Are Metal-Metal Interactions Involved in The Rising Enthalpies Observed in The Kubas Binding of H_2 to Hydrazine Linked Hydrogen Storage Materials?

Claire V. J. Skipper[a], David M. Antonelli[b]* and Nikolas Kaltsoyannis[a]*

[a] *Department of Chemistry, University College, London, 20 Gordon Street, London WC1H OAJ, United Kingdom.*

b Sustainable Environment Research Centre, University of Glamorgan, Pontypridd CF37 1DL, United Kingdom.

Supporting Information

Figure S1: Schematic representations of A-H dimers 1-8 where M= Ti^{2+}, V^{2+} or Cr^{2+}.

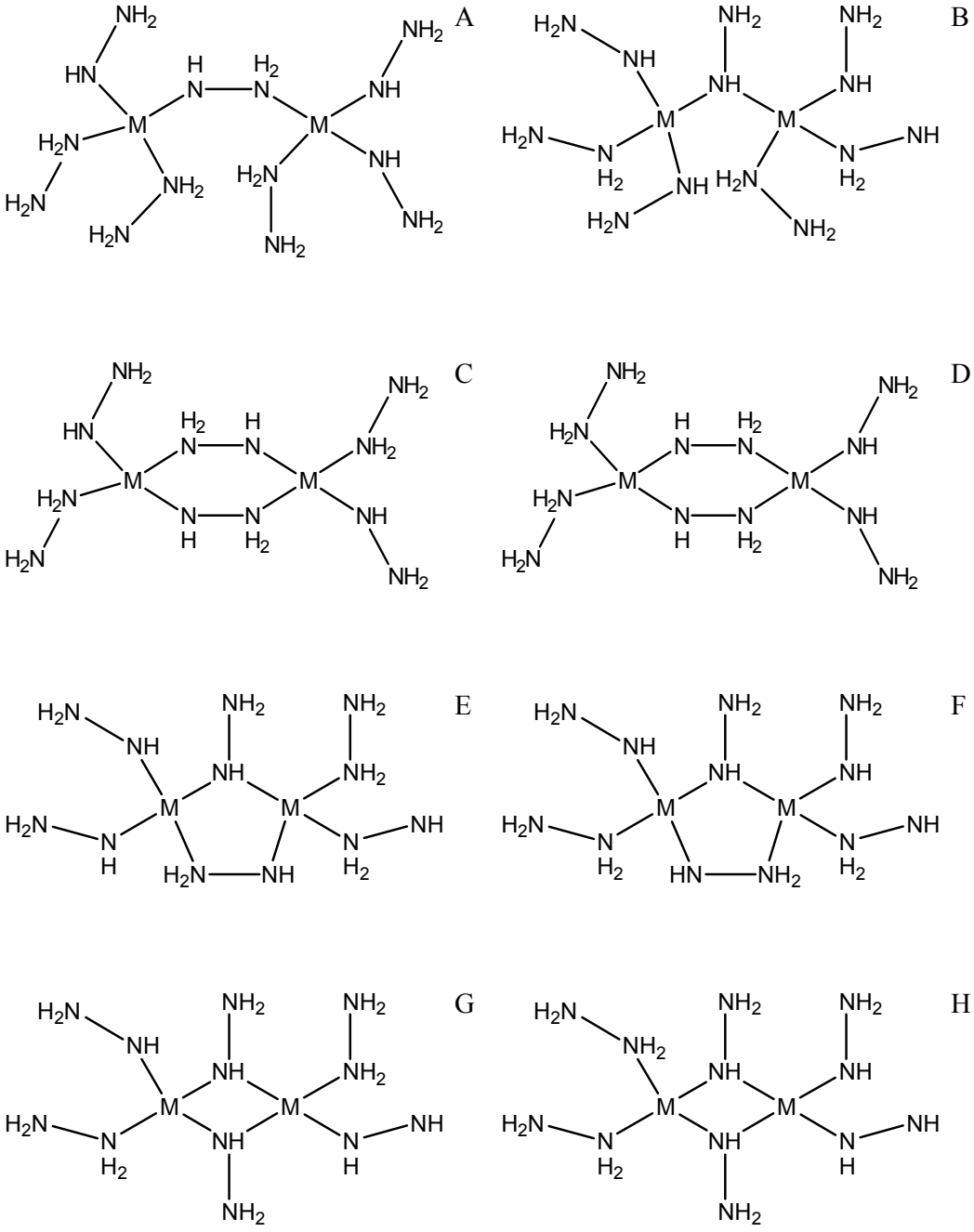


Figure S2: Schematic representations of A-E dimers 1, 2, 3, 6 and 7 with Ti^{2+} and a hydride ligand.

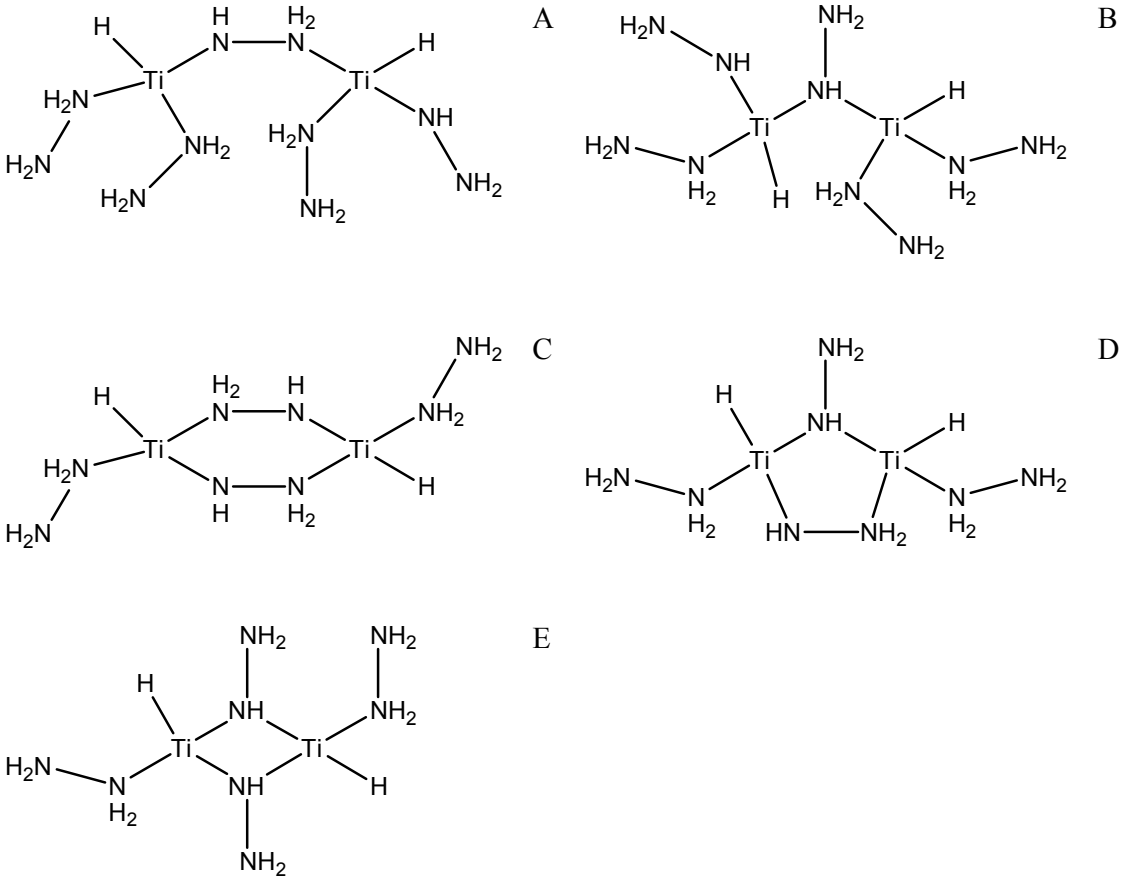
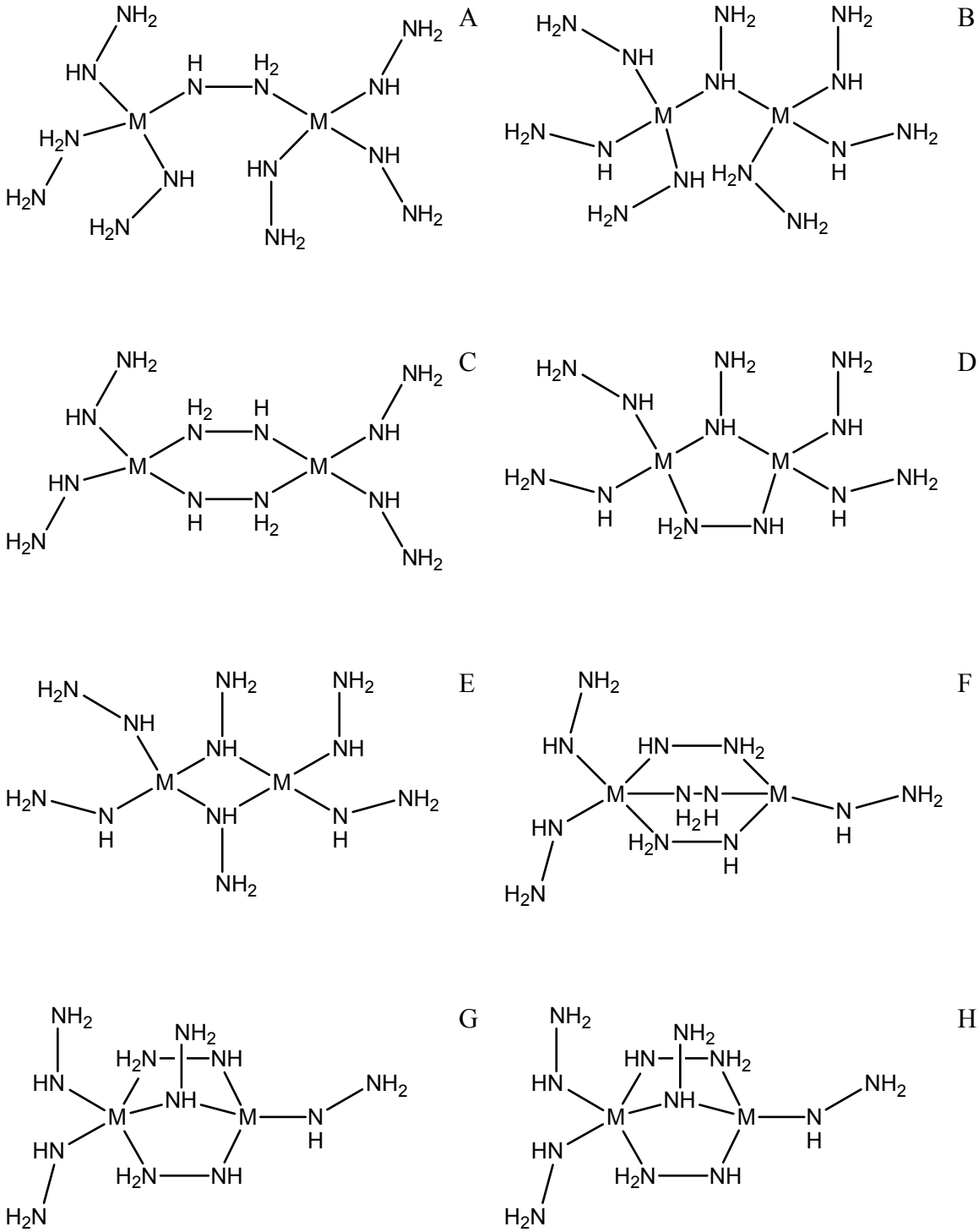
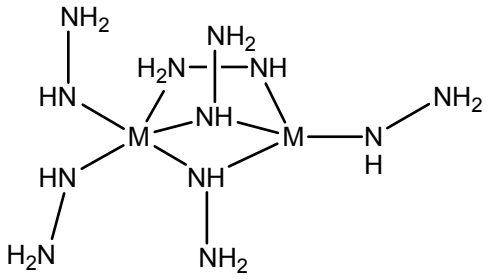
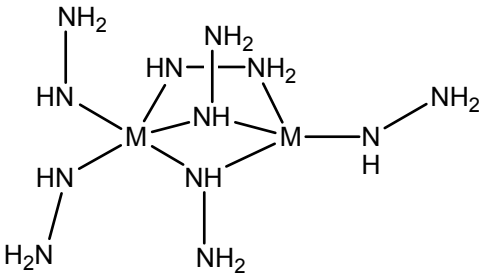


