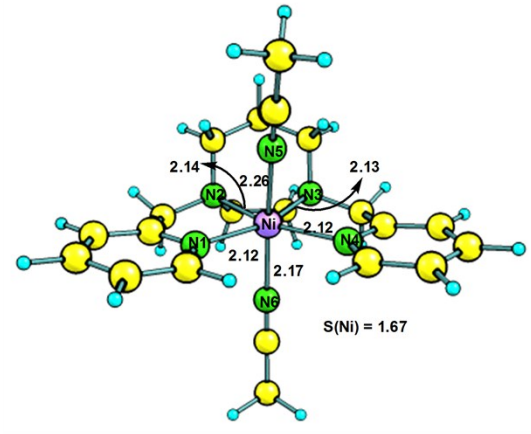
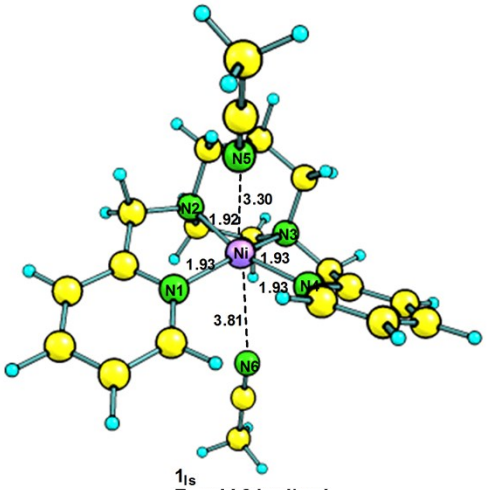
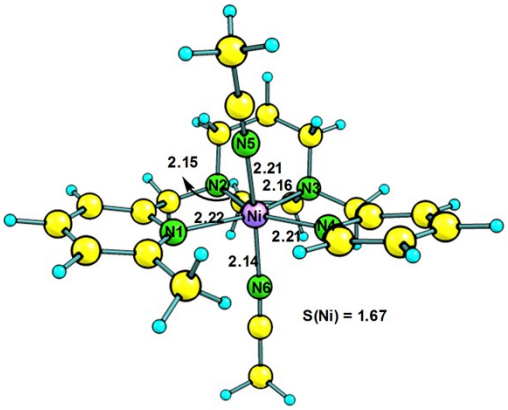


