1.015342
29	1	0	0.247615	-2.184748	1.192073
30	1	0	4.943977	-1.727510	-0.366513
31	1	0	1.841463	-4.000657	1.560320
32	1	0	4.187624	-3.822358	0.716030
33	14	0	0.035979	2.775992	-0.008487
34	8	0	-0.418081	3.819497	-1.216967
35	1	0	-0.360657	4.761891	-1.002784
36	8	0	0.529095	3.807567	1.214744
37	1	0	0.829670	3.409768	2.044417

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.429274	-3.047469	0.572774
2	6	0	2.094091	-3.120207	1.041151
3	6	0	3.866183	-1.897960	-0.049381
4	6	0	1.217269	-2.077645	0.820189
5	6	0	2.999515	-0.786388	-0.249204
6	6	0	1.611220	-0.895086	0.125783
7	6	0	3.495784	0.447226	-0.746505
8	6	0	-1.239682	1.562796	0.342415
9	6	0	0.745582	0.231867	-0.111928
10	6	0	-2.607267	1.744535	0.649332
11	6	0	2.680196	1.559859	-0.769522
12	6	0	-0.748618	0.278764	0.068324
13	6	0	1.310841	1.473749	-0.431849
14	6	0	-3.487147	0.682129	0.657914
15	6	0	-1.678152	-0.801880	-0.142716
16	6	0	-3.060265	-0.597433	0.214702

17	6	0	-1.351052	-2.029945	-0.791116
18	6	0	-3.990411	-1.661871	0.046659
19	6	0	-2.286689	-3.026507	-0.981561
20	6	0	-3.618291	-2.857782	-0.528526
21	1	0	4.110338	-3.881161	0.731817
22	1	0	1.757980	-3.999901	1.586327
23	1	0	4.902869	-1.806700	-0.370819
24	1	0	0.207376	-2.147218	1.206765
25	1	0	4.542483	0.511391	-1.042538
26	1	0	-2.967392	2.746133	0.878613
27	1	0	3.092167	2.525933	-1.057253
28	1	0	-4.532400	0.820534	0.932841
29	1	0	-0.345131	-2.173535	-1.167268
30	1	0	-5.022294	-1.497021	0.353839
31	1	0	-1.999620	-3.943853	-1.491599
32	1	0	-4.346752	-3.654819	-0.663726
33	14	0	0.068725	2.894377	-0.087960
34	8	0	0.641854	3.573573	1.376922
35	1	0	0.646007	4.536082	1.258400
36	8	0	-0.304614	3.971218	-1.170117

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.205217	4.066478	-1.134565
2	6	0	-2.503497	2.766896	-1.612863
3	6	0	-1.175946	4.243879	-0.236278
4	6	0	-1.783079	1.674744	-1.176854
5	6	0	-0.407626	3.139415	0.224617
6	6	0	-0.720601	1.816973	-0.237327
7	6	0	1.926004	-0.774169	-1.477320
8	6	0	0.675518	3.312560	1.125778
9	6	0	0.602679	-1.377799	-1.064377
10	6	0	0.051537	0.698374	0.232131
11	6	0	0.280563	-2.695237	-1.494066
12	6	0	1.425659	2.234473	1.531886
13	6	0	-0.276915	-0.693778	-0.223252
14	6	0	1.131778	0.912755	1.091451
15	6	0	-0.878324	-3.317596	-1.097546
16	6	0	-1.476520	-1.340672	0.235766