Figure S3: Schematic representations of A-K dimers 1, 2, 3, 6, 7, 9, 10,11, 12, 13 and 14 where M= Ti^{3+}, V^{3+} or Cr^{3+}

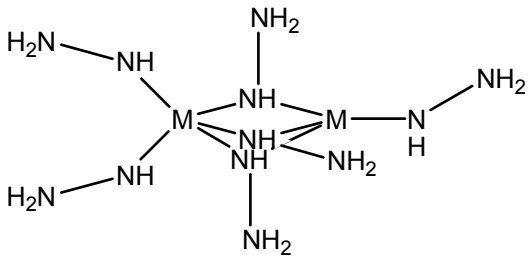



NH2
NH2
H2N
NH
HN
NH2
M
NH
M
N
H
HN
NH
H2N
NH2

I

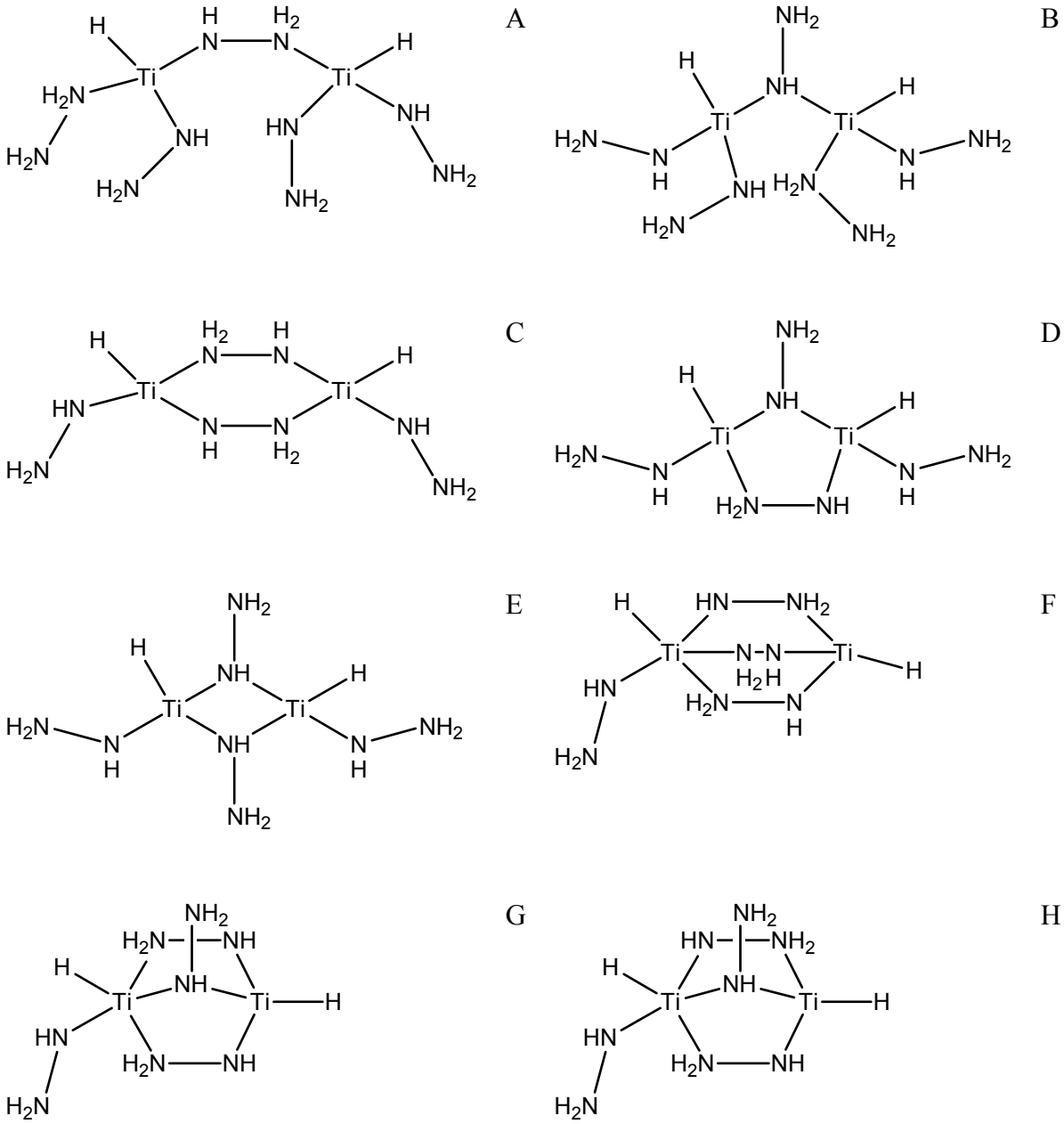

NH2
NH2
HN
NH2
HN
NH2
M
NH
M
N
H
HN
NH
H2N
NH2

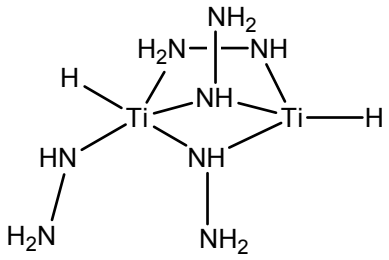
J


NH2
H2N
NH
NH2
M
NH
M
N
H
NH
NH
NH2
H2N
NH2

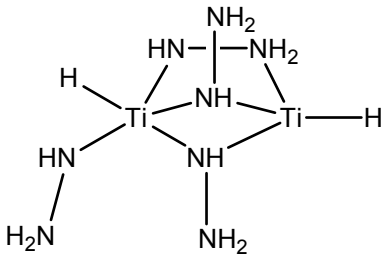
K

Figure S4: Schematic representations of A-K dimers 1, 2 , 3, 6, 7, 9, 10,11, 12, 13 and 14 with Ti^{3+} and a hydride ligand

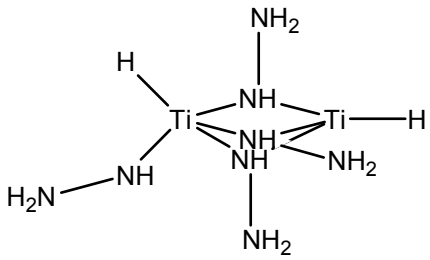



NH2
H2N
NH
H
Ti
NH
Ti
H
HN
NH
H2N
NH2

I


NH2
HN
NH2
H
Ti
NH
Ti
H
HN
NH
H2N
NH2

J


NH2
H
NH
Ti
Ti
H
NH
NH
NH2
NH
H2N
NH2

K

Table S1: Partial charges on the Ti(II) atoms in D2 with varying numbers of H_2 molecules bound. Numbers highlighted in red indicate that the Ti(II) has the greater number of H_2 molecules bound.

Number of H_2 bound	Mulliken		Hirshfeld		Voronoi		Gaussian Mulliken	
	Ti 1	Ti 2	Ti 1	Ti 2	Ti 1	Ti 2	Ti 1	Ti 2
0	0.805	0.746	0.262	0.187	0.093	0.089	0.219	0.686
1	1.035	0.756	0.244	0.183	0.092	0.051	0.223	0.734
2	0.852	0.875	0.247	0.227	0.067	0.071	-0.182	0.513
3	0.895	0.867	0.251	0.226	0.054	0.069	-0.399	0.454
4	0.729	0.864	0.229	0.241	0.036	0.052	-0.219	0.068

Table S2: Partial charges on the Ti(II) atoms in D7 with varying numbers of H_2 molecules bound. Numbers highlighted in red indicate that the Ti(II) has the greater number of H_2 molecules bound. /= calculation not computationally accessible

Number of H_2 bound	Mulliken		Hirshfeld		Voronoi		Gaussian Mulliken		Bader	
	Ti 1	Ti 2	Ti 1	Ti 2	Ti 1	Ti 2	Ti 1	Ti 2	Ti 1	Ti 2
0	1.022	0.690	0.246	0.134	0.146	0.034	0.810	0.644	1.495	1.238
1	0.970	0.843	0.253	0.192	0.149	0.058	0.853	0.162	1.493	1.384
2	/	/	/	/	/	/	0.566	0.160	1.475	1.37
3	0.969	0.961	0.250	0.259	0.084	0.079	0.361	-0.041	1.556	1.44
4	0.855	0.831	0.221	0.243	0.060	0.044	-0.148	0.147	1.491	1.462

Table S3: Partial charges on the V(II) atoms in D2 with varying numbers of H_2 molecules bound. Numbers highlighted in red indicate that the V(II) has the greater number of H_2 molecules bound.

Number of H_2 bound	Mulliken		Hirshfeld		Voronoi		Gaussian Mulliken		Bader	
	V 1	V 2	V 1	V 2	V 1	V 2	V 1	V 2	V 1	V 2
0	0.712	0.792	0.142	0.155	0.021	0.048	0.248	0.493	1.163	1.269
1	0.723	0.765	0.140	0.185	0.012	0.054	0.399	0.479	1.177	1.312
2	0.753	0.821	0.174	0.149	-0.012	-0.017	0.020	0.124	1.283	1.340
3	0.907	0.892	0.191	0.150	-0.025	-0.021	-0.348	0.048	1.340	1.346
4	0.805	0.848	0.193	0.186	-0.025	-0.015	-0.503	0.113	1.332	1.366

Table S4: Partial charges on the V(II) atoms in D5 with varying numbers of H_2 molecules bound. Numbers highlighted in red indicate that the V(II) has the greater number of H_2 molecules bound.

Number of H_2 bound	Mulliken		Hirshfeld		Voronoi		Gaussian Mulliken		Bader	
	V 1	V 2	V 1	V 2	V 1	V 2	V 1	V 2	V 1	V 2
0	0.531	1.098	0.064	0.232	-0.059	0.126	0.1361	0.549	0.991	1.507
1	-0.145	0.734	0.121	0.211	-0.041	0.097	0.748	0.991	1.177	1.434
2	0.713	0.959	0.124	0.222	-0.053	0.079	0.682	0.315	1.174	1.428
3	0.754	0.919	0.147	0.203	-0.043	0.044	0.754	0.919		
4	0.892	0.823	0.186	0.176	-0.020	0.006	0.020	-0.094		

Cartesian coordinates, SCF energies and spin data of optimised structures

Ti(III) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2477.220100 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.929559	-0.429668	-0.126186
2	7	0	-2.125546	-2.172378	0.691357
3	7	0	-3.559982	1.064203	-0.484054
4	7	0	-0.515686	-0.366796	-1.498392
5	7	0	-1.374904	0.846721	1.214662
6	7	0	0.626719	0.542791	-1.484149
7	1	0	-0.173030	-1.237670	-1.920158
8	1	0	0.916113	0.749117	-2.451418
9	1	0	0.316678	1.460823	-1.118060
10	7	0	-2.289730	-3.094223	-0.397207
11	1	0	-2.340679	-2.642838	1.570977
12	1	0	-3.093461	-2.879137	-0.997386
13	1	0	-1.437696	-3.199302	-0.952590
14	1	0	-0.438986	0.750612	1.655766
15	7	0	-2.137081	1.939607	1.782303
16	1	0	-3.222964	1.694422	-1.226244
17	7	0	-4.924056	0.638084	-0.702655
18	1	0	-3.491704	1.594499	0.413513
19	1	0	-5.478527	1.405751	-1.101506
20	1	0	-4.896465	-0.117437	-1.395968
21	1	0	-2.331489	1.748855	2.773286
22	1	0	-1.573989	2.799817	1.760402
23	22	0	2.265445	0.228870	-0.052563
24	7	0	1.577893	-0.083187	1.785356
25	1	0	2.008613	-0.139381	2.714131
26	7	0	1.407906	-1.385904	1.190767
27	1	0	2.138994	-2.076525	1.400866
28	1	0	0.455497	-1.759655	1.286413
29	7	0	2.792874	2.110077	-0.270053
30	1	0	3.682610	2.575937	-0.039125
31	7	0	1.761760	3.107340	-0.528797
32	1	0	1.621394	3.692152	0.306499
33	1	0	2.074360	3.748607	-1.271544
34	7	0	3.820848	-0.807052	-0.636893