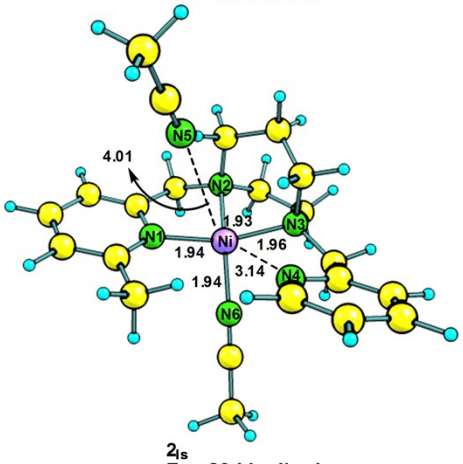
1_{hs}
E = 0.0 kcal/mol



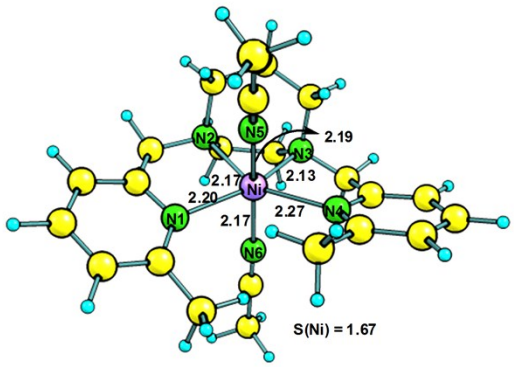
1_{ls}
E = +11.0 kcal/mol



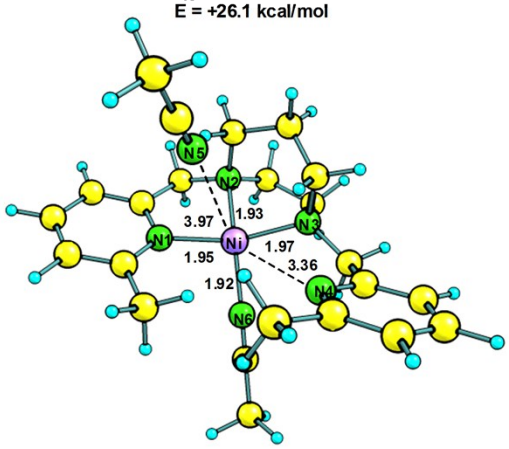
2_{hs}
E = 0.0 kcal/mol



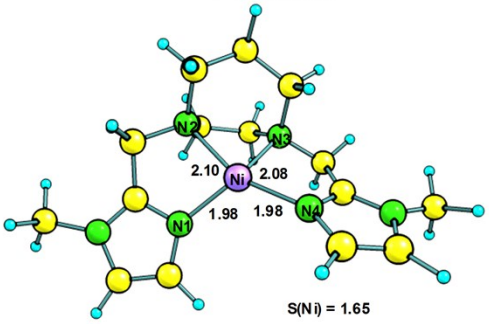
2_{ls}
E = +26.1 kcal/mol



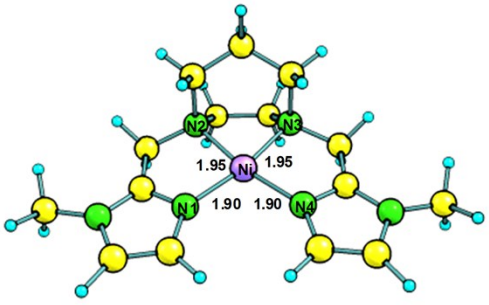
3_{hs}
E = 0.0 kcal/mol



3_{ls}
E = +19.4 kcal/mol



4_{hs}
E = 0.0 kcal/mol



4_{ls}
E = -5.8 kcal/mol

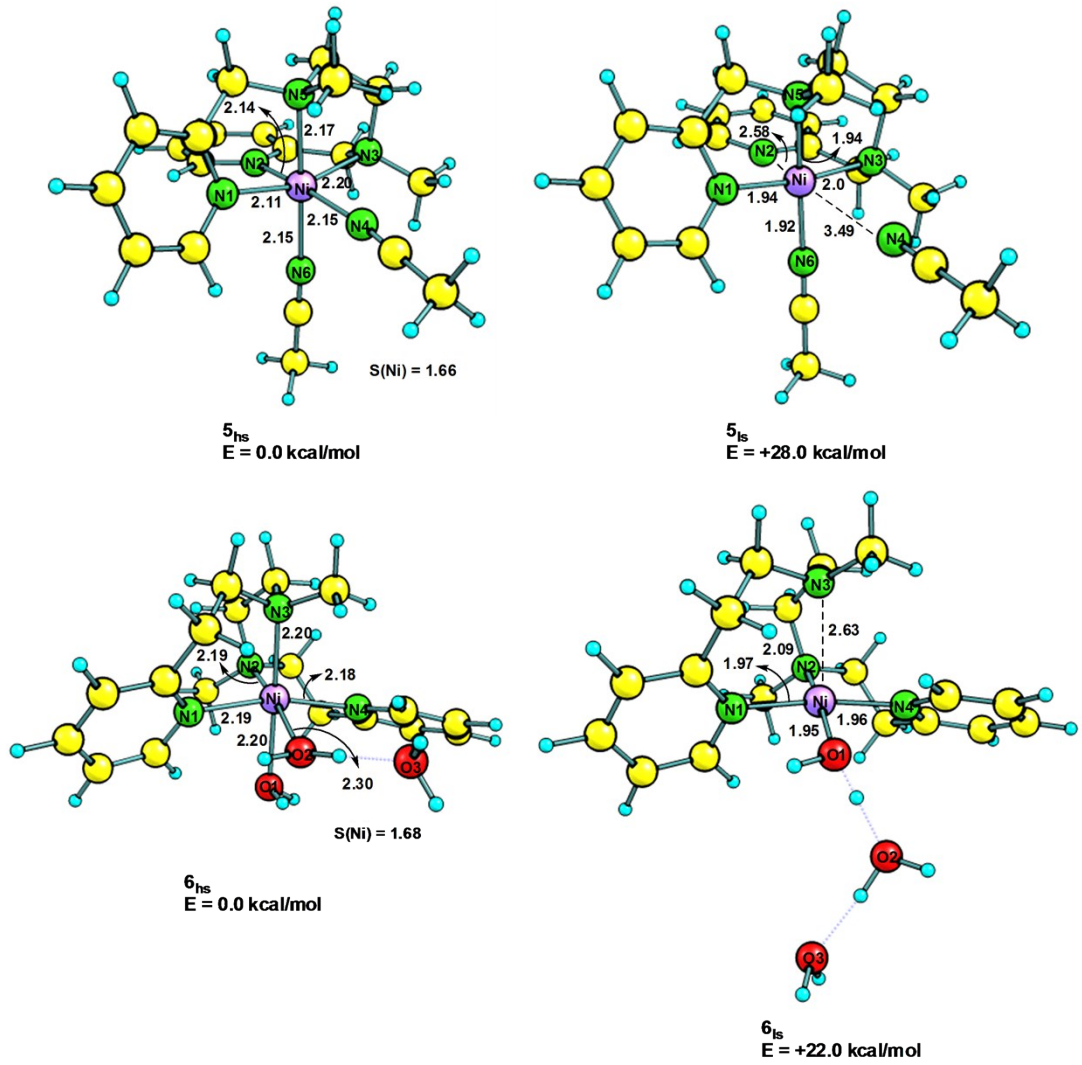


Fig S1. DFT optimized structures of **1**-**6** in the high spin (S = 1) and low spin (S = 0) states. The bond lengths are shown in Å along with the spin density on Ni centre. The optimized structure of **5**(cis-β configuration) is based on computation, and that of **6** (cis-α configuration) on the X-ray crystal structure of $[Ni(pdao)(H_2O)_2]^{2+}$.

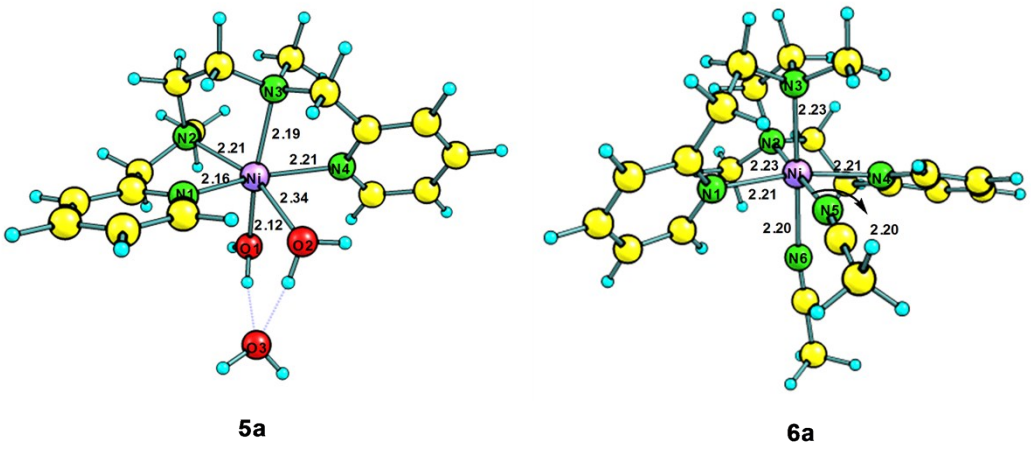


Fig. S2. DFT optimized structure of **5a** with H_2O as coordinating ligand and that of **6a** with CH_3CN as coordinating ligand in the high spin (S = 1) state. The ligands L5 and L6 display cis-α mode of coordination.

Coordinates of the optimized geometries:

$\mathbf{1}_{hs}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.000254	-0.183189	0.044126
2	7	0	-1.820686	0.643938	0.744610
3	7	0	-1.329061	-1.390882	-1.106410
4	6	0	0.001972	2.704488	-1.769322
5	7	0	1.328090	-1.391516	-1.106370
6	7	0	1.820556	0.642759	0.745168
7	7	0	0.000944	1.655315	-1.276892
8	7	0	-0.000654	-1.519222	1.751934
9	6	0	-0.000509	-2.039208	2.787008
10	6	0	1.999449	1.749852	1.490499
11	6	0	2.904197	0.032487	0.219652
12	6	0	2.682139	-1.280345	-0.508533
13	6	0	-2.904608	0.033884	0.219396
14	6	0	0.003250	4.019675	-2.397721
15	6	0	4.193154	0.531369	0.414563
16	6	0	-1.999108	1.751336	1.489586
17	6	0	4.372116	1.674222	1.191035
18	6	0	-0.779973	-2.775810	-1.037440
19	6	0	3.251773	2.293655	1.747499
20	6	0	-4.371841	1.676342	1.190596
21	6	0	-4.193371	0.533223	0.414386
22	6	0	-3.251210	2.295617	1.746636
23	6	0	-1.317364	-0.897137	-2.521257
24	6	0	1.316682	-0.897894	-2.521255
25	6	0	0.778333	-2.776171	-1.037340
26	6	0	-0.000429	-1.199214	-3.253831
27	6	0	-2.683066	-1.279137	-0.508598
28	1	0	1.103012	2.210506	1.891567
29	1	0	3.463686	-1.431723	-1.262912
30	1	0	2.798946	-2.085017	0.225176
31	1	0	0.799485	4.636593	-1.971350
32	1	0	-0.958731	4.513402	-2.232706
33	1	0	0.170621	3.918476	-3.474050
34	1	0	5.042818	0.024189	-0.031343
35	1	0	-1.102476	2.211972	1.890213
36	1	0	5.366956	2.074582	1.358463
37	1	0	-1.175491	-3.385656	-1.858040
38	1	0	-1.128307	-3.223365	-0.106954
39	1	0	3.343103	3.181705	2.362903
40	1	0	-5.366527	2.077054	1.358101
41	1	0	-5.043265	0.026200	-0.031264
42	1	0	-3.342113	3.183946	2.361694
43	1	0	-1.530320	0.172532	-2.498946
44	1	0	-2.131945	-1.384993	-3.074358
45	1	0	2.130984	-1.386279	-3.074305
46	1	0	1.530346	0.171641	-2.498953
47	1	0	-0.000716	-2.249062	-3.562137
48	1	0	-0.000297	-0.630032	-4.189133
49	1	0	1.173673	-3.386297	-1.857823
50	1	0	1.126354	-3.223782	-0.106762
51	6	0	-0.000237	-2.695683	4.087706
52	1	0	0.112513	-3.776478	3.961333
53	1	0	0.829105	-2.319201	4.693565
54	1	0	-0.941904	-2.493653	4.606419
55	1	0	-3.464664	-1.430308	-1.262968
56	1	0	-2.800159	-2.083706	0.225177