17	6	0	-1.783050	-2.667127	-0.218168
18	6	0	2.051666	-0.215302	1.496033
19	6	0	-2.375687	-0.728825	1.156995
20	6	0	-2.970770	-3.306009	0.232662
21	6	0	-3.515255	-1.378229	1.583315
22	6	0	-3.824231	-2.678085	1.113066
23	1	0	-2.783869	4.918575	-1.481815
24	1	0	-3.307968	2.629171	-2.331001
25	1	0	-0.929828	5.237896	0.131631
26	1	0	1.787833	0.247352	-1.857562
27	1	0	-2.024404	0.686940	-1.554998
28	1	0	2.384879	-1.356296	-2.284941
29	1	0	0.908771	4.312263	1.486334
30	1	0	0.974947	-3.212965	-2.151693
31	1	0	2.259171	2.381847	2.215450
32	1	0	-1.109062	-4.322605	-1.444402
33	1	0	-2.154116	0.265256	1.530652
34	1	0	2.693099	0.075824	2.335529
35	1	0	1.490976	-1.105918	1.806610
36	1	0	-3.189380	-4.309264	-0.127369
37	1	0	-4.181969	-0.888266	2.288556
38	1	0	-4.727553	-3.177890	1.453210
39	8	0	4.362023	0.390111	-0.287401
40	8	0	3.875651	-2.137207	0.306554
41	14	0	3.112643	-0.689419	0.004743
42	1	0	4.137180	1.287624	-0.570513
43	1	0	4.800791	-2.203228	0.030197

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.889902	-2.596761	1.087186
2	6	0	-3.557563	-1.300744	1.552455
3	6	0	-3.032360	-3.247496	0.224437
4	6	0	-2.396287	-0.681099	1.137140
5	6	0	-1.825146	-2.639393	-0.213677
6	6	0	-1.495662	-1.312980	0.229090
7	6	0	2.072478	-0.254107	1.473339
8	6	0	-0.913604	-3.317258	-1.066683
9	6	0	1.190389	0.878780	1.064751

10	6	0	-0.281258	-0.689489	-0.220101
11	6	0	1.525410	2.205065	1.472081
12	6	0	0.260466	-2.718266	-1.450358
13	6	0	0.076835	0.693701	0.232436
14	6	0	0.606278	-1.394035	-1.045878
15	6	0	0.792990	3.298681	1.082508
16	6	0	-0.676008	1.828495	-0.226347
17	6	0	-0.323784	3.148626	0.217439
18	6	0	1.929355	-0.831624	-1.447999
19	6	0	-1.760946	1.712392	-1.145359
20	6	0	-1.078491	4.266068	-0.230572
21	6	0	-2.469864	2.817682	-1.570703
22	6	0	-2.134893	4.112701	-1.104575
23	1	0	-4.808787	-3.076689	1.417438
24	1	0	-4.221196	-0.789803	2.247171
25	1	0	-3.263832	-4.251190	-0.129780
26	1	0	1.490545	-1.132881	1.776575
27	1	0	-2.153929	0.308843	1.509373
28	1	0	2.718015	0.028042	2.313479
29	1	0	-1.151604	-4.327376	-1.397082
30	1	0	2.398413	2.336787	2.107325
31	1	0	0.966763	-3.260094	-2.075157
32	1	0	1.070138	4.297092	1.418180
33	1	0	-2.026501	0.728744	-1.518618
34	1	0	2.357063	-1.388988	-2.289489
35	1	0	1.847992	0.222188	-1.741375
36	1	0	-0.797263	5.256488	0.125144
37	1	0	-3.290997	2.692452	-2.273658
38	1	0	-2.700825	4.978233	-1.442761
39	8	0	3.982297	-2.232388	0.278423
40	8	0	4.233613	0.453965	-0.324036
41	14	0	3.212935	-0.885700	0.021751
42	1	0	5.147028	0.131699	-0.290033

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.514001	2.595380	0.683330
2	6	0	-0.508622	2.581177	1.651354
3	6	0	0.070524	1.368062	2.042163