35	1	0	4.581934	-0.500342	-1.258299
36	7	0	4.100044	-2.102163	-0.063004
37	1	0	4.143428	-2.816860	-0.800785
38	1	0	5.022459	-2.093716	0.389019

Ti (III) D2 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2477.237781 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.434788	-0.306464	0.347272
2	7	0	-2.777962	-1.294304	-0.707595
3	7	0	-2.091369	1.770033	0.167760
4	7	0	0.096250	-0.887440	-0.974339
5	7	0	-0.975228	-0.649405	2.169672
6	7	0	-0.001369	-0.615339	-2.420358
7	1	0	0.211187	-1.907008	-0.910482
8	1	0	-0.374776	0.339466	-2.495333
9	1	0	0.966325	-0.543199	-2.772799
10	7	0	-2.676279	-2.124053	-1.896633
11	1	0	-3.571066	-1.671715	-0.173858
12	1	0	-3.448532	-1.872661	-2.530397
13	1	0	-1.821120	-1.811796	-2.381212
14	1	0	-0.355355	-0.790775	2.973968
15	7	0	-2.390815	-0.657521	2.438700
16	1	0	-1.210624	2.367918	0.174299
17	7	0	-2.832724	2.032882	-1.071097
18	1	0	-2.687450	2.112268	0.931005
19	1	0	-2.161635	2.434012	-1.735973
20	1	0	-3.088269	1.100907	-1.429886
21	1	0	-2.748908	-1.567882	2.750686
22	1	0	-2.685212	0.061791	3.110547
23	22	0	1.498119	0.173420	0.140238
24	7	0	2.078058	-0.455918	1.924684
25	1	0	2.959007	-0.252699	2.409663
26	7	0	2.174030	-1.659526	1.147342
27	1	0	3.111966	-1.877719	0.775468
28	1	0	1.697174	-2.457722	1.572779
29	7	0	1.422583	2.160013	-0.039532
30	1	0	2.343523	2.618250	-0.103698
31	7	0	0.400032	3.168576	0.111863
32	1	0	0.545086	3.687392	0.990196
33	1	0	0.482737	3.866061	-0.641165
34	7	0	3.112414	0.110105	-1.018959
35	1	0	3.340986	0.776835	-1.768282
36	7	0	4.145893	-0.875418	-0.847249

37	1	0	4.271734	-1.424833	-1.707187
38	1	0	5.045338	-0.418703	-0.653376

Ti(III) D12 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2365.532809 Hartree/particle
Input spin multiplicity ($2S+1$) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.601031	0.064543	-0.112974
2	7	0	1.262911	-1.677759	-0.985115
3	7	0	0.302782	-0.379230	1.485241
4	7	0	0.220078	1.148867	-1.218598
5	7	0	-3.329044	1.788367	0.768371
6	7	0	0.742669	2.195744	-0.353264
7	1	0	0.099742	1.466799	-2.184395
8	1	0	1.202564	2.944244	-0.887827
9	1	0	-0.040776	2.581497	0.200859
10	7	0	-0.101226	-2.077558	-0.709769
11	1	0	1.830835	-2.485325	-1.264700
12	1	0	-0.505497	-2.616364	-1.490403
13	1	0	-0.117609	-2.637308	0.163530
14	1	0	-3.334034	2.817878	0.754256
15	7	0	-1.960646	1.338027	0.979466
16	1	0	-3.542750	1.504182	-0.198326
17	1	0	0.294232	0.324921	2.238570
18	7	0	0.389333	-1.712903	2.079277
19	1	0	1.304290	-1.823838	2.534355
20	1	0	-0.325107	-1.799890	2.813323
21	1	0	-1.797246	1.385790	1.990723
22	22	0	-1.137831	-0.079286	-0.139204
23	7	0	3.385602	0.258095	0.742208
24	1	0	3.996043	0.688718	1.441380
25	7	0	-2.684841	-0.354807	-1.380587
26	1	0	-3.075320	-0.689031	-2.266461
27	7	0	3.678440	0.708527	-0.595615
28	1	0	3.909564	1.706813	-0.673738
29	1	0	4.410178	0.160090	-1.060500
30	7	0	-2.995383	-1.235636	-0.279170
31	1	0	-3.848700	-0.969461	0.225808
32	1	0	-3.025531	-2.233496	-0.515665

Ti(III) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2365.541889 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.381347	-0.007963	0.045642
2	7	0	0.000190	-0.660726	1.533897
3	7	0	-2.578680	1.144029	1.113506
4	7	0	-0.052666	1.302448	-0.942956
5	7	0	-1.910463	-1.855951	-0.471695
6	7	0	-0.127124	2.718394	-0.557741
7	1	0	-0.069567	1.274693	-1.966384
8	1	0	-0.891648	2.786627	0.128122
9	1	0	0.723696	2.911746	-0.012586
10	7	0	0.075830	-2.086747	1.877498
11	1	0	-0.109550	-0.116908	2.400289
12	1	0	0.731655	-2.200145	2.661496
13	1	0	-0.844387	-2.388650	2.222871
14	1	0	-1.343235	-2.694462	-0.300797
15	7	0	-1.502864	-1.240759	-1.705571
16	7	0	-3.316351	1.098518	-0.114185
17	1	0	-3.122454	1.476855	1.913707
18	1	0	-3.466746	2.010858	-0.557841
19	1	0	-4.199896	0.577205	-0.071719
20	1	0	-0.543338	-1.503617	-2.012080
21	1	0	-2.211124	-1.298752	-2.440853
22	22	0	1.339282	0.097857	0.081519
23	7	0	2.564938	1.370249	0.943291
24	1	0	2.986193	2.061931	1.571604
25	7	0	1.377969	-1.288591	-1.493464
26	1	0	2.115733	-1.160190	-2.197474
27	7	0	3.327695	1.156621	-0.258912
28	1	0	3.422963	1.989014	-0.851941
29	1	0	4.258102	0.753408	-0.096999
30	7	0	2.012799	-1.888235	-0.324514
31	1	0	2.967387	-2.223208	-0.475228
32	1	0	1.422737	-2.618824	0.094170

Ti(III) D7 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2366.679741 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = S(S+1) = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.314457	-0.124162	-0.218015
2	7	0	-0.102357	-0.615815	1.478391
3	7	0	-2.543256	0.840349	1.019404
4	7	0	0.115692	1.119599	-1.175472
5	7	0	-1.682027	-2.026936	-0.653029
6	7	0	0.071561	2.581095	-1.082698
7	1	0	0.365332	0.903056	-2.145220
8	1	0	-0.902320	2.877490	-1.236085
9	1	0	0.261354	2.794938	-0.095849
10	7	0	-0.023879	-2.008797	1.931838
11	1	0	-0.379993	-0.022920	2.274564
12	1	0	0.491888	-2.032487	2.821308
13	1	0	-0.976741	-2.334071	2.142226
14	1	0	-1.166587	-2.836898	-0.290107
15	7	0	-1.060918	-1.546380	-1.854334
16	7	0	-3.819833	1.318202	0.554862
17	1	0	-2.458845	0.930663	2.042013
18	1	0	-3.968908	2.294345	0.839595
19	1	0	-4.585318	0.766180	0.961481
20	1	0	-0.053439	-1.786672	-1.949615
21	1	0	-1.611906	-1.736842	-2.695406
22	22	0	1.373815	0.129585	0.194615
23	7	0	2.229873	1.620097	1.134179
24	1	0	2.353954	2.464936	1.700527
25	7	0	1.790541	-1.356630	-1.209105
26	1	0	2.600682	-1.279804	-1.835137
27	7	0	3.059683	1.590082	-0.038988
28	1	0	2.911220	2.380989	-0.677224
29	1	0	4.060120	1.474571	0.155477
30	7	0	2.281625	-1.804125	0.088381
31	1	0	3.278046	-2.032395	0.120896
32	1	0	1.709902	-2.569069	0.469024
33	1	0	-2.454685	0.745470	-1.984524
34	1	0	-2.996566	0.904042	-1.457135

Ti(III) D7 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2367.802439 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = S(S+1) = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.468974	0.007333	-0.120785
2	7	0	0.172083	1.185678	-0.975414
3	7	0	-3.106407	-1.093639	-0.248993
4	7	0	-0.183473	-0.991930	1.179725
5	7	0	-2.544702	1.690256	0.067924
6	7	0	-0.401577	-2.416450	0.990789
7	1	0	-0.221713	-0.820770	2.188023
8	1	0	-1.409608	-2.619034	0.973491
9	1	0	0.026069	-2.661214	0.084862
10	7	0	0.247050	2.582696	-0.539803
11	1	0	0.330640	1.144666	-1.991438
12	1	0	1.245466	2.802639	-0.407537
13	1	0	-0.104134	3.199180	-1.284813
14	1	0	-2.284561	2.586548	-0.360339
15	7	0	-1.812137	1.561489	1.296162
16	7	0	-4.453360	-0.608757	-0.377787
17	1	0	-3.159255	-2.116842	-0.293157
18	1	0	-4.748490	-0.670302	-1.362829
19	1	0	-4.385314	0.396542	-0.166540
20	1	0	-1.015092	2.216008	1.343227
21	1	0	-2.401837	1.585579	2.132337
22	22	0	1.475951	-0.163068	0.038414
23	7	0	1.662298	-1.801299	-1.095186
24	1	0	1.897137	-2.135104	-2.034200
25	7	0	3.007879	1.063298	-0.287561
26	1	0	3.159588	1.634355	-1.124603
27	7	0	2.745301	-1.986910	-0.161643
28	1	0	2.699319	-2.882770	0.334587
29	1	0	3.678284	-1.852307	-0.566544
30	7	0	4.234281	1.110166	0.473342
31	1	0	4.378482	0.184721	0.892822
32	1	0	4.119250	1.755980	1.266957
33	1	0	1.737631	0.565795	2.004944
34	1	0	1.284459	1.151121	1.727383
35	1	0	-0.597468	-1.048186	-1.797698
36	1	0	-1.353009	-1.052646	-1.997644

Ti(III) D7 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2368.949456 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = $S(S+1)$ = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.324884	-0.170898	0.559550
2	7	0	-0.455922	0.450671	1.591545
3	7	0	2.768498	-1.534668	0.486226
4	7	0	0.276491	-0.455095	-1.217171
5	7	0	2.240558	1.380516	-0.208821
6	7	0	0.026663	-1.823507	-1.626960
7	1	0	0.714233	0.128773	-1.946160
8	1	0	-0.327609	-1.850790	-2.590508
9	1	0	0.909887	-2.348109	-1.593625
10	7	0	-0.522575	1.867534	1.899905
11	1	0	-0.785331	-0.102914	2.396902
12	1	0	-1.488877	2.108313	2.153013
13	1	0	0.075664	2.082445	2.706826
14	1	0	3.000254	1.883774	0.272020
15	7	0	1.858383	2.064896	-1.419658
16	7	0	3.956221	-1.475693	-0.336132
17	1	0	2.685266	-2.505274	0.801336
18	1	0	4.779800	-1.397917	0.279353
19	1	0	3.898487	-0.577530	-0.828713
20	1	0	1.484500	2.995106	-1.190536
21	1	0	2.684665	2.224276	-2.009459
22	22	0	-1.543278	-0.040319	-0.210665
23	7	0	-2.574972	-1.393379	0.744234
24	1	0	-2.539327	-1.641605	1.744050
25	7	0	-2.495507	1.607478	-0.472785
26	1	0	-3.435125	1.992445	-0.370029
27	7	0	-3.300054	-2.369123	-0.022316
28	1	0	-2.891548	-3.305520	0.090365
29	1	0	-4.278763	-2.415090	0.285939
30	7	0	-1.571190	2.654051	-0.827597
31	1	0	-1.112292	2.441681	-1.718837
32	1	0	-0.856262	2.722299	-0.085509
33	1	0	-2.719533	-1.101545	-1.823370
34	1	0	-2.416069	-0.500551	-2.208188
35	1	0	2.689773	0.089082	2.340676
36	1	0	2.332278	0.747884	2.513195