$\mathbf{1}_{ls}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.083451	0.013600	-0.252656
2	7	0	0.185594	1.578954	0.872933
3	7	0	0.356468	1.174701	-1.758706
4	6	0	4.469852	-0.148832	0.504273
5	7	0	-0.597460	-1.200592	-1.588686
6	7	0	0.048608	-1.484162	0.955511
7	7	0	3.340401	-0.078855	0.242103
8	7	0	-3.714935	0.016099	0.093107
9	6	0	-4.812820	0.188774	0.430112
10	6	0	0.755540	-1.627700	2.094719
11	6	0	-0.616690	-2.552148	0.446721
12	6	0	-1.339625	-2.270985	-0.843126
13	6	0	0.357450	2.724876	0.168747
14	6	0	5.889463	-0.238110	0.831678
15	6	0	-0.628165	-3.780723	1.098332
16	6	0	-0.119552	1.659071	2.185355
17	6	0	0.067282	-3.915606	2.300554
18	6	0	-0.949969	1.107615	-2.495468
19	6	0	0.778768	-2.824192	2.800669
20	6	0	-0.025930	4.053200	2.133669
21	6	0	0.259141	3.975933	0.771453
22	6	0	-0.223864	2.872746	2.851192
23	6	0	1.497449	0.620857	-2.584661
24	6	0	0.529882	-1.765062	-2.405772
25	6	0	-1.510362	-0.338726	-2.425622
26	6	0	1.163619	-0.692474	-3.294358
27	6	0	0.706962	2.552540	-1.287062
28	1	0	1.327468	-0.766845	2.418846
29	1	0	-1.449540	-3.171043	-1.457218
30	1	0	-2.335755	-1.882387	-0.610589
31	1	0	6.466003	0.429567	0.185284
32	1	0	6.244416	-1.262374	0.687565
33	1	0	6.054359	0.051134	1.873316
34	1	0	-1.167205	-4.617820	0.667532
35	1	0	-0.296493	0.722868	2.699045
36	1	0	0.069379	-4.864151	2.827943
37	1	0	-0.817456	1.458505	-3.525242
38	1	0	-1.643523	1.785739	-1.994425
39	1	0	1.354390	-2.897324	3.716375
40	1	0	-0.105228	5.018383	2.623491
41	1	0	0.400951	4.874547	0.179951
42	1	0	-0.466085	2.886882	3.907766
43	1	0	2.338842	0.497773	-1.898616
44	1	0	1.764841	1.373253	-3.336892
45	1	0	0.138453	-2.575098	-3.033649
46	1	0	1.257062	-2.195402	-1.711875
47	1	0	0.523391	-0.501848	-4.160848
48	1	0	2.096331	-1.092900	-3.704035
49	1	0	-1.637275	-0.785281	-3.416409
50	1	0	-2.478797	-0.313403	-1.928725
51	6	0	-6.193095	0.404174	0.851033
52	1	0	-6.878053	0.114912	0.048988
53	1	0	-6.413302	-0.196687	1.737796
54	1	0	-6.353373	1.459409	1.088917
55	1	0	1.786828	2.686338	-1.406044
56	1	0	0.219991	3.308073	-1.912356

$\underline{2_{hs}}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.043495	0.219219	-0.116421
2	7	0	-1.985912	-0.589000	-0.485222
3	7	0	-1.110753	1.853351	0.675311
4	6	0	-0.133605	-1.892173	2.489947
5	7	0	1.516976	1.656656	0.520890
6	7	0	1.893336	-0.935092	-0.448794
7	7	0	-0.069961	-1.077824	1.668403
8	7	0	0.088827	0.912199	-2.136507
9	6	0	0.065867	1.085865	-3.281271
10	6	0	2.048860	-2.259050	-0.642968
11	6	0	3.000726	-0.196147	-0.215976
12	6	0	2.813689	1.298788	-0.098441
13	6	0	-2.921655	0.251581	0.019319
14	6	0	-0.213130	-2.907419	3.532557
15	6	0	4.275538	-0.760873	-0.165312
16	6	0	-2.373849	-1.821104	-0.889715
17	6	0	4.425775	-2.128941	-0.380751
18	6	0	-0.501841	3.102506	0.137857
19	6	0	3.286307	-2.893089	-0.628859
20	6	0	-4.641751	-1.409580	-0.172538
21	6	0	-4.246753	-0.128551	0.209437
22	6	0	-3.698089	-2.251876	-0.747233
23	6	0	-1.018324	1.832846	2.170687
24	6	0	1.596617	1.601445	2.015329
25	6	0	1.045721	2.996288	0.071943
26	6	0	0.370384	2.222053	2.702251
27	6	0	-2.517059	1.693538	0.236218
28	1	0	3.654437	1.749483	0.443797
29	1	0	2.828367	1.716266	-1.110732
30	1	0	0.672180	-3.548892	3.497976
31	1	0	-1.106631	-3.521742	3.388877
32	1	0	-0.266341	-2.428509	4.514765
33	1	0	5.136359	-0.131327	0.035759
34	1	0	5.408998	-2.587591	-0.351427
35	1	0	-0.816461	3.968826	0.732171
36	1	0	-0.887775	3.248271	-0.871238
37	1	0	3.347966	-3.961545	-0.803562
38	1	0	-5.669047	-1.734651	-0.041667
39	1	0	-4.958519	0.574458	0.629309
40	1	0	-3.973967	-3.243051	-1.090935
41	1	0	-1.314205	0.837714	2.504087
42	1	0	-1.748321	2.545685	2.578502
43	1	0	2.487855	2.152405	2.346839
44	1	0	1.732909	0.556702	2.299950
45	1	0	0.465371	3.311821	2.677285
46	1	0	0.409880	1.959081	3.764300
47	1	0	1.527252	3.787111	0.658603
48	1	0	1.362283	3.129510	-0.962515
49	6	0	0.037142	1.304599	-4.721225
50	1	0	0.171712	2.367787	-4.941083
51	1	0	0.841033	0.737069	-5.199171
52	1	0	-0.923731	0.975479	-5.127619
53	1	0	-3.207921	2.182317	0.933517
54	1	0	-2.631051	2.206206	-0.725085
55	1	0	1.145771	-2.828180	-0.814771
56	6	0	-1.356422	-2.734467	-1.514606
57	1	0	-1.827062	-3.383256	-2.257129
58	1	0	-0.566393	-2.164590	-2.006802
59	1	0	-0.905303	-3.390442	-0.760660