4	6	0	-0.626807	0.201618	1.689410
5	6	0	-1.644462	0.180352	0.717585
6	6	0	-1.956678	1.409881	0.077971
7	1	0	-1.846771	3.552437	0.283983
8	1	0	-0.082694	3.523185	1.992789
9	1	0	-0.284263	-0.740393	2.113405
10	6	0	1.486062	1.301036	2.578927
11	1	0	1.678641	2.139961	3.258262
12	1	0	1.617244	0.384423	3.165497
13	6	0	2.624877	1.329244	1.437356
14	1	0	3.224349	2.234275	1.588208
15	1	0	3.294532	0.482952	1.612183
16	6	0	2.070475	1.335128	0.023330
17	6	0	1.726342	2.577599	-0.529844
18	6	0	1.639346	0.167726	-0.662221
19	6	0	0.722758	2.691841	-1.492954
20	1	0	2.136845	3.484146	-0.088177
21	6	0	0.635049	0.314801	-1.637773
22	6	0	0.043036	1.551652	-1.933750
23	1	0	0.377252	3.680829	-1.788921
24	1	0	0.209958	-0.572508	-2.096499
25	6	0	-2.506540	1.489427	-1.336247
26	1	0	-3.099506	0.604370	-1.574790
27	1	0	-3.173037	2.355423	-1.430485
28	6	0	-1.370390	1.625229	-2.471038
29	1	0	-1.540322	0.828404	-3.203404
30	1	0	-1.521253	2.578608	-2.990877
31	14	0	-2.432898	-1.500486	0.301500
32	14	0	2.301633	-1.581469	-0.431685
33	6	0	-4.300961	-1.389838	0.079715
34	1	0	-4.774216	-0.954900	0.969134
35	1	0	-4.599514	-0.789263	-0.785870
36	1	0	-4.712703	-2.397251	-0.062054
37	6	0	-2.077909	-2.703108	1.720355
38	1	0	-2.416351	-2.316007	2.689782
39	1	0	-2.613225	-3.642213	1.530065
40	1	0	-1.012860	-2.950168	1.809945
41	6	0	3.807404	-1.868737	-1.533672
42	1	0	4.635790	-1.211895	-1.238241
43	1	0	4.170973	-2.903407	-1.471257
44	1	0	3.573206	-1.650541	-2.582490
45	6	0	2.717207	-2.152868	1.320686
46	1	0	3.653379	-1.718481	1.691077
47	1	0	1.925280	-1.922811	2.041431

48	1	0	2.849022	-3.243573	1.316103
49	8	0	-1.831595	-2.129632	-1.132580
50	1	0	-0.868304	-2.300291	-1.134644
51	8	0	1.026222	-2.564274	-1.003388
52	1	0	1.258982	-3.470292	-1.251910

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.415142	2.617820	0.848689
2	6	0	-0.342486	2.523395	1.735532
3	6	0	0.233123	1.272574	1.992925
4	6	0	-0.513503	0.145161	1.617183
5	6	0	-1.615894	0.208041	0.738435
6	6	0	-1.945984	1.481195	0.211435
7	1	0	-1.741516	3.605621	0.523391
8	1	0	0.138781	3.434139	2.091851
9	1	0	-0.113286	-0.834847	1.874222
10	6	0	1.692231	1.121243	2.382436
11	1	0	1.953720	1.758996	3.239316
12	1	0	1.865156	0.083404	2.687176
13	6	0	2.706337	1.470930	1.196873
14	1	0	3.056250	2.501563	1.343119
15	1	0	3.579107	0.820812	1.308812
16	6	0	2.071857	1.371644	-0.182520
17	6	0	1.630397	2.571830	-0.771180
18	6	0	1.657723	0.144098	-0.755911
19	6	0	0.555558	2.595846	-1.660314
20	1	0	2.031670	3.518376	-0.407632
21	6	0	0.563648	0.208264	-1.644017
22	6	0	-0.102498	1.399085	-1.974417
23	1	0	0.140723	3.553281	-1.976071
24	1	0	0.113294	-0.727764	-1.971178
25	6	0	-2.569400	1.686725	-1.160879
26	1	0	-3.471120	1.085252	-1.310876
27	1	0	-2.873366	2.738152	-1.246589
28	6	0	-1.567703	1.364428	-2.368449
29	1	0	-1.803691	0.364605	-2.751173
30	1	0	-1.790396	2.076956	-3.175815
31	14	0	-2.379136	-1.501629	0.343898