37	1	0	0.717054	-1.858430	1.789242
38	1	0	0.237395	-1.979805	1.183265

Ti(III) D7 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2370.088525 Hartreee/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = S(S+1) = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.698236	0.323762	-0.301879
2	7	0	-0.178955	1.778597	-0.884103
3	7	0	-3.241601	-0.785774	-0.798596
4	7	0	-0.081521	-1.042131	-0.289533
5	7	0	-1.828765	0.265453	1.645603
6	7	0	-0.080405	-1.947133	-1.425157
7	1	0	-0.113721	-1.543930	0.612182
8	1	0	0.763331	-2.534112	-1.382279
9	1	0	-0.905631	-2.557744	-1.364663
10	7	0	-0.223996	3.001593	-0.101623
11	1	0	-0.185159	2.006617	-1.889517
12	1	0	0.624782	3.553984	-0.278037
13	1	0	-1.015247	3.579636	-0.413278
14	1	0	-2.403822	0.910073	2.205454
15	7	0	-0.889535	-0.428975	2.493536
16	7	0	-4.054897	-1.583797	0.082721
17	1	0	-3.519029	-1.031147	-1.753356
18	1	0	-4.992292	-1.159156	0.142563
19	1	0	-3.636539	-1.462553	1.011992
20	1	0	-0.170136	0.234305	2.812706
21	1	0	-1.370190	-0.794947	3.323253
22	22	0	1.484121	0.389234	-0.429981
23	7	0	3.025566	-0.698123	-1.076624
24	1	0	3.315515	-0.802149	-2.057767
25	7	0	1.941599	0.552046	1.433897
26	1	0	2.252449	1.371761	1.963529
27	7	0	4.015983	-1.224596	-0.178777
28	1	0	4.251959	-2.187731	-0.444505
29	1	0	4.885024	-0.678165	-0.236231
30	7	0	2.232214	-0.612557	2.241869
31	1	0	2.942662	-1.148320	1.714317
32	1	0	1.375482	-1.181514	2.280364
33	1	0	0.989823	-0.252202	-2.655825
34	1	0	1.341219	0.430764	-2.749993
35	1	0	2.462943	2.124658	-1.067326
36	1	0	2.569722	2.178378	-0.288796

37	1	0	-1.880723	0.488847	-2.501222
38	1	0	-1.413368	-0.132306	-2.470123
39	1	0	-2.995822	1.972255	-0.595757
40	1	0	-2.912520	2.006561	0.180732

Ti(III) D14 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2365.525593 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = S(S+1) = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.045705	-0.298055	0.053377
2	7	0	-0.366500	0.107224	1.582512
3	7	0	2.720092	-1.359259	0.218498
4	7	0	-0.194623	1.104734	-1.013323
5	7	0	2.227719	1.325622	0.054007
6	7	0	-1.017353	0.699586	-2.120347
7	1	0	0.282609	2.016266	-1.124629
8	1	0	-1.462131	1.503113	-2.575351
9	1	0	-0.484977	0.163305	-2.823467
10	7	0	-0.264829	1.342378	2.365182
11	1	0	-0.441733	-0.640853	2.276328
12	1	0	0.577512	1.824516	2.030264
13	1	0	-1.058649	1.937546	2.099848
14	1	0	3.109512	1.261010	0.580740
15	7	0	2.043952	2.646188	-0.480640
16	7	0	4.040321	-1.147735	-0.325407
17	1	0	2.731911	-2.306375	0.607935
18	1	0	3.956904	-0.346398	-0.959525
19	1	0	4.663683	-0.829694	0.433087
20	1	0	2.082016	3.352137	0.266054
21	1	0	2.798559	2.874741	-1.138942
22	22	0	-1.697131	0.027496	-0.097766
23	7	0	-0.483132	-1.615869	-0.697698
24	1	0	-0.555975	-2.168589	-1.559503
25	7	0	-3.449679	0.326065	0.721576
26	1	0	-4.161194	0.378636	1.454205
27	7	0	0.143988	-2.379546	0.350080
28	1	0	-0.547265	-2.755185	1.010072
29	1	0	0.736461	-3.136061	-0.012784
30	7	0	-3.853214	-0.454368	-0.415769
31	1	0	-4.477965	0.036493	-1.064740
32	1	0	-4.245102	-1.377443	-0.193727

Ti(III) D11 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2365.518325 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = $S(S+1)$ = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.768128	0.420672	-0.059416
2	7	0	0.326611	-0.479970	-1.282425
3	7	0	3.587195	0.147053	-0.663285
4	7	0	0.953417	2.182545	-0.188203
5	7	0	1.364813	0.130003	2.093898
6	7	0	-0.468306	2.126220	0.049690
7	1	0	1.268935	3.146751	-0.350563
8	1	0	-0.730599	2.622027	0.913090
9	1	0	-1.057186	2.527553	-0.700931
10	7	0	0.509497	-1.879135	-1.693416
11	1	0	0.205989	0.046355	-2.156714
12	1	0	1.233835	-2.260037	-1.071268
13	1	0	-0.347367	-2.372636	-1.407793
14	1	0	1.435222	0.952426	2.710554
15	7	0	-0.012427	-0.296134	1.905300
16	1	0	1.924548	-0.619957	2.523199
17	1	0	4.392064	0.307106	-1.278313
18	7	0	3.461070	-1.229392	-0.245846
19	1	0	3.514816	-1.895705	-1.026356
20	1	0	4.159630	-1.498870	0.455946
21	1	0	-0.324964	-0.797976	2.748370
22	22	0	-1.135786	-0.078524	0.234575
23	7	0	-2.875652	0.757853	-0.262927
24	1	0	-3.754028	0.294462	0.012293
25	7	0	-1.939172	-1.849295	0.538947
26	1	0	-1.457157	-2.582555	1.072142
27	7	0	-3.149445	2.046208	-0.855662
28	1	0	-3.622265	1.920391	-1.759180
29	1	0	-3.793262	2.588720	-0.265332
30	7	0	-3.134310	-2.460269	0.005493
31	1	0	-3.890145	-2.394345	0.702794
32	1	0	-3.432632	-1.880789	-0.786394

Ti(III) D10 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2365.529824 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.815632	-0.349391	0.028888
2	7	0	-0.681054	1.150846	-0.822229
3	7	0	-3.563318	-0.921939	-0.622616
4	7	0	-0.277233	-1.597171	-0.483839
5	7	0	0.135043	0.284234	1.981241
6	7	0	0.716482	-1.366314	-1.521235
7	1	0	-0.083222	-2.515624	-0.069745
8	1	0	1.471591	-2.075301	-1.447089
9	1	0	0.292964	-1.337516	-2.454662
10	7	0	-0.950589	2.569695	-0.562153
11	1	0	-0.572997	1.088050	-1.843165
12	1	0	-1.811537	2.617477	-0.003247
13	1	0	-0.202795	2.904648	0.060147
14	1	0	0.353654	1.215384	2.361294
15	7	0	-1.296819	0.067541	1.892597
16	1	0	0.584336	-0.417415	2.584461
17	1	0	-4.200627	-1.275506	-1.339115
18	7	0	-3.989131	0.295660	0.001860
19	1	0	-4.330863	1.013964	-0.646538
20	1	0	-4.678085	0.155721	0.747868
21	1	0	-1.747954	0.238070	2.795674
22	22	0	1.153591	0.111267	-0.023086
23	7	0	2.628210	-1.086815	0.604401
24	1	0	3.334069	-0.917715	1.336784
25	7	0	2.206768	1.728002	-0.376273
26	1	0	1.815713	2.500116	-0.928586
27	7	0	2.830422	-2.422119	0.051595
28	1	0	3.789609	-2.512171	-0.309813
29	1	0	2.739226	-3.132795	0.789498
30	7	0	3.647723	1.910954	-0.414385
31	1	0	3.925774	2.431377	0.429535
32	1	0	4.040513	0.969935	-0.293703

V(III) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2666.260745 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0011 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.978819	-0.001592	-0.358158
2	7	0	-2.729120	-1.646047	-0.906684
3	7	0	-3.813735	1.119351	0.243223
4	7	0	-0.321099	0.325069	-1.252859
5	7	0	-1.410071	0.317921	1.438081
6	7	0	0.784070	1.072262	-0.690851
7	1	0	0.019572	-0.127527	-2.105824
8	1	0	1.083137	1.873831	-1.277722
9	1	0	0.408171	1.495035	0.170646
10	7	0	-4.074346	-1.971605	-1.324904
11	1	0	-2.244665	-2.536472	-0.756864
12	1	0	-4.734551	-1.499137	-0.694796
13	1	0	-4.228015	-1.589428	-2.264628
14	1	0	-0.465722	0.023482	1.766238
15	7	0	-2.314589	0.537880	2.547707
16	1	0	-3.643892	2.121866	0.083143
17	7	0	-5.164645	0.741415	-0.119664
18	1	0	-3.675399	0.956667	1.269230
19	1	0	-5.835905	1.424085	0.254124
20	1	0	-5.228014	0.785131	-1.140926
21	1	0	-2.382445	-0.315014	3.118042
22	1	0	-1.927329	1.265153	3.162166
23	23	0	2.583554	0.093629	0.049166
24	7	0	1.555031	-0.542889	1.640680
25	1	0	2.092256	-0.925739	2.429702
26	7	0	1.433547	-1.560955	0.630536
27	1	0	2.040736	-2.388731	0.726253
28	1	0	0.460822	-1.761076	0.380527
29	7	0	3.495297	1.778274	-0.284460
30	1	0	4.468177	1.969196	-0.007943
31	7	0	2.916415	2.935979	-0.926471
32	1	0	2.945061	3.747113	-0.294563
33	1	0	3.470128	3.193637	-1.752911
34	7	0	4.063418	-1.079686	-0.268268
35	1	0	4.893864	-0.794859	-0.803626
36	7	0	4.077663	-2.496492	0.002592

37	1	0	4.217252	-3.027153	-0.867467
38	1	0	4.873002	-2.720252	0.613396

V(III) D12 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.556020 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0016 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.671938	0.059147	0.152086
2	7	0	1.336641	-1.121593	-1.477800
3	7	0	0.335022	-0.991819	1.313143
4	7	0	0.306897	1.246111	-0.788694
5	7	0	-3.353576	1.196994	1.300961
6	7	0	0.131917	2.667252	-0.530086
7	1	0	0.505389	1.152246	-1.792733
8	1	0	-0.850430	2.894378	-0.742703
9	1	0	0.200257	2.771307	0.489277
10	7	0	-0.044112	-1.593661	-1.368286
11	1	0	1.935052	-1.957561	-1.550627
12	1	0	-0.410236	-1.827847	-2.301274
13	1	0	-0.081894	-2.433396	-0.759732
14	1	0	-3.454651	2.062793	1.845733
15	7	0	-1.996989	0.733369	1.361900
16	1	0	-3.506828	1.428477	0.306515
17	1	0	0.252391	-0.656096	2.284549
18	7	0	0.371576	-2.451066	1.311224
19	1	0	1.233462	-2.774175	1.767706
20	1	0	-0.413630	-2.807972	1.870829
21	1	0	-1.793045	0.533722	2.348784
22	23	0	-1.073590	-0.112401	-0.072981
23	7	0	3.393574	0.395015	0.951751
24	1	0	4.275555	0.065256	1.353544
25	7	0	-2.647198	0.310907	-1.316930
26	1	0	-2.521222	0.142634	-2.323404
27	7	0	3.547486	0.996759	-0.342671
28	1	0	3.728495	2.005195	-0.316652
29	1	0	4.200907	0.529496	-0.981544
30	7	0	-2.867619	-0.986855	-0.689395
31	1	0	-3.675900	-0.940189	-0.057319
32	1	0	-2.981010	-1.773331	-1.336186