2_{ls}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.260961	0.916736	0.186363
2	7	0	-1.879837	0.593328	-0.837945
3	7	0	-1.417754	0.967640	1.734384
4	6	0	-1.347889	-4.134807	0.170797
5	7	0	1.135997	0.773448	1.559499
6	7	0	2.309215	-0.681583	-0.645897
7	7	0	-1.167646	-2.991051	0.259094
8	7	0	0.738094	1.807169	-1.218535
9	6	0	1.242716	2.477583	-2.014602
10	6	0	2.826699	-1.610101	-1.464334
11	6	0	3.133990	-0.092102	0.234641
12	6	0	2.558651	0.988095	1.133434
13	6	0	-3.002764	0.875698	-0.123856
14	6	0	-1.575408	-5.572576	0.061365
15	6	0	4.492888	-0.405300	0.326422
16	6	0	-1.983830	0.009333	-2.058001
17	6	0	5.022503	-1.358856	-0.543660
18	6	0	-0.763846	1.943136	2.674232
19	6	0	4.172378	-1.976973	-1.458709
20	6	0	-4.399836	0.102257	-1.899740
21	6	0	-4.275553	0.647269	-0.620032
22	6	0	-3.250425	-0.226831	-2.606721
23	6	0	-1.556632	-0.392139	2.362815
24	6	0	0.986224	-0.631530	2.126305
25	6	0	0.773604	1.807349	2.583594
26	6	0	-0.244014	-0.825814	3.010999
27	6	0	-2.736246	1.473160	1.229187
28	1	0	3.171982	1.064549	2.039682
29	1	0	2.599184	1.960444	0.633562
30	1	0	-1.175688	-6.084520	0.941165
31	1	0	-1.080073	-5.965922	-0.830614
32	1	0	-2.646925	-5.779159	-0.009626
33	1	0	5.125253	0.083778	1.061294
34	1	0	6.075018	-1.619876	-0.497758
35	1	0	-1.137058	1.785050	3.691224
36	1	0	-1.059420	2.947617	2.369029
37	1	0	4.536717	-2.731940	-2.146948
38	1	0	-5.380692	-0.084500	-2.325141
39	1	0	-5.147501	0.882875	-0.019629
40	1	0	-3.316918	-0.686673	-3.586591
41	1	0	-1.850031	-1.092806	1.578663
42	1	0	-2.351488	-0.344008	3.117329
43	1	0	1.887024	-0.846098	2.713643
44	1	0	0.964570	-1.314186	1.277103
45	1	0	-0.110185	-0.328289	3.976657
46	1	0	-0.315833	-1.894570	3.234010
47	1	0	1.227598	1.552609	3.547374
48	1	0	1.206345	2.756037	2.259927
49	6	0	1.887410	3.304348	-3.024286
50	1	0	2.214822	4.249080	-2.579984
51	1	0	2.755928	2.779576	-3.433602
52	1	0	1.182937	3.519133	-3.833423
53	1	0	-3.536188	1.245690	1.941808
54	1	0	-2.671662	2.562697	1.142460
55	1	0	2.131240	-2.083021	-2.153569
56	6	0	-0.746044	-0.397610	-2.807004
57	1	0	-0.419405	0.402656	-3.480092
58	1	0	0.076384	-0.637672	-2.131995
59	1	0	-0.962971	-1.271335	-3.425405

3_{hs}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.026395	-0.265102	0.114133
2	7	0	-2.021620	0.604128	0.418563
3	7	0	-1.211022	-1.966946	-0.522932
4	6	0	-0.127174	1.192558	-2.895195
5	7	0	1.387159	-1.848554	-0.076523
6	7	0	1.924979	0.899122	0.209723
7	7	0	-0.093598	0.607636	-1.896043
8	7	0	-0.015917	-0.579048	2.257527
9	6	0	-0.089591	-0.578093	3.413438
10	6	0	2.216314	2.202731	-0.019213
11	6	0	2.958297	0.027336	0.339189
12	6	0	2.616039	-1.416419	0.625363
13	6	0	-2.950731	-0.164492	-0.201249
14	6	0	-0.169951	1.924969	-4.154186
15	6	0	4.291235	0.416260	0.271064
16	6	0	-2.380847	1.836172	0.851838
17	6	0	4.592032	1.762936	0.074099
18	6	0	-0.763821	-3.075651	0.365770
19	6	0	3.541669	2.656135	-0.076809
20	6	0	-4.550646	1.622696	-0.184242
21	6	0	-4.211261	0.316585	-0.538762
22	6	0	-3.637455	2.373587	0.544866
23	6	0	-0.931323	-2.311477	-1.955697
24	6	0	1.647924	-2.104788	-1.528398
25	6	0	0.777533	-3.047310	0.567846
26	6	0	0.487519	-2.840135	-2.211464
27	6	0	-2.651490	-1.643742	-0.357410
28	1	0	3.465602	-2.063657	0.372951
29	1	0	2.438854	-1.522799	1.699897
30	1	0	0.842722	2.049087	-4.548765
31	1	0	-0.615722	2.911347	-3.995990
32	1	0	-0.772161	1.377181	-4.884986
33	1	0	5.077552	-0.324504	0.370561
34	1	0	5.622166	2.101038	0.024112
35	1	0	-1.093173	-4.044606	-0.029614
36	1	0	-1.249661	-2.934905	1.331848
37	1	0	3.730526	3.710314	-0.250731
38	1	0	-5.522788	2.030686	-0.442618
39	1	0	-4.921230	-0.326275	-1.048751
40	1	0	-3.889385	3.368932	0.895448
41	1	0	-1.140522	-1.422320	-2.548823
42	1	0	-1.640808	-3.088842	-2.270766
43	1	0	2.552021	-2.721411	-1.628340
44	1	0	1.853791	-1.143421	-2.003506
45	1	0	0.527642	-3.898987	-1.939346
46	1	0	0.662345	-2.819472	-3.292143
47	1	0	1.250541	-3.961497	0.193229
48	1	0	0.990545	-2.996972	1.635113
49	6	0	-0.180798	-0.577146	4.867611
50	1	0	0.272567	-1.487085	5.271706
51	1	0	0.346388	0.291975	5.271980
52	1	0	-1.229737	-0.535205	5.175172
53	1	0	-3.239518	-2.060058	-1.181946
54	1	0	-3.016685	-2.134781	0.551817
55	6	0	1.112910	3.206819	-0.219906
56	1	0	0.151705	2.733016	-0.403448
57	1	0	1.020384	3.854721	0.658020
58	1	0	1.349517	3.859507	-1.065730
59	6	0	-1.456744	2.592953	1.768782
60	1	0	-1.880106	2.584891	2.780473
61	1	0	-0.465255	2.145903	1.815792
62	1	0	-1.366750	3.641788	1.475430