32	14	0	2.224089	-1.664918	-0.338988
33	6	0	-3.934090	-1.438621	-0.744903
34	1	0	-4.701550	-0.758127	-0.352833
35	1	0	-3.708619	-1.153598	-1.779060
36	1	0	-4.366096	-2.448353	-0.775538
37	6	0	-2.937470	-2.193779	2.026275
38	1	0	-3.678107	-1.543145	2.512136
39	1	0	-3.386879	-3.187397	1.892543
40	1	0	-2.087354	-2.304816	2.710416
41	6	0	2.640613	-2.400975	-2.059198
42	1	0	3.422522	-1.830533	-2.581856
43	1	0	2.994869	-3.434686	-1.937758
44	1	0	1.756457	-2.432865	-2.708936
45	6	0	3.904145	-1.670738	0.581783
46	1	0	4.656124	-1.014321	0.120368
47	1	0	3.803605	-1.396714	1.639545
48	1	0	4.297557	-2.697159	0.555561
49	8	0	-1.318033	-2.505153	-0.405965
50	1	0	-0.326900	-2.533710	-0.063129
51	8	0	1.085650	-2.467405	0.457539

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.852492	-0.195503	0.000064
2	8	0	-1.178136	-0.796546	1.288587
3	8	0	-1.178570	-0.796753	-1.288228
4	6	0	1.016157	0.042551	-0.000077
5	7	0	-1.346415	1.398995	-0.000242
6	1	0	-1.839715	1.653908	-0.852241
7	1	0	-1.837558	1.655121	0.852647
8	9	0	1.393039	0.719185	-1.090378
9	9	0	1.602565	-1.157895	-0.000615
10	9	0	1.393146	0.718392	1.090754

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Standard orientation:

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

1	16	0	-0.944209	-0.057971	0.017656
2	8	0	-1.177689	0.070518	1.484820
3	8	0	-1.177365	-1.381310	-0.600852
4	6	0	0.963307	0.021528	-0.020275
5	7	0	-1.457103	1.115859	-0.882671
6	1	0	-1.487188	1.948129	-0.288120
7	9	0	1.463199	-0.126338	-1.271778
8	9	0	1.552267	-0.929045	0.749567
9	9	0	1.412849	1.224889	0.437125

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.258991	-0.901325	0.097817
2	8	0	-1.718793	-1.793043	1.151081
3	8	0	-0.859308	-1.324757	-1.228626
4	6	0	-2.607091	0.413428	-0.107879
5	9	0	-3.698001	-0.189525	-0.579038
6	9	0	-2.206910	1.357088	-0.953736
7	9	0	-2.872092	0.959579	1.083136
8	7	0	-0.000010	0.000022	0.809593
9	1	0	-0.000005	0.000015	1.829979
10	16	0	1.258995	0.901333	0.097816
11	8	0	0.859332	1.324742	-1.228641
12	8	0	1.718795	1.793068	1.151066
13	6	0	2.607086	-0.413437	-0.107836
14	9	0	2.872057	-0.959573	1.083193
15	9	0	2.206914	-1.357105	-0.953687
16	9	0	3.698012	0.189499	-0.578981

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.152766	0.858619	0.081335
2	8	0	1.656092	1.858815	1.030739

3	8	0	0.907482	1.251882	-1.311843
4	6	0	2.581282	-0.376102	-0.032290
5	9	0	3.647942	0.214862	-0.613505
6	9	0	2.250752	-1.450642	-0.767151
7	9	0	2.961822	-0.802658	1.186245
8	7	0	-0.000004	0.000027	0.825921
9	16	0	-1.152763	-0.858611	0.081371
10	8	0	-0.907472	-1.251936	-1.311788
11	8	0	-1.656085	-1.858767	1.030818
12	6	0	-2.581286	0.376097	-0.032315
13	9	0	-2.961827	0.802714	1.186198
14	9	0	-2.250760	1.450600	-0.767233
15	9	0	-3.647943	-0.214902	-0.613500