V(III) D12 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2555.702078 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0014 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.651209	-0.383623	0.051411
2	7	0	1.067586	-1.629732	-1.416891
3	7	0	0.219094	-0.727160	1.455077
4	7	0	0.489165	0.972850	-0.866693
5	7	0	-3.267145	1.724535	1.047405
6	7	0	0.614012	2.399514	-0.638056
7	1	0	0.547155	0.824510	-1.881900
8	1	0	0.026956	2.616437	0.174042
9	1	0	1.605138	2.560741	-0.384182
10	7	0	-0.347646	-1.834407	-1.151532
11	1	0	1.503284	-2.545095	-1.588252
12	1	0	-0.837126	-2.119621	-2.012301
13	1	0	-0.479995	-2.565628	-0.431356
14	1	0	-3.268659	2.675344	1.437217
15	7	0	-1.963452	1.141230	1.191826
16	1	0	-3.398341	1.804813	0.025491
17	1	0	0.231248	-0.124260	2.291857
18	7	0	0.009288	-2.117185	1.838560
19	1	0	0.753605	-2.423201	2.480051
20	1	0	-0.875672	-2.187758	2.356030
21	1	0	-1.749760	1.122089	2.196212
22	23	0	-1.167780	-0.027335	-0.082692
23	7	0	3.400726	0.409849	0.295935
24	1	0	4.286398	-0.029709	0.577651
25	7	0	-2.679378	0.376676	-1.389436
26	1	0	-2.635179	0.079600	-2.372411
27	7	0	3.609391	1.765120	-0.141717
28	1	0	4.054656	2.311977	0.604729
29	1	0	4.238576	1.793367	-0.954554
30	7	0	-3.057455	-0.779496	-0.586302
31	1	0	-3.854778	-0.546530	0.018616
32	1	0	-3.267052	-1.634728	-1.111774
33	1	0	2.836306	-1.817807	1.184700
34	1	0	2.505079	-2.255088	0.642357

V(III) D12 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2556.848561 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.493707	-0.706449	-0.116679
2	7	0	-1.031613	-1.673528	1.545110
3	7	0	0.228703	-0.700425	-1.230748
4	7	0	-0.821885	0.939255	0.855712
5	7	0	1.765920	3.215499	-0.490365
6	7	0	-1.257360	2.275512	0.488220
7	1	0	-1.062953	0.819389	1.847369
8	1	0	-0.792441	2.463609	-0.408599
9	1	0	-2.271257	2.191996	0.284403
10	7	0	0.398007	-1.447263	1.578719
11	1	0	-1.225882	-2.663325	1.738617
12	1	0	0.765246	-1.456110	2.539768
13	1	0	0.912088	-2.154917	1.032169
14	1	0	1.091479	3.552535	0.208551
15	7	0	1.415292	1.858498	-0.828031
16	1	0	2.686226	3.215465	-0.032791
17	1	0	0.298490	-0.156755	-2.103134
18	7	0	0.749879	-2.046517	-1.404105
19	1	0	0.397444	-2.445819	-2.281487
20	1	0	1.787022	-1.981207	-1.440603
21	1	0	1.365846	1.807941	-1.851113
22	23	0	1.185578	0.366403	0.334145
23	7	0	-3.274115	-0.273126	-0.698636
24	1	0	-3.952186	-0.906757	-1.141439
25	7	0	2.925968	-0.538465	0.473398
26	1	0	3.667933	-0.264392	1.129343
27	7	0	-3.914001	0.942391	-0.267639
28	1	0	-4.338034	1.418491	-1.072850
29	1	0	-4.671889	0.737351	0.396059
30	7	0	3.477135	-1.301856	-0.614634
31	1	0	4.105919	-0.716175	-1.180871
32	1	0	4.036060	-2.088189	-0.260465
33	1	0	2.125340	1.388576	1.829295
34	1	0	1.373386	1.417718	2.030441
35	1	0	-1.698378	-2.723864	-0.792829
36	1	0	-2.146003	-2.384313	-1.320576

V(III) D12 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2557.991006 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0010 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.848762	-0.483767	-0.192438
2	7	0	1.115716	-1.913401	-1.313875
3	7	0	0.175687	-0.527926	1.007667
4	7	0	0.748033	0.768204	-1.377674
5	7	0	-2.529042	2.711114	0.019272
6	7	0	0.955880	2.205044	-1.423787
7	1	0	0.839188	0.433986	-2.344261
8	1	0	0.296631	2.577611	-0.722207
9	1	0	1.903533	2.398077	-1.074391
10	7	0	-0.330675	-1.919614	-1.300881
11	1	0	1.474581	-2.807314	-1.667199
12	1	0	-0.714796	-2.317671	-2.166698
13	1	0	-0.657822	-2.489620	-0.500626
14	1	0	-2.361458	3.159456	-0.888924
15	7	0	-1.431070	1.822088	0.308851
16	1	0	-3.383684	2.147087	-0.087529
17	1	0	0.327886	0.189098	1.739672
18	7	0	-0.163843	-1.815236	1.594035
19	1	0	0.442079	-1.986052	2.405312
20	1	0	-1.147258	-1.752499	1.920403
21	1	0	-1.098579	2.051683	1.251401
22	23	0	-1.147328	0.081375	-0.469103
23	7	0	2.728955	0.746425	1.046504
24	1	0	3.744615	0.886040	1.132669
25	7	0	-2.770721	-0.870017	0.043037
26	1	0	-3.609730	-0.945031	-0.547035
27	7	0	2.030070	1.559041	2.012423
28	1	0	2.552814	1.602279	2.894603
29	1	0	1.952343	2.524530	1.666057
30	7	0	-3.054667	-1.307252	1.385081
31	1	0	-3.605422	-0.593445	1.880782
32	1	0	-3.616627	-2.167210	1.374601
33	1	0	-2.407234	0.750440	-1.942380
34	1	0	-1.847097	0.384665	-2.343740
35	1	0	2.488199	-2.321540	0.807895
36	1	0	2.956596	-1.822784	1.161012

37	1	0	3.324553	-0.197071	-1.622747
38	1	0	3.693453	-0.658983	-1.115797

V(III) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.544004 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0029 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.574597	-0.084313	0.085605
2	7	0	-0.169941	-1.578116	-0.246954
3	7	0	-3.154225	-1.069911	-0.331200
4	7	0	-0.198763	0.567640	1.452626
5	7	0	-1.898459	1.751309	-0.401126
6	7	0	0.495393	-0.316468	2.366441
7	1	0	-0.273477	1.546504	1.767399
8	1	0	1.019777	0.198042	3.081647
9	1	0	-0.160363	-0.957365	2.828664
10	7	0	-0.155819	-2.254731	-1.540326
11	1	0	-0.164073	-2.333457	0.452052
12	1	0	-0.973854	-1.917319	-2.064455
13	1	0	0.665980	-1.911969	-2.050713
14	1	0	-2.311686	2.032646	-1.301192
15	7	0	-1.341695	2.888939	0.291591
16	7	0	-4.539030	-0.674069	-0.294152
17	1	0	-3.134000	-2.060504	-0.592255
18	1	0	-4.909744	-0.832716	0.653164
19	1	0	-4.551260	0.342217	-0.427726
20	1	0	-0.698405	3.407625	-0.319866
21	1	0	-2.097247	3.535167	0.548260
22	23	0	1.294181	-0.210953	0.295816
23	7	0	3.110495	-0.607508	0.757427
24	1	0	3.361621	-1.057618	1.647712
25	7	0	1.508852	0.826947	-1.244863
26	1	0	0.672844	1.248292	-1.672385
27	7	0	4.280637	-0.356862	-0.043354
28	1	0	4.985540	0.147076	0.509601
29	1	0	4.706610	-1.246158	-0.333655
30	7	0	2.659354	1.452135	-1.804073
31	1	0	3.469999	0.939225	-1.410858
32	1	0	2.663710	1.306284	-2.822328

V(III) D13 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.544669 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0010 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.283387	-0.013212	-0.295397
2	7	0	0.240249	-1.558124	-1.319429
3	7	0	0.047432	-0.520442	1.362845
4	7	0	-0.224157	1.024094	-1.358090
5	7	0	-4.415860	-0.258694	0.091593
6	7	0	-0.288695	2.468435	-1.386633
7	1	0	-0.262459	0.596448	-2.294152
8	1	0	0.520360	2.839604	-1.900026
9	1	0	-1.132125	2.768730	-1.887756
10	7	0	-1.111440	-1.690638	-0.781248
11	1	0	0.651674	-2.505071	-1.316704
12	1	0	-1.763606	-2.038444	-1.495528
13	1	0	-1.113343	-2.323525	0.041920
14	1	0	-4.465181	-0.369776	-0.926810
15	7	0	-3.227475	0.503524	0.415086
16	1	0	-4.316854	-1.200222	0.485808
17	1	0	0.411839	0.078793	2.126917
18	7	0	-0.072193	-1.901758	1.811079
19	1	0	0.863696	-2.248208	2.056066
20	1	0	-0.622854	-1.917805	2.678484
21	1	0	-3.560531	1.334321	0.920786
22	23	0	-1.369613	0.204520	0.101352
23	7	0	1.535982	1.614401	0.736432
24	1	0	1.014670	2.452916	0.450169
25	7	0	2.897501	-0.453520	-1.318776
26	1	0	2.898700	-1.131021	-2.090230
27	7	0	1.764802	1.663759	2.160650
28	1	0	2.764380	1.509702	2.333678
29	1	0	1.554789	2.599259	2.526358
30	7	0	3.077789	-1.147320	-0.060615
31	1	0	3.017755	-2.169833	-0.114003
32	1	0	3.954717	-0.881973	0.397800

V(III) D14 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.554139 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0015 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.084492	-0.143083	0.137759
2	7	0	-0.486633	-0.705809	1.457249
3	7	0	2.033853	-1.770932	0.408160
4	7	0	-0.220984	1.617074	0.107413
5	7	0	2.695329	0.895262	0.043672
6	7	0	-0.008712	2.405259	-1.083304
7	1	0	-0.181563	2.196210	0.958758
8	1	0	-0.661489	3.197169	-1.103936
9	1	0	0.962522	2.761266	-1.035334
10	7	0	-0.509767	-0.154387	2.810422
11	1	0	-0.563206	-1.723899	1.574055
12	1	0	0.336202	0.413428	2.935781
13	1	0	-1.309582	0.484038	2.887839
14	1	0	3.570531	0.493205	0.406614
15	7	0	2.847820	2.295635	-0.251853
16	7	0	3.282132	-2.172111	-0.169469
17	1	0	1.892501	-2.352003	1.242751
18	1	0	3.206673	-3.121020	-0.561853
19	1	0	3.457161	-1.537231	-0.955598
20	1	0	3.177630	2.797446	0.582834
21	1	0	3.574969	2.414615	-0.968419
22	23	0	-1.562810	0.130179	-0.046569
23	7	0	-0.261029	-0.509748	-1.435881
24	1	0	-0.024385	0.096051	-2.234386
25	7	0	-3.435241	0.480793	-0.075973
26	1	0	-3.938566	1.370509	-0.092711
27	7	0	-0.554705	-1.878079	-1.802632
28	1	0	-0.968242	-1.905206	-2.740770
29	1	0	0.316528	-2.421302	-1.821127
30	7	0	-4.418734	-0.578295	-0.133462
31	1	0	-4.273625	-1.148012	-0.973691
32	1	0	-4.316031	-1.191128	0.681422