3_{ls}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.500665	-0.985294	0.128649
2	7	0	-2.079742	-0.164399	0.935520
3	7	0	-1.672522	-1.454529	-1.331551
4	6	0	-0.976717	3.843842	-1.536173
5	7	0	0.894131	-1.485985	-1.170413
6	7	0	2.493654	0.528503	0.284303
7	7	0	-0.906467	2.730461	-1.212657
8	7	0	0.479681	-1.290678	1.750369
9	6	0	0.988980	-1.626466	2.732554
10	6	0	3.221616	1.609044	0.629956
11	6	0	3.113883	-0.501012	-0.312268
12	6	0	2.296241	-1.728694	-0.676620
13	6	0	-3.228899	-0.576392	0.334111
14	6	0	-1.066085	5.242464	-1.944684
15	6	0	4.484226	-0.514193	-0.582225
16	6	0	-2.129741	0.813269	1.876136
17	6	0	5.244220	0.590359	-0.198433
18	6	0	-1.142058	-2.751645	-1.874415
19	6	0	4.604998	1.665511	0.409867
20	6	0	-4.546426	0.875047	1.698237
21	6	0	-4.474724	-0.084310	0.686921
22	6	0	-3.368524	1.328896	2.277111
23	6	0	-1.665215	-0.375430	-2.381155
24	6	0	0.895800	-0.352724	-2.185033
25	6	0	0.399164	-2.761061	-1.787918
26	6	0	-0.322144	-0.334877	-3.107601
27	6	0	-3.031779	-1.622927	-0.724438
28	1	0	2.826583	-2.272900	-1.467237
29	1	0	2.215756	-2.405577	0.178546
30	1	0	-1.218867	5.881433	-1.070526
31	1	0	-1.905271	5.379781	-2.632340
32	1	0	-0.144354	5.547089	-2.448142
33	1	0	4.947132	-1.361004	-1.079288
34	1	0	6.312900	0.616172	-0.386765
35	1	0	-1.504686	-2.901542	-2.896311
36	1	0	-1.546480	-3.558752	-1.262507
37	1	0	5.163605	2.547568	0.704513
38	1	0	-5.505008	1.278555	2.008372
39	1	0	-5.365550	-0.438011	0.179321
40	1	0	-3.388879	2.102450	3.036769
41	1	0	-1.864747	0.574905	-1.882075
42	1	0	-2.472700	-0.581937	-3.094359
43	1	0	1.803297	-0.454574	-2.791944
44	1	0	0.973256	0.575304	-1.618660
45	1	0	-0.262375	-1.141463	-3.844804
46	1	0	-0.278868	0.595442	-3.682028
47	1	0	0.871263	-2.905384	-2.765889
48	1	0	0.723907	-3.582020	-1.145528
49	6	0	1.643550	-2.030053	3.967815
50	1	0	1.750807	-3.118621	3.994966
51	1	0	2.634016	-1.568963	4.028579
52	1	0	1.045378	-1.711865	4.826957
53	1	0	-3.808165	-1.575890	-1.495608
54	1	0	-3.079379	-2.617594	-0.269342
55	6	0	2.487537	2.759150	1.269564
56	1	0	1.567684	2.978782	0.719920
57	1	0	2.210628	2.517202	2.302542
58	1	0	3.104387	3.659786	1.297517
59	6	0	-0.863245	1.359503	2.471152
60	1	0	-0.590714	0.808927	3.378088
61	1	0	-0.029252	1.312013	1.771101
62	1	0	-1.015769	2.401510	2.760234

4_{hs}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.007245	-0.156156	0.356816
2	7	0	-1.592728	-1.199687	-0.146226
3	6	0	-1.246656	1.903728	-1.134609
4	7	0	-1.356675	1.434218	0.287158
5	7	0	1.126306	1.284591	-0.633428
6	7	0	1.747233	-1.070481	0.565189
7	6	0	2.685650	-0.520912	-0.220450
8	6	0	-5.218370	-0.997800	-0.037046
9	7	0	-3.793949	-1.324523	-0.194468
10	6	0	-2.737341	-0.531585	0.066489
11	6	0	-2.715296	0.887361	0.563717
12	6	0	-1.938210	-2.474452	-0.556463
13	6	0	2.353729	-2.100348	1.259443
14	6	0	-3.300194	-2.561450	-0.586160
15	6	0	0.326347	3.209210	0.839355
16	6	0	0.221718	1.859065	-1.665637
17	6	0	1.489455	2.298215	0.426619
18	6	0	-0.968514	2.505264	1.259895
19	7	0	3.863108	-1.155405	-0.053246
20	6	0	2.346368	0.606404	-1.159524
21	6	0	3.663958	-2.162537	0.879540
22	6	0	5.126984	-0.900051	-0.758484
23	1	0	-1.669025	2.910569	-1.225080
24	1	0	-1.859104	1.235697	-1.742123
25	1	0	-5.560442	-1.266441	0.965233
26	1	0	-5.790095	-1.556545	-0.778170
27	1	0	-5.375672	0.067914	-0.206158
28	1	0	-2.882729	0.916023	1.646732
29	1	0	-3.496206	1.504500	0.101897
30	1	0	-1.199545	-3.221065	-0.803665
31	1	0	1.822082	-2.705875	1.977266
32	1	0	-3.957831	-3.375934	-0.849323
33	1	0	0.115672	3.923145	0.037839
34	1	0	0.669631	3.817159	1.682557
35	1	0	0.563480	2.852613	-1.974878
36	1	0	0.265071	1.213077	-2.544547
37	1	0	2.301826	2.927218	0.041030
38	1	0	1.886991	1.748455	1.286902
39	1	0	-1.772008	3.249281	1.336780
40	1	0	-0.863312	2.031712	2.242096
41	1	0	3.177710	1.312477	-1.272915
42	1	0	2.121294	0.209700	-2.155810
43	1	0	4.465635	-2.816563	1.187071
44	1	0	5.954122	-1.172796	-0.103080
45	1	0	5.210837	0.159845	-1.001000
46	1	0	5.177933	-1.493475	-1.674456

4_{ls}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.000019	0.016260	-0.103569
2	7	0	-1.493190	-1.148089	0.011239
3	6	0	-0.775917	2.450678	-1.190964
4	7	0	-1.294777	1.470565	-0.175959
5	7	0	1.294785	1.470501	-0.176221
6	7	0	1.493140	-1.148106	0.011374
7	6	0	2.657817	-0.511293	-0.168628
8	6	0	-5.119656	-1.072743	-0.209329
9	7	0	-3.690561	-1.366296	-0.033169
10	6	0	-2.657878	-0.511212	-0.168450
11	6	0	-2.660374	0.940778	-0.521554
12	6	0	-1.798203	-2.469413	0.271935
13	6	0	1.798173	-2.469330	0.272544