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.469413	0.000061	-0.153406
2	8	0	1.889247	1.287327	-0.721454
3	8	0	1.889267	-1.286820	-0.722312
4	7	0	1.950397	-0.000499	1.476962
5	1	0	2.489951	-0.840843	1.677838
6	1	0	2.489838	0.839769	1.678456
7	6	0	-0.325801	0.000023	-0.063867
8	6	0	-1.005743	-1.219376	-0.033649
9	6	0	-1.005794	1.219388	-0.033613
10	6	0	-2.400173	-1.212370	0.042142
11	1	0	-0.452645	-2.151578	-0.085261
12	6	0	-2.400228	1.212318	0.042171
13	1	0	-0.452725	2.151609	-0.085186
14	6	0	-3.095746	-0.000040	0.083088
15	1	0	-2.941905	-2.154053	0.061775
16	1	0	-2.942000	2.153978	0.061825
17	1	0	-4.181104	-0.000066	0.138816

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.560566	-0.008022	-0.028423
2	8	0	-1.894033	-1.190402	-0.868414
3	8	0	-1.904381	1.340164	-0.590093
4	7	0	-2.017217	-0.248584	1.466792
5	1	0	-2.031298	0.672705	1.913772
6	6	0	0.281563	0.002472	-0.053161
7	6	0	0.987197	1.209839	-0.044796
8	6	0	0.983719	-1.208337	-0.015881
9	6	0	2.385582	1.207640	0.008350
10	1	0	0.429300	2.140354	-0.100624
11	6	0	2.379421	-1.209856	0.038220
12	1	0	0.423751	-2.138826	-0.038806
13	6	0	3.087958	-0.001247	0.053457
14	1	0	2.927940	2.152332	0.007673
15	1	0	2.918596	-2.155865	0.063962
16	1	0	4.175953	-0.003424	0.092162

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.587948	1.296778	0.164682
2	8	0	-0.153557	1.309870	1.575041
3	8	0	-0.943549	2.579563	-0.470817
4	7	0	0.472788	0.579836	-0.872771
5	6	0	-2.097061	0.286797	0.106686
6	6	0	-3.079386	0.587207	-0.839451
7	6	0	-2.263518	-0.766072	1.008795
8	6	0	-4.245782	-0.181142	-0.884566
9	1	0	-2.924282	1.419588	-1.518435
10	6	0	-3.433954	-1.527682	0.957743
11	1	0	-1.479664	-0.985040	1.725138
12	6	0	-4.424676	-1.238443	0.013620
13	1	0	-5.015156	0.048603	-1.618682
14	1	0	-3.568659	-2.351713	1.654849
15	1	0	-5.333487	-1.835760	-0.022495
16	16	0	1.312096	-0.740853	-0.521497

17	8	0	0.790234	-1.597422	0.561824
18	8	0	1.737469	-1.377928	-1.777053
19	6	0	2.958290	-0.105945	0.172368
20	9	0	3.569194	0.723681	-0.697262
21	9	0	3.791590	-1.149601	0.394422
22	9	0	2.805560	0.549218	1.333388

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.703216	1.355498	0.213782
2	8	0	-0.187355	1.357623	1.574234
3	8	0	-0.958862	2.576118	-0.549422
4	7	0	0.502066	0.583132	-0.785365
5	1	0	0.558144	0.950441	-1.734380
6	6	0	-2.143612	0.296731	0.127639
7	6	0	-3.081699	0.520471	-0.884539
8	6	0	-2.304572	-0.708579	1.084306
9	6	0	-4.209581	-0.299411	-0.941017
10	1	0	-2.937376	1.326601	-1.596355
11	6	0	-3.439369	-1.518075	1.012349
12	1	0	-1.560229	-0.851765	1.859286
13	6	0	-4.385895	-1.316305	0.003136
14	1	0	-4.952252	-0.138010	-1.717122
15	1	0	-3.581782	-2.305599	1.746667
16	1	0	-5.266970	-1.950463	-0.045325
17	16	0	1.396133	-0.803664	-0.509557
18	8	0	0.766143	-1.584598	0.543404
19	8	0	1.751567	-1.337923	-1.818180
20	6	0	3.005212	-0.120501	0.211686
21	9	0	3.532577	0.765258	-0.641906
22	9	0	3.853672	-1.140172	0.373774
23	9	0	2.783136	0.468446	1.383189