V(III) D14 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2555.706909 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0020 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.536948	0.074251	-0.034446
2	7	0	0.256367	-1.066317	-1.162899
3	7	0	3.218499	-0.682927	-0.485932
4	7	0	0.254313	-0.467555	1.444401
5	7	0	0.442401	1.473587	-0.896340
6	7	0	0.284745	0.250270	2.701577
7	1	0	0.176984	-1.485658	1.598630
8	1	0	-0.633076	0.173880	3.155707
9	1	0	0.971043	-0.185460	3.329353
10	7	0	0.238727	-2.516406	-1.076249
11	1	0	0.284532	-0.852555	-2.166958
12	1	0	1.066521	-2.823798	-0.552829
13	1	0	-0.588715	-2.785838	-0.532500
14	1	0	0.247237	1.484944	-1.907559
15	7	0	0.474287	2.802824	-0.341098
16	7	0	4.585124	-0.415940	-0.099211
17	1	0	3.259472	-1.402532	-1.215934
18	1	0	4.813492	0.557344	-0.330607
19	1	0	4.660519	-0.503198	0.919345
20	1	0	0.803142	3.473526	-1.043247
21	1	0	-0.502482	3.027291	-0.073046
22	23	0	-1.192599	0.075496	-0.033489
23	7	0	-2.158559	1.804813	0.215502
24	1	0	-2.894164	1.925786	0.920442
25	7	0	-2.383238	-1.283789	0.565342
26	1	0	-2.180132	-1.861107	1.389273
27	7	0	-2.738275	1.220583	-0.983199
28	1	0	-3.710003	0.908825	-0.881088
29	1	0	-2.681849	1.863781	-1.779060
30	7	0	-3.587361	-1.828939	-0.010303
31	1	0	-4.410812	-1.344954	0.374451
32	1	0	-3.567269	-1.636400	-1.016319
33	1	0	2.074559	1.729997	1.067978
34	1	0	2.681758	1.260521	1.205325

V(III) D14 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2556.847180 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = S(S+1) = 6 (formal), 6.0008 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.136609	-0.234509	0.459878
2	7	0	-0.830850	-0.808878	1.110217
3	7	0	1.650953	-2.100832	0.299049
4	7	0	-0.171823	1.651729	0.451863
5	7	0	2.815578	0.736456	0.377603
6	7	0	0.245680	2.739986	-0.410232
7	1	0	-0.304077	1.970432	1.419073
8	1	0	-0.136523	3.626241	-0.064011
9	1	0	1.281262	2.784586	-0.410990
10	7	0	-1.444051	-0.443500	2.376653
11	1	0	-0.980519	-1.817855	1.008077
12	1	0	-0.730889	-0.038199	2.993603
13	1	0	-2.134558	0.295105	2.190553
14	1	0	3.611545	0.418816	0.947657
15	7	0	3.127271	1.981559	-0.270859
16	7	0	2.695946	-2.516224	-0.603592
17	1	0	1.550452	-2.838670	1.002865
18	1	0	2.285567	-2.814875	-1.499217
19	1	0	3.254652	-1.680167	-0.814510
20	1	0	3.674632	2.583986	0.355389
21	1	0	3.711854	1.813017	-1.100054
22	23	0	-1.381179	0.358163	-0.489856
23	7	0	0.297924	-0.285361	-1.449668
24	1	0	0.817125	-0.000368	-2.285307
25	7	0	-3.284550	0.429130	-0.264744
26	1	0	-3.890661	1.223977	-0.490169
27	7	0	-0.576652	-1.416883	-1.695838
28	1	0	-0.742626	-1.565937	-2.695478
29	1	0	-0.156451	-2.260551	-1.270743
30	7	0	-4.162787	-0.652623	0.119099
31	1	0	-4.316486	-1.272098	-0.687939
32	1	0	-3.666338	-1.213679	0.819498
33	1	0	1.563108	0.035159	2.543850
34	1	0	1.643045	-0.728550	2.459003
35	1	0	-1.931598	1.512599	-2.131701
36	1	0	-1.315885	1.921089	-1.876795

V(III) D11 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.546552 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0009 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.828597	-0.376319	-0.059519
2	7	0	-0.634442	1.049866	-0.784056
3	7	0	-3.641962	-0.378565	-0.616385
4	7	0	-0.983103	-2.075187	-0.514291
5	7	0	-0.988835	-0.375706	1.923020
6	7	0	0.428476	-1.851001	-0.712881
7	1	0	-1.330727	-2.755026	-1.199907
8	1	0	1.043155	-2.535917	-0.238707
9	1	0	0.678826	-1.884068	-1.709513
10	7	0	-0.806167	2.390586	-0.227921
11	1	0	-0.575834	1.176027	-1.801199
12	1	0	-1.802010	2.506354	0.005762
13	1	0	-0.289761	2.392288	0.661229
14	1	0	-1.069390	-1.337896	2.288686
15	7	0	0.393473	0.013506	1.751503
16	1	0	-1.473037	0.248052	2.586109
17	1	0	-4.524782	-0.889940	-0.719192
18	7	0	-3.799523	0.928725	-0.038658
19	1	0	-4.118291	1.620854	-0.727178
20	1	0	-4.436076	0.949151	0.766403
21	1	0	0.883892	-0.001045	2.651883
22	23	0	1.216722	0.116927	-0.017804
23	7	0	2.917815	-0.799405	-0.225901
24	1	0	3.796769	-0.309957	-0.439265
25	7	0	2.071090	1.795131	-0.358910
26	1	0	1.527625	2.596971	-0.695481
27	7	0	3.144565	-2.201974	0.013525
28	1	0	3.743984	-2.599667	-0.719981
29	1	0	3.642908	-2.333788	0.903238
30	7	0	3.409672	2.266179	-0.136680
31	1	0	3.810593	1.712764	0.627219
32	1	0	3.987869	2.075773	-0.968253

V(III) D10 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.545804 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0014 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.720117	-0.478474	0.191436
2	7	0	-0.606787	0.773417	-0.896419
3	7	0	-3.553992	-0.378647	-0.325936
4	7	0	-0.984687	-2.261850	-0.132164
5	7	0	0.391912	0.077259	1.943637
6	7	0	0.428023	-2.009183	-0.360869
7	1	0	-1.316206	-2.976201	-0.790029
8	1	0	1.039985	-2.672545	0.135659
9	1	0	0.681264	-2.121878	-1.352142
10	7	0	-0.952900	2.187012	-0.679915
11	1	0	-0.572114	0.662874	-1.916460
12	1	0	-1.968830	2.251265	-0.873236
13	1	0	-0.893170	2.306012	0.340891
14	1	0	0.829288	0.848687	2.467634
15	7	0	-1.058367	0.226133	1.918957
16	1	0	0.674269	-0.800569	2.404448
17	1	0	-4.349496	-1.003105	-0.137914
18	7	0	-3.974420	0.939645	-0.718287
19	1	0	-4.444690	0.908939	-1.631332
20	1	0	-4.639953	1.337372	-0.043565
21	1	0	-1.433632	-0.005008	2.847216
22	23	0	1.264526	0.099767	-0.055354
23	7	0	2.960983	-0.707328	-0.503552
24	1	0	3.724154	-0.166204	-0.933573
25	7	0	1.910562	1.855317	-0.234525
26	1	0	1.263394	2.578309	-0.583321
27	7	0	3.294364	-2.108342	-0.436432
28	1	0	3.687203	-2.427038	-1.331167
29	1	0	4.026960	-2.254664	0.269147
30	7	0	3.123068	2.484140	0.163635
31	1	0	3.764078	1.744332	0.469734
32	1	0	3.561777	2.956652	-0.638776

V(III) D9 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2554.543648 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.828125	0.171576	-0.383794
2	7	0	0.220951	-0.511013	1.562422
3	7	0	-3.669138	0.151522	0.111692
4	7	0	-1.311394	1.881699	-1.043299
5	7	0	0.286732	-1.577264	-1.327160
6	7	0	0.108133	1.555678	-0.969288
7	1	0	-1.465044	2.860722	-0.783750
8	1	0	0.503859	1.582974	-1.916859
9	1	0	0.646162	2.235751	-0.383369
10	7	0	-1.218724	-0.524487	1.516432
11	1	0	0.553057	-0.783404	2.493850
12	1	0	-1.620630	-1.464884	1.647227
13	1	0	-1.639328	0.065928	2.247366
14	1	0	0.467672	-2.542625	-1.013182
15	7	0	-1.133049	-1.325649	-1.400439
16	1	0	0.731326	-1.486558	-2.250866
17	1	0	-4.446890	0.473194	-0.480728
18	7	0	-4.136122	-0.641793	1.220194
19	1	0	-4.761530	-0.080265	1.811326
20	1	0	-4.689326	-1.440847	0.883255
21	1	0	-1.554881	-1.834774	-2.182854
22	23	0	1.390496	-0.200604	0.054588
23	7	0	2.623472	1.275811	0.314319
24	1	0	3.634265	1.159931	0.455998
25	7	0	2.810275	-1.477129	-0.110610
26	1	0	2.621313	-2.458954	-0.342256
27	7	0	2.217449	2.635647	0.564622
28	1	0	2.240306	2.840474	1.571748
29	1	0	2.853466	3.298145	0.105077
30	7	0	4.204328	-1.433819	0.258741
31	1	0	4.689952	-0.787511	-0.374573
32	1	0	4.281332	-1.034101	1.200937

Cr(III) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2867.169892 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = $S(S+1)$ = 12 (formal), 12.0023 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-2.178170	0.328844	0.027490
2	7	0	-2.997059	0.934779	-1.673147
3	7	0	-4.088776	-0.581754	0.521332
4	7	0	-0.469765	1.222759	-0.421971
5	7	0	-1.362763	-1.015871	1.073606
6	7	0	0.667335	1.164134	0.494632
7	1	0	-0.082727	0.964150	-1.338383
8	1	0	1.029916	2.117638	0.690293
9	1	0	0.311833	0.796875	1.387274
10	7	0	-3.099842	2.029828	-0.747699
11	1	0	-2.350596	1.209820	-2.423879
12	1	0	-4.051465	2.398652	-0.670952
13	1	0	-2.395623	2.767791	-0.864218
14	1	0	-0.342299	-1.232903	1.079528
15	7	0	-2.086450	-2.064997	1.758238
16	1	0	-4.698839	0.023799	1.085900
17	7	0	-4.764692	-1.120377	-0.639037
18	1	0	-3.741378	-1.364540	1.119767
19	1	0	-5.774805	-1.159389	-0.475023
20	1	0	-4.560511	-0.460429	-1.406104
21	1	0	-1.783513	-2.979063	1.398034
22	1	0	-1.828258	-2.052341	2.752813
23	24	0	2.432974	0.057364	0.006658
24	7	0	1.523929	-1.595625	0.621901
25	1	0	2.230174	-2.324733	0.798986
26	7	0	1.382032	-1.504630	-0.805851
27	1	0	2.025218	-2.136484	-1.317745
28	1	0	0.399381	-1.532042	-1.094780
29	7	0	3.443852	1.592192	0.533183
30	1	0	4.466100	1.544580	0.628048
31	7	0	2.923787	2.835752	1.025044
32	1	0	3.231805	3.003991	1.991284
33	1	0	3.275484	3.617921	0.459316
34	7	0	4.088507	-0.845240	-0.573492
35	1	0	4.894767	-0.284827	-0.873175
36	7	0	4.063350	-2.111112	-1.259141