14	6	0	-3.156432	-2.613383	0.242042
15	6	0	0.000230	2.813163	1.537595
16	6	0	0.775766	2.450638	-1.191124
17	6	0	1.298772	2.068457	1.213805
18	6	0	-1.298406	2.068500	1.214084
19	7	0	3.690510	-1.366330	-0.033129
20	6	0	2.660255	0.940600	-0.522131
21	6	0	3.156401	-2.613315	0.242583
22	6	0	5.119591	-1.072847	-0.209512
23	1	0	-1.189886	3.446258	-0.999632
24	1	0	-1.130837	2.128781	-2.170660
25	1	0	-5.696936	-1.777206	0.389298
26	1	0	-5.402450	-1.172198	-1.260064
27	1	0	-5.336996	-0.062039	0.138873
28	1	0	-3.439009	1.505586	0.002558
29	1	0	-2.830283	1.075254	-1.594773
30	1	0	-1.051407	-3.218344	0.471154
31	1	0	1.051399	-3.218169	0.472196
32	1	0	-3.782397	-3.479075	0.395249
33	1	0	0.000191	3.785000	1.035673
34	1	0	0.000345	3.040236	2.608440
35	1	0	1.189825	3.446196	-0.999881
36	1	0	1.130467	2.128718	-2.170892
37	1	0	2.136875	2.771865	1.287141
38	1	0	1.483760	1.250472	1.915714
39	1	0	-2.136467	2.771936	1.287629
40	1	0	-1.483265	1.250508	1.916021
41	1	0	3.439084	1.505528	0.001563
42	1	0	2.829792	1.074781	-1.595446
43	1	0	3.782377	-3.478951	0.396060
44	1	0	5.696918	-1.777122	0.389291
45	1	0	5.336972	-0.062032	0.138341
46	1	0	5.402290	-1.172646	-1.260240

5_{hs}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	*28*	*0*	*-0.122968*	*0.409929*	*-0.011387*
2	*7*	*0*	*0.171142*	*1.163724*	*1.977561*
3	*7*	*0*	*-0.445448*	*-0.399660*	*-1.996403*
4	*7*	*0*	*-1.762214*	*1.796886*	*-0.112445*
5	*7*	*0*	*1.332153*	*1.702382*	*-1.026421*
6	*7*	*0*	*1.655854*	*-0.732215*	*0.300934*
7	*6*	*0*	*-3.200325*	*-3.325738*	*0.661318*
8	*1*	*0*	*-3.891268*	*-4.158642*	*0.744621*
9	*7*	*0*	*-1.431160*	*-1.188613*	*0.436129*
10	*6*	*0*	*-1.561503*	*-2.074748*	*-0.577044*
11	*6*	*0*	*-1.623667*	*0.153028*	*-2.713379*
12	*1*	*0*	*-1.708186*	*-0.291040*	*-3.713141*
13	*1*	*0*	*-1.540466*	*1.234499*	*-2.812489*
14	*6*	*0*	*-2.171317*	*-1.352850*	*1.547588*
15	*1*	*0*	*-2.033625*	*-0.610187*	*2.326656*
16	*6*	*0*	*-2.441672*	*-3.152556*	*-0.496974*
17	*1*	*0*	*-2.531259*	*-3.842956*	*-1.329433*
18	*6*	*0*	*2.942394*	*-2.654547*	*0.952408*
19	*1*	*0*	*2.955872*	*-3.658429*	*1.361972*
20	*6*	*0*	*4.040491*	*-0.718404*	*0.048134*
21	*1*	*0*	*4.935276*	*-0.187499*	*-0.260907*
22	*6*	*0*	*2.792541*	*-0.101207*	*-0.054193*
23	*6*	*0*	*-0.656823*	*-1.851802*	*-1.773517*
24	*1*	*0*	*0.314770*	*-2.316208*	*-1.577084*
25	*1*	*0*	*-1.071281*	*-2.339009*	*-2.665012*
26	*6*	*0*	*1.736103*	*-1.980435*	*0.803156*
27	*1*	*0*	*0.797798*	*-2.441498*	*1.091801*
28	*6*	*0*	*0.813151*	*-0.094030*	*-2.726870*
29	*1*	*0*	*1.587511*	*-0.779871*	*-2.379083*
30	*6*	*0*	*1.225908*	*1.357967*	*-2.481372*
31	*1*	*0*	*0.695958*	*-0.256358*	*-3.806750*
32	*6*	*0*	*-3.063354*	*-2.408669*	*1.704125*

33	1	0	-3.637279	-2.504272	2.619092
34	6	0	2.665065	1.346211	-0.471186
35	1	0	2.817211	1.956597	0.426153
36	1	0	3.465958	1.617637	-1.171506
37	6	0	4.118015	-2.013449	0.557115
38	1	0	5.077880	-2.512314	0.645730
39	6	0	1.122293	3.164651	-0.852014
40	1	0	1.148561	3.410862	0.210879
41	1	0	1.894797	3.745098	-1.371755
42	1	0	0.483531	2.028742	-2.918741
43	1	0	2.173703	1.563335	-2.995542
44	6	0	-2.671076	2.510655	-0.042347
45	6	0	0.372076	1.509965	3.064173
46	6	0	-3.814696	3.409972	0.038188
47	1	0	-4.260987	3.535612	-0.952694
48	1	0	-4.566471	2.996379	0.716664
49	1	0	-3.495524	4.387317	0.411666
50	6	0	0.626298	1.943909	4.431921
51	1	0	1.107642	2.926241	4.428241
52	1	0	-0.315988	2.012522	4.983163
53	1	0	1.282230	1.226773	4.933930
54	1	0	-2.530672	-0.068145	-2.149434
55	1	0	0.145726	3.441729	-1.249035

5ls

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.177396	-0.129529	0.031775
2	7	0	0.483868	-0.719374	1.826737
3	7	0	0.042777	0.463701	-1.816757
4	7	0	3.458739	-1.226576	-0.370237
5	7	0	-0.514381	-1.914506	-0.561293
6	7	0	-2.370112	0.109422	0.433421
7	6	0	1.436964	4.391579	0.500998
8	1	0	1.691648	5.446575	0.567713
9	7	0	0.780233	1.687066	0.348589
10	6	0	0.406362	2.543967	-0.636045
11	6	0	1.372956	0.362663	-2.500083
12	1	0	1.250824	0.636347	-3.557931
13	1	0	1.749893	-0.654214	-2.428770
14	6	0	1.478966	2.167027	1.398054
15	1	0	1.769111	1.437000	2.146126
16	6	0	0.717467	3.897556	-0.591846
17	1	0	0.402297	4.548027	-1.404156
18	6	0	-4.649184	0.914299	0.490310
19	1	0	-5.300776	1.752611	0.624691
20	6	0	-4.192385	-1.411911	0.035981
21	1	0	-4.525849	-2.416366	-0.174887
22	6	0	-2.826941	-1.126986	0.178871
23	6	0	-0.371539	1.895140	-1.746383
24	1	0	-1.442595	1.930594	-1.515898
25	1	0	-0.220637	2.410568	-2.698358
26	6	0	-3.258576	1.096588	0.583807
27	1	0	-2.855518	2.077741	0.792320
28	6	0	-0.985714	-0.398206	-2.477202
29	1	0	-1.972819	-0.069047	-2.155937
30	6	0	-0.724291	-1.833063	-2.057642
31	1	0	-0.918667	-0.298412	-3.566977
32	6	0	1.827330	3.503868	1.506022
33	1	0	2.397023	3.844387	2.366202
34	6	0	-1.803205	-2.237664	0.149118
35	1	0	-1.528042	-2.484750	1.180087
36	1	0	-2.222170	-3.146456	-0.295199
37	6	0	-5.105659	-0.375321	0.194776
38	1	0	-6.169091	-0.558686	0.100273
39	6	0	0.453514	-3.026310	-0.283392
40	1	0	0.545275	-3.167114	0.791438
41	1	0	0.110236	-3.954843	-0.752402
42	1	0	0.180992	-2.208545	-2.538488
43	1	0	-1.550854	-2.485244	-2.368216

44	6	0	4.561420	-1.590339	-0.456214
45	6	0	0.671442	-1.054443	2.911645
46	6	0	5.943704	-2.038478	-0.564543
47	1	0	6.256226	-2.038888	-1.611355
48	1	0	6.602742	-1.367746	-0.006400
49	1	0	6.050653	-3.051251	-0.166228
50	6	0	0.905247	-1.485579	4.286597
51	1	0	1.248682	-2.525145	4.302122
52	1	0	1.669641	-0.853530	4.746868
53	1	0	-0.022214	-1.401302	4.862711
54	1	0	2.084630	1.022838	-2.005569
55	1	0	1.437146	-2.762809	-0.683692

6_{hs}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.029577	-0.081788	-0.154466
2	8	0	-0.188358	-0.179063	-2.342292
3	1	0	-0.138729	0.787650	-2.453771
4	1	0	-1.036907	-0.443841	-2.723431
5	8	0	0.227050	2.074435	-0.921233
6	1	0	-0.253363	2.932413	-0.768363
7	1	0	1.159418	2.299468	-1.040503
8	7	0	-2.132566	0.151900	-0.204075
9	7	0	-0.123206	-2.216852	0.327778
10	7	0	0.350710	0.149641	2.010766
11	7	0	2.173512	0.027332	-0.570473
12	6	0	-2.670681	1.373150	0.012387
13	1	0	-1.992624	2.155200	0.327703
14	6	0	-4.019472	1.659750	-0.155370
15	1	0	-4.386129	2.660906	0.041752
16	6	0	-4.869982	0.638323	-0.574426
17	1	0	-5.931211	0.816475	-0.716370
18	6	0	-4.326911	-0.623233	-0.802619
19	1	0	-4.958759	-1.444636	-1.123394
20	6	0	-2.959237	-0.845490	-0.612308
21	6	0	-2.384585	-2.225791	-0.837520
22	1	0	-3.214528	-2.923094	-0.977889
23	1	0	-1.808630	-2.271441	-1.770355
24	6	0	-1.531703	-2.727988	0.329230
25	1	0	-1.499303	-3.824601	0.319148
26	1	0	-2.012319	-2.434714	1.264355
27	6	0	0.687921	-3.080211	-0.573301
28	1	0	0.656145	-4.124726	-0.239989
29	1	0	1.724243	-2.745318	-0.574040
30	1	0	0.301318	-3.028862	-1.592408
31	6	0	0.422143	-2.317406	1.713846
32	1	0	1.512349	-2.310563	1.643581
33	1	0	0.140342	-3.275986	2.169154
34	6	0	-0.069169	-1.165856	2.579723
35	1	0	-1.159750	-1.167866	2.642788
36	1	0	0.307488	-1.279325	3.604877
37	6	0	-0.484634	1.222863	2.612160
38	1	0	-0.364809	1.244342	3.702443
39	1	0	-1.534764	1.050235	2.380603
40	1	0	-0.187919	2.194057	2.211769
41	6	0	1.779802	0.401064	2.387670
42	1	0	1.802258	0.772130	3.419811
43	1	0	2.317387	-0.548862	2.382800
44	6	0	2.505901	1.382953	1.464579
45	1	0	3.346816	1.814516	2.013414
46	1	0	1.844644	2.221756	1.216013
47	6	0	3.035861	0.732654	0.208063
48	6	0	4.388205	0.848587	-0.126255
49	1	0	5.048990	1.415709	0.520674
50	6	0	4.878906	0.236553	-1.277417
51	1	0	5.928387	0.319344	-1.541792
52	6	0	3.991927	-0.480404	-2.078273
53	1	0	4.317135	-0.972026	-2.988370

54	6	0	2.659466	-0.555272	-1.691903
55	1	0	1.938783	-1.081345	-2.303634
56	8	0	-1.097818	4.354083	-0.483201
57	1	0	-1.549132	4.780933	-1.224733
58	1	0	-0.753684	5.076882	0.059473

6_{ls}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.009535	0.015233	0.015193
2	8	0	0.094046	1.334897	-1.422423
3	1	0	0.712607	2.138972	-1.209242
4	1	0	-0.768467	1.697221	-1.665585
5	8	0	1.607020	3.265068	-0.830557
6	1	0	1.193944	4.132856	-0.574029
7	1	0	2.334063	3.465887	-1.433786
8	7	0	-1.931978	0.449886	0.035284
9	7	0	-0.523339	-2.394518	-0.903976
10	7	0	-0.038371	-1.078509	1.793667
11	7	0	1.925315	-0.139778	-0.217056
12	6	0	-2.294032	1.476813	0.845502
13	1	0	-1.505803	1.908555	1.451532
14	6	0	-3.585472	1.973377	0.916639
15	1	0	-3.812004	2.795050	1.586640
16	6	0	-4.563229	1.388581	0.110636
17	1	0	-5.591386	1.735221	0.141094
18	6	0	-4.188462	0.365444	-0.753484
19	1	0	-4.918792	-0.086528	-1.415554
20	6	0	-2.862533	-0.086769	-0.803366
21	6	0	-2.476907	-1.130726	-1.826773
22	1	0	-3.361457	-1.331278	-2.436795
23	1	0	-1.723189	-0.720186	-2.509932
24	6	0	-1.958273	-2.460307	-1.254402
25	1	0	-2.133372	-3.255650	-1.991791
26	1	0	-2.548833	-2.730181	-0.374913
27	6	0	0.288886	-2.877445	-2.035712
28	1	0	0.088436	-3.934176	-2.267493
29	1	0	1.351800	-2.771424	-1.808577
30	1	0	0.067385	-2.289253	-2.930785
31	6	0	-0.216828	-3.148499	0.319911
32	1	0	0.863949	-3.313029	0.355936
33	1	0	-0.676672	-4.149967	0.320406
34	6	0	-0.692050	-2.414834	1.568942
35	1	0	-1.768076	-2.235292	1.514627
36	1	0	-0.518975	-3.041138	2.453316
37	6	0	-0.817988	-0.390393	2.869931
38	1	0	-0.809407	-1.001432	3.779229
39	1	0	-1.851018	-0.252378	2.561411
40	1	0	-0.374375	0.578874	3.102823
41	6	0	1.342703	-1.299165	2.345332
42	1	0	1.244953	-1.574663	3.401173
43	1	0	1.792844	-2.149366	1.831024
44	6	0	2.259677	-0.081884	2.194681
45	1	0	3.081500	-0.164942	2.910077
46	1	0	1.730008	0.847136	2.438354
47	6	0	2.814464	-0.036633	0.799174
48	6	0	4.187328	0.011980	0.551866
49	1	0	4.872716	0.098589	1.387964
50	6	0	4.661536	-0.066254	-0.754853
51	1	0	5.727613	-0.035776	-0.956803
52	6	0	3.740549	-0.199869	-1.794268
53	1	0	4.057136	-0.283419	-2.827922
54	6	0	2.387719	-0.223814	-1.487355
55	1	0	1.640042	-0.297707	-2.264743
56	8	0	0.397115	5.517078	-0.087701
57	1	0	0.119186	6.175993	-0.738348