37	1	0	4.315734	-2.011447	-2.251782
38	1	0	4.750189	-2.754892	-0.847925

Cr(III) D1 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2868.299250 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0018 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	2.048559	0.246133	-0.322627
2	7	0	2.881497	1.678751	0.764447
3	7	0	3.994697	-0.707915	-0.396527
4	7	0	0.302194	1.156051	-0.314425
5	7	0	1.296477	-1.473889	-0.452775
6	7	0	-0.907044	0.626315	-0.886486
7	1	0	-0.028798	1.653904	0.524052
8	1	0	-1.458269	1.398502	-1.312650
9	1	0	-0.663522	-0.058371	-1.610556
10	7	0	2.907825	2.136205	-0.599011
11	1	0	2.250010	2.287796	1.300295
12	1	0	3.841197	2.429640	-0.900355
13	1	0	2.187868	2.822547	-0.849915
14	1	0	0.305118	-1.699213	-0.198953
15	7	0	2.063717	-2.696235	-0.549240
16	1	0	4.542356	-0.462274	-1.231593
17	7	0	4.747515	-0.535213	0.827429
18	1	0	3.681033	-1.701702	-0.478551
19	1	0	5.751750	-0.602646	0.638483
20	1	0	4.516914	0.415233	1.158703
21	1	0	1.833560	-3.304029	0.247877
22	1	0	1.764691	-3.207401	-1.389112
23	24	0	-2.310484	-0.120237	0.403380
24	7	0	-1.330283	-1.844974	0.746653
25	1	0	-1.801670	-2.691368	1.088186
26	7	0	-0.994102	-0.992481	1.878231
27	1	0	-1.280276	-1.352972	2.794606
28	1	0	0.015220	-0.797122	1.888672
29	7	0	-2.595382	1.806951	0.837567
30	1	0	-3.130183	2.123993	1.656690
31	7	0	-2.885358	2.647504	-0.304167
32	1	0	-3.894539	2.684361	-0.507465
33	1	0	-2.586767	3.612928	-0.119828
34	7	0	-3.504365	-0.447340	-1.089767
35	1	0	-4.001484	0.334088	-1.536755
36	7	0	-4.333015	-1.617517	-0.991128

37	1	0	-5.314591	-1.374507	-0.804857
38	1	0	-4.315876	-2.137098	-1.876884
39	1	0	-3.745129	-1.100879	1.432210
40	1	0	-3.693019	-0.448404	1.854003

Cr(III) D2 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2867.163561 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0054 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.781152	0.075766	-0.329503
2	7	0	3.046526	-1.097221	-1.036958
3	7	0	1.057745	0.457554	1.602180
4	7	0	0.130730	-1.111375	-0.678783
5	7	0	2.084475	1.950656	-0.691985
6	7	0	0.319912	-2.529936	-0.316064
7	1	0	0.127348	-1.124574	-1.711059
8	1	0	0.336998	-2.512649	0.713587
9	1	0	-0.573715	-3.005115	-0.513235
10	7	0	2.952205	-2.401776	-1.587061
11	1	0	4.025873	-0.797360	-1.093199
12	1	0	3.674058	-3.003817	-1.169458
13	1	0	2.032830	-2.775596	-1.273574
14	1	0	2.388431	2.296323	-1.611338
15	7	0	2.129807	3.007237	0.292128
16	1	0	0.610673	-0.369128	2.033352
17	7	0	1.911440	1.100143	2.603086
18	1	0	0.257165	1.105780	1.405671
19	1	0	2.765101	0.530038	2.646899
20	1	0	2.190514	1.975812	2.120651
21	1	0	3.000759	3.543018	0.193874
22	1	0	1.355904	3.667017	0.140890
23	24	0	-1.746119	-0.259020	-0.152283
24	7	0	-1.296242	1.564559	0.380173
25	1	0	-2.136445	2.096021	0.645434
26	7	0	-1.224146	1.558100	-1.059050
27	1	0	-2.052133	1.975910	-1.512948
28	1	0	-0.305599	1.888520	-1.382195
29	7	0	-2.146035	-1.589439	1.204264
30	1	0	-3.096593	-1.611440	1.596499
31	7	0	-1.177410	-1.822719	2.255827
32	1	0	-1.383198	-1.235260	3.076658
33	1	0	-1.254012	-2.794973	2.584115
34	7	0	-3.603819	-0.003474	-0.660065
35	1	0	-4.369723	-0.475430	-0.161216
36	7	0	-4.062367	1.239131	-1.230993

37	1	0	-4.577513	1.051796	-2.099873
38	1	0	-4.717280	1.723115	-0.603569

Cr(III) D3 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.421146 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0033 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.905944	-0.370953	0.022095
2	7	0	-1.717439	1.520822	-0.422970
3	7	0	-3.621219	-0.646549	-0.856639
4	7	0	-0.795342	-1.662853	-0.882803
5	7	0	-0.732931	-0.372022	1.854632
6	7	0	0.639610	-1.861920	-0.794121
7	1	0	-1.148088	-2.132116	-1.723605
8	1	0	0.829748	-2.807453	-0.432499
9	1	0	1.062505	-1.833074	-1.734447
10	7	0	-0.885263	2.371437	0.393751
11	1	0	-1.369255	1.626754	-1.383850
12	1	0	-1.489147	2.881435	1.045576
13	1	0	-0.208705	1.806890	0.950217
14	1	0	-0.726951	-1.328994	2.239029
15	7	0	0.614372	0.141933	1.696739
16	1	0	-1.243476	0.207981	2.535629
17	1	0	-3.864560	-0.023199	-1.638125
18	7	0	-3.920882	0.048501	0.374563
19	1	0	-4.095690	1.054908	0.264110
20	1	0	-4.654299	-0.419366	0.913424
21	1	0	1.051843	0.243322	2.620164
22	24	0	1.813284	-0.333497	0.213812
23	7	0	3.548473	0.126120	0.921553
24	1	0	4.027715	1.033708	0.892278
25	7	0	1.586513	0.698770	-1.415578
26	1	0	0.701399	0.444210	-1.876887
27	7	0	3.880465	-0.666909	-0.232370
28	1	0	4.170827	-0.149904	-1.070382
29	1	0	4.533846	-1.425585	-0.017537
30	7	0	1.587513	2.125067	-1.404852
31	1	0	0.857092	2.522530	-0.784353
32	1	0	2.501938	2.447997	-1.083863

Cr(III) D12 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.463167 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1)$ = 12 (formal), 12.0012 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.671199	0.225464	-0.058623
2	7	0	1.404399	-1.461134	-1.036350
3	7	0	0.259443	-0.350398	1.342706
4	7	0	0.098866	1.088225	-0.970371
5	7	0	-3.147438	2.051227	0.327207
6	7	0	0.525668	2.124208	-0.046108
7	1	0	0.041830	1.428089	-1.933905
8	1	0	0.785520	2.990592	-0.528148
9	1	0	-0.304205	2.267446	0.589975
10	7	0	0.001976	-1.873985	-0.872634
11	1	0	1.977719	-2.228384	-0.654663
12	1	0	-0.280735	-2.408788	-1.703709
13	1	0	-0.057599	-2.483526	-0.037075
14	1	0	-2.784510	2.887937	-0.143323
15	7	0	-2.004900	1.342096	0.884922
16	1	0	-3.535319	1.458517	-0.424042
17	1	0	0.197542	0.346329	2.098760
18	7	0	0.474761	-1.674871	1.906072
19	1	0	1.422968	-1.727232	2.298514
20	1	0	-0.183064	-1.824940	2.680073
21	1	0	-2.274518	1.107210	1.849081
22	24	0	-1.246084	-0.197709	-0.115225
23	7	0	3.533607	0.040143	0.630934
24	1	0	3.900104	0.732606	1.297492
25	7	0	-2.917339	-0.545355	-1.158009
26	1	0	-2.876496	-1.164863	-1.978505
27	7	0	3.603536	0.637941	-0.697246
28	1	0	4.016299	1.575391	-0.740466
29	1	0	4.092534	0.024077	-1.355428
30	7	0	-2.930204	-1.391389	0.027670
31	1	0	-3.719247	-1.151870	0.635574
32	1	0	-2.938221	-2.401653	-0.149391

Cr(III) D12 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2756.601968 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0018 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.693908	0.372537	0.291065
2	7	0	1.553191	-1.370733	-0.585043
3	7	0	0.054584	-0.058510	1.550122
4	7	0	0.221577	1.082692	-0.851250
5	7	0	-3.789461	1.196724	-0.002141
6	7	0	0.053866	2.443085	-0.376853
7	1	0	0.391329	1.058201	-1.863261
8	1	0	0.282019	3.110835	-1.119833
9	1	0	-0.958904	2.511700	-0.110064
10	7	0	0.191840	-1.878609	-0.452732
11	1	0	2.182289	-2.054603	-0.135753
12	1	0	0.010858	-2.549550	-1.209356
13	1	0	0.093936	-2.351273	0.465245
14	1	0	-4.187221	2.143404	0.035731
15	7	0	-2.386774	1.282273	0.438828
16	1	0	-3.728551	0.955548	-1.001983
17	1	0	-0.186989	0.734746	2.162422
18	7	0	0.162330	-1.276782	2.338506
19	1	0	0.942230	-1.200653	3.003366
20	1	0	-0.691871	-1.401674	2.895820
21	1	0	-2.453129	1.239343	1.466980
22	24	0	-1.215331	-0.232281	-0.146408
23	7	0	3.537457	0.482808	-0.118375
24	1	0	4.094481	1.314941	0.102230
25	7	0	-2.544422	-0.823359	-1.509904
26	1	0	-2.239396	-1.577899	-2.140126
27	7	0	4.264763	-0.241882	-1.126610
28	1	0	4.895520	-0.910754	-0.663274
29	1	0	3.563528	-0.807851	-1.622287
30	7	0	-2.871853	-1.443195	-0.227788
31	1	0	-3.729531	-0.998399	0.135852
32	1	0	-2.958558	-2.463833	-0.240039
33	1	0	1.790609	2.269660	1.190966
34	1	0	2.271823	1.850359	1.638271

Cr(III) D12 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2757.740349 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = $S(S+1)$ = 12 (formal), 12.0024 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.687561	0.360975	0.313942
2	7	0	1.495188	-1.340793	-0.646309
3	7	0	-0.066187	-0.035095	1.308988
4	7	0	0.390879	1.379104	-0.911923
5	7	0	-3.743099	1.522835	0.457702
6	7	0	0.244649	2.758311	-0.489699
7	1	0	0.625115	1.333370	-1.913006
8	1	0	0.884986	3.358127	-1.020485
9	1	0	-0.723793	3.053106	-0.688122
10	7	0	0.130722	-1.438149	-1.171411
11	1	0	1.528523	-2.045532	0.106966
12	1	0	0.207818	-1.523950	-2.191279
13	1	0	-0.379666	-2.284448	-0.837331
14	1	0	-4.251284	1.380971	-0.420660
15	7	0	-2.338099	1.590894	0.156593
16	1	0	-3.953327	0.709298	1.054953
17	1	0	-0.445490	0.702851	1.922327
18	7	0	-0.158774	-1.329574	1.954935
19	1	0	0.185200	-1.250966	2.918463
20	1	0	-1.160056	-1.579936	1.968731
21	1	0	-1.944670	2.249380	0.839073
22	24	0	-1.194370	0.091091	-0.375046
23	7	0	3.565157	0.207003	0.301595
24	1	0	4.198719	0.903886	0.707387
25	7	0	-2.479373	-1.364044	0.102277
26	1	0	-3.485574	-1.163765	0.169519
27	7	0	4.368883	-0.683394	-0.479261
28	1	0	4.868172	-1.327556	0.150123
29	1	0	3.691512	-1.253918	-1.006880
30	7	0	-2.260056	-2.722985	-0.333402
31	1	0	-2.461406	-3.381307	0.428341
32	1	0	-2.878596	-2.979878	-1.113999
33	1	0	-2.322831	-0.166672	-2.084093
34	1	0	-1.970272	0.493095	-2.284130
35	1	0	1.740119	2.279029	1.266836
36	1	0	2.160997	1.836451	1.743161