58	1	0	0.781253	6.023382	0.640896

5a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.083778	0.037751	0.365077
2	8	0	-0.088145	1.341409	2.029949
3	7	0	0.795630	-1.697850	-0.769010
4	8	0	0.506907	2.061087	-0.720056
5	7	0	-1.204401	-1.573740	1.160940
6	7	0	-1.848138	0.464955	-0.492419
7	6	0	4.871560	0.701327	-0.636037
8	1	0	5.883569	0.888626	-0.980866
9	7	0	2.279233	0.208187	0.245378
10	6	0	2.676623	-0.215026	-0.979323
11	6	0	1.638106	-2.747843	-0.125684
12	1	0	2.003774	-3.444362	-0.890679
13	1	0	1.067275	-3.319427	0.600609
14	6	0	3.156465	0.856884	1.031623
15	1	0	2.786758	1.169746	2.003191
16	6	0	3.965011	0.019052	-1.451740
17	1	0	4.259162	-0.338443	-2.433397
18	6	0	-3.392913	1.412994	-2.072601
19	1	0	-3.544554	2.001984	-2.970449
20	6	0	-4.208260	0.086044	-0.245046
21	1	0	-5.015935	-0.380351	0.309835
22	6	0	-2.888357	-0.089458	0.166342
23	6	0	1.626596	-0.993682	-1.767352
24	1	0	0.991589	-0.316480	-2.351327
25	1	0	2.111791	-1.682389	-2.471769
26	6	0	-2.102967	1.196081	-1.598994
27	1	0	-1.240111	1.615074	-2.101896
28	6	0	-0.486855	-2.284042	-1.200263
29	1	0	-1.003537	-1.563735	-1.836343
30	6	0	-1.319259	-2.613955	0.062202
31	1	0	-0.347608	-3.204293	-1.784224
32	6	0	4.464700	1.120130	0.631399
33	1	0	5.144695	1.635074	1.300971
34	6	0	-2.517321	-0.910472	1.373790
35	1	0	-2.431807	-0.260299	2.251920
36	1	0	-3.299126	-1.647457	1.598426
37	6	0	-4.467458	0.854000	-1.380138
38	1	0	-5.486425	1.000595	-1.724195
39	6	0	-0.771803	-2.187278	2.445239
40	1	0	-0.722151	-1.417100	3.218614
41	1	0	-1.474009	-2.961419	2.777975
42	1	0	-1.010753	-3.576303	0.474349
43	1	0	-2.366797	-2.730969	-0.228402
44	1	0	2.490913	-2.304759	0.385168
45	1	0	0.218133	-2.629348	2.342225
46	1	0	-0.330294	1.093246	2.930708
47	1	0	-0.387826	2.264886	1.870159
48	1	0	0.071671	2.814039	-0.272193
49	1	0	1.443519	2.292894	-0.771803
50	8	0	-0.674654	3.859689	1.129191
51	1	0	-1.574220	4.201206	1.017806
52	1	0	-0.155841	4.605873	1.466044

6a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.000020	-0.127320	-0.000009
2	7	0	-0.390356	1.504801	-1.420057
3	7	0	-2.152464	0.093460	0.422497
4	7	0	-0.415842	-1.797423	-1.413682
5	7	0	0.415847	-1.797566	1.413518
6	7	0	2.152464	0.093507	-0.422484
7	6	0	-2.538405	0.636107	1.598118
8	1	0	-1.752071	0.819338	2.317962
9	6	0	-3.853038	0.960459	1.906094
10	1	0	-4.092717	1.386283	2.874125
11	6	0	-4.836676	0.721066	0.948297
12	1	0	-5.877969	0.956021	1.144885
13	6	0	-4.452444	0.164205	-0.267650
14	1	0	-5.190176	-0.045243	-1.034941
15	6	0	-3.108752	-0.141665	-0.510112
16	6	0	-2.711428	-0.772080	-1.822932
17	1	0	-3.622497	-1.036258	-2.366396
18	1	0	-2.183412	-0.047753	-2.451667
19	6	0	-1.874725	-2.041396	-1.656038
20	1	0	-1.971957	-2.670066	-2.550254
21	1	0	-2.277593	-2.619013	-0.822354
22	6	0	0.249078	-1.617965	-2.730517
23	1	0	0.105893	-2.503085	-3.362996
24	1	0	1.317153	-1.460331	-2.587633
25	1	0	-0.172124	-0.752945	-3.245422
26	6	0	0.157894	-3.000862	-0.744417
27	1	0	1.237613	-2.992806	-0.910129
28	1	0	-0.226286	-3.918727	-1.209378
29	6	0	-0.157905	-3.000932	0.744139
30	1	0	-1.237624	-2.992878	0.909853
31	1	0	0.226263	-3.918848	1.209010
32	6	0	-0.249056	-1.618235	2.730377
33	1	0	-0.105876	-2.503421	3.362765
34	1	0	-1.317131	-1.460573	2.587520
35	1	0	0.172160	-0.753272	3.245367
36	6	0	1.874728	-2.041571	1.655831
37	1	0	1.971967	-2.670338	2.549978
38	1	0	2.277587	-2.619103	0.822082
39	6	0	2.711440	-0.772279	1.822849
40	1	0	3.622514	-1.036522	2.366273
41	1	0	2.183438	-0.048016	2.451671
42	6	0	3.108755	-0.141724	0.510093
43	6	0	4.452448	0.164166	0.267659
44	1	0	5.190184	-0.045372	1.034922
45	6	0	4.836677	0.721161	-0.948228
46	1	0	5.877971	0.956130	-1.144796
47	6	0	3.853035	0.960666	-1.905993
48	1	0	4.092711	1.386598	-2.873977
49	6	0	2.538402	0.636285	-1.598046
50	1	0	1.752066	0.819599	-2.317864
51	7	0	0.390346	1.504631	1.420193
52	6	0	-1.016520	3.659107	-2.765032
53	6	0	1.016551	3.658800	2.765376
54	1	0	1.875322	4.153406	2.302332
55	1	0	0.170003	4.351358	2.779948
56	1	0	1.273293	3.390924	3.794579
57	1	0	-1.272476	3.391421	-3.794480
58	1	0	-1.875795	4.153243	-2.302421
59	1	0	-0.170241	4.352010	-2.778851
60	6	0	-0.667517	2.461240	-2.011741
61	6	0	0.667522	2.461002	2.011980