Cr(III) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.432259 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0060 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.390521	-0.491310	0.309881
2	7	0	0.475598	-1.298261	0.687459
3	7	0	-1.533152	0.022409	2.096785
4	7	0	-0.384106	0.320261	-1.277373
5	7	0	-3.045193	-0.750395	-0.589501
6	7	0	-0.965508	1.566734	-1.730952
7	1	0	-0.411285	-0.372911	-2.045007
8	1	0	-0.449157	1.888004	-2.559280
9	1	0	-1.932899	1.344048	-2.026135
10	7	0	0.758373	-2.669873	0.253194
11	1	0	0.779272	-1.272449	1.669080
12	1	0	-0.045556	-3.266461	0.492955
13	1	0	0.803244	-2.653932	-0.771323
14	1	0	-3.752394	-1.409428	-0.238684
15	7	0	-3.478463	-0.103755	-1.797583
16	7	0	-2.400515	1.064465	2.550626
17	1	0	-0.935709	-0.253582	2.881817
18	1	0	-1.971810	1.981635	2.366359
19	1	0	-3.253789	1.019417	1.985378
20	1	0	-3.672258	-0.802260	-2.526409
21	1	0	-4.359202	0.399102	-1.630506
22	24	0	1.447691	0.232702	-0.326961
23	7	0	1.471650	2.086511	-0.121674
24	1	0	0.718074	2.651922	-0.532931
25	7	0	3.130234	-0.587708	-0.477892
26	1	0	3.884098	-0.092787	-0.966362
27	7	0	2.383305	2.947112	0.560289
28	1	0	1.981131	3.236743	1.462941
29	1	0	3.215258	2.392048	0.781799
30	7	0	3.721646	-1.735089	0.150047
31	1	0	2.941252	-2.296194	0.519401
32	1	0	4.152564	-2.323200	-0.577151

Cr(III) D13 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.422586 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1)$ = 12 (formal), 12.0101 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.290696	0.225258	-0.163009
2	7	0	1.036234	-1.580459	-0.813870
3	7	0	-0.127183	-0.063794	1.250161
4	7	0	-0.350281	0.624994	-1.398158
5	7	0	-4.653194	-0.222523	0.168852
6	7	0	-0.730845	2.016194	-1.538816
7	1	0	-0.140678	0.203677	-2.315179
8	1	0	-0.021454	2.507287	-2.097935
9	1	0	-1.623554	2.080406	-2.042113
10	7	0	-0.266496	-2.147263	-0.562029
11	1	0	1.794088	-2.253430	-0.624765
12	1	0	-0.498651	-2.865330	-1.260312
13	1	0	-0.264267	-2.582851	0.377900
14	1	0	-4.981759	0.705632	-0.136294
15	7	0	-3.279168	-0.123137	0.591242
16	1	0	-4.662770	-0.814625	-0.666761
17	1	0	-0.212563	0.832238	1.764168
18	7	0	0.153417	-1.162226	2.157383
19	1	0	1.036336	-0.986348	2.654482
20	1	0	-0.588172	-1.198108	2.867529
21	1	0	-3.309269	0.247273	1.547861
22	24	0	-1.636635	-0.506904	-0.247751
23	7	0	1.580957	2.017889	0.472826
24	1	0	2.472926	2.343716	0.859351
25	7	0	3.167178	-0.129301	-0.043268
26	1	0	3.834635	0.585428	0.278889
27	7	0	0.529463	2.792402	1.021468
28	1	0	0.823494	3.760045	1.191248
29	1	0	-0.226612	2.797615	0.310823
30	7	0	3.805622	-1.395243	-0.220208
31	1	0	4.421205	-1.369938	-1.042093
32	1	0	4.389659	-1.625900	0.592352

Cr(III) D14 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.439787 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0028 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.078772	-0.016404	0.126320
2	7	0	-0.446395	-1.208183	1.056851
3	7	0	2.330160	-1.533253	-0.131789
4	7	0	-0.440970	1.452002	0.316658
5	7	0	2.528250	1.158701	0.167622
6	7	0	-0.321655	2.443943	-0.718900
7	1	0	-0.574640	1.881902	1.244964
8	1	0	-1.050247	3.158613	-0.611435
9	1	0	0.610933	2.883084	-0.590987
10	7	0	-0.564791	-1.268001	2.494519
11	1	0	-0.358520	-2.168892	0.700428
12	1	0	0.181978	-0.697783	2.908157
13	1	0	-1.454853	-0.843022	2.778904
14	1	0	3.454163	0.721557	0.013949
15	7	0	2.532963	2.591572	0.107146
16	7	0	3.758519	-1.342240	-0.136059
17	1	0	2.092676	-2.375744	0.410484
18	1	0	4.179382	-1.627463	0.756718
19	1	0	4.183606	-1.923528	-0.866511
20	1	0	2.886345	2.971547	0.994688
21	1	0	3.190030	2.901114	-0.619821
22	24	0	-1.649058	-0.069466	-0.083586
23	7	0	-0.204797	-0.572518	-1.409011
24	1	0	-0.042128	0.066751	-2.200235
25	7	0	-3.369686	0.644270	0.071973
26	1	0	-3.727819	1.562710	0.344532
27	7	0	-0.066910	-1.963043	-1.760031
28	1	0	-0.478240	-2.136694	-2.682101
29	1	0	0.945172	-2.176081	-1.771071
30	7	0	-4.501031	-0.202725	-0.209328
31	1	0	-4.485415	-0.515478	-1.184733
32	1	0	-4.501141	-1.025395	0.400914

Cr(III) D10 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.449685 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0026 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.919058	-0.092881	-0.300748
2	7	0	-0.412771	1.349400	-0.330397
3	7	0	-3.778852	-0.565509	-0.493467
4	7	0	-0.882369	-1.270945	-1.423056
5	7	0	0.082113	-0.745167	1.553980
6	7	0	0.558045	-1.237183	-1.316843
7	1	0	-1.184121	-2.215191	-1.686613
8	1	0	0.976798	-2.095190	-0.902692
9	1	0	0.985275	-1.100152	-2.243405
10	7	0	-0.633319	2.399219	0.675616
11	1	0	-0.421318	1.839186	-1.234305
12	1	0	-1.055990	1.903400	1.473298
13	1	0	0.291294	2.713972	1.005228
14	1	0	0.481410	-0.523955	2.475969
15	7	0	-1.339886	-0.411102	1.549406
16	1	0	0.245193	-1.750654	1.392958
17	1	0	-4.420239	-1.248181	-0.074420
18	7	0	-3.814037	0.692489	0.209034
19	1	0	-4.353562	1.415505	-0.275621
20	1	0	-4.079077	0.656921	1.199498
21	1	0	-1.834486	-1.192611	2.002872
22	24	0	1.280540	0.225962	0.021840
23	7	0	2.802320	-1.025906	0.429586
24	1	0	3.502450	-0.787876	1.145268
25	7	0	2.445229	1.645743	-0.371437
26	1	0	2.115876	2.542264	-0.747628
27	7	0	2.529345	-2.448124	0.460579
28	1	0	3.295282	-2.961656	0.007011
29	1	0	2.480030	-2.813014	1.421965
30	7	0	3.849838	1.577821	-0.633496
31	1	0	4.361352	2.112175	0.082068
32	1	0	4.098663	0.585954	-0.514190

Cr(III) D9 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2755.432534 Hartree/particle
Input spin multiplicity ($2S+1$) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0030 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	2.087702	-0.015307	-0.213807
2	7	0	-0.377346	-1.829164	-0.728540
3	7	0	3.762858	0.942524	-0.107988
4	7	0	0.995733	1.112441	-1.294899
5	7	0	-0.028168	0.176374	1.648145
6	7	0	-0.436459	0.947851	-1.382133
7	1	0	1.222192	2.107094	-1.396326
8	1	0	-0.963703	1.841696	-1.254374
9	1	0	-0.668588	0.549135	-2.300802
10	7	0	1.058453	-1.893099	-0.514872
11	1	0	-0.749860	-2.781308	-0.608844
12	1	0	1.295075	-2.393123	0.357342
13	1	0	1.492418	-2.418881	-1.286874
14	1	0	-0.412389	-0.309952	2.469632
15	7	0	1.413392	-0.029509	1.618037
16	1	0	-0.316616	1.165564	1.725015
17	1	0	4.044316	1.660611	0.571343
18	7	0	4.102951	-0.373681	0.387326
19	1	0	4.885712	-0.790378	-0.124822
20	1	0	4.270558	-0.446562	1.397180
21	1	0	1.827778	0.715943	2.196137
22	24	0	-1.408771	-0.292035	0.032860
23	7	0	-2.332858	1.410124	0.661861
24	1	0	-3.118133	1.402878	1.327518
25	7	0	-2.969085	-1.340030	0.006739
26	1	0	-2.933157	-2.317209	-0.307442
27	7	0	-2.448349	2.547863	-0.224859
28	1	0	-3.355767	2.574842	-0.710753
29	1	0	-2.368707	3.425357	0.301882
30	7	0	-4.352706	-0.985257	0.056589
31	1	0	-4.795455	-1.438475	0.869303
32	1	0	-4.368930	0.023921	0.239786

Ti(III) D1 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2256.018567 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.576927	0.223580	-0.621342
2	1	0	1.621485	1.784764	-1.496435
3	7	0	3.414043	-0.752124	0.169918
4	7	0	0.297642	-0.973719	-1.480514
5	7	0	1.189254	0.618386	1.211822
6	7	0	-1.013338	-1.367404	-1.001133
7	1	0	0.236980	-0.896333	-2.504649
8	1	0	-1.409445	-2.104236	-1.603192
9	1	0	-0.938715	-1.817373	-0.064149
10	1	0	0.251071	0.995627	1.447725
11	7	0	2.157372	0.741964	2.275086
12	1	0	3.247636	-1.760544	0.294781
13	7	0	4.700087	-0.473784	-0.434907
14	1	0	3.385539	-0.308508	1.115948
15	1	0	5.389298	-1.180596	-0.151993
16	1	0	4.583895	-0.533361	-1.451011
17	1	0	2.342607	1.732209	2.477630
18	1	0	1.779906	0.330043	3.136903
19	22	0	-2.383196	0.251811	-0.471402
20	7	0	-1.659658	1.711662	0.636694
21	1	0	-2.047885	2.405780	1.282191
22	7	0	-1.409771	2.253775	-0.677269
23	1	0	-1.999269	3.048720	-0.939969
24	1	0	-0.415748	2.465964	-0.844858
25	7	0	-3.191191	-1.042777	0.752282
26	1	0	-4.138907	-1.015049	1.150808
27	7	0	-2.391790	-2.064312	1.411914
28	1	0	-2.243748	-1.818030	2.399253
29	1	0	-2.897571	-2.959819	1.411107
30	1	0	-3.657747	0.610492	-1.666978

Ti(III) D2 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2256.047425 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.379297	-0.207540	0.174796
2	1	0	2.449573	0.259954	1.547086
3	7	0	1.297758	1.784509	-0.675302
4	7	0	-0.062233	-0.737469	1.577506
5	7	0	2.000650	-1.710974	-0.850443
6	7	0	-0.128983	-0.165936	2.915422
7	1	0	-0.064741	-1.757423	1.705540
8	1	0	0.669835	0.470215	3.018687
9	1	0	-1.004906	0.365291	2.985300
10	1	0	2.120686	-2.695052	-1.100894
11	7	0	3.142288	-0.883626	-1.097726
12	1	0	0.458900	2.028781	-1.261730
13	7	0	1.096488	2.539199	0.572406
14	1	0	2.132194	2.177782	-1.125987
15	1	0	0.106439	2.367499	0.816087
16	1	0	1.678909	2.054090	1.283372
17	1	0	4.004725	-1.188648	-0.635482
18	1	0	3.316066	-0.707797	-2.092898
19	22	0	-1.519406	-0.270614	0.146634
20	7	0	-2.115029	-1.379765	-1.303295
21	1	0	-2.502777	-1.645174	-2.210261
22	7	0	-1.752482	-2.456971	-0.445198
23	1	0	-2.540768	-3.027753	-0.125201
24	1	0	-0.993173	-3.045948	-0.803010
25	7	0	-1.828627	1.640444	-0.299092
26	1	0	-2.729592	2.000096	0.046286
27	7	0	-1.351323	2.432085	-1.410749
28	1	0	-1.925679	2.254573	-2.243823
29	1	0	-1.447029	3.432764	-1.197174
30	1	0	-2.735803	-0.254345	1.437948

Ti(III) D7 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2144.337812 Hartree/particle
Input spin multiplicity ($2S+1$) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.316001	-0.014912	0.409224
2	7	0	-0.077114	1.500442	0.732656
3	1	0	1.373546	-0.332279	2.166723
4	7	0	0.114640	-1.291162	-0.652323
5	7	0	2.887840	0.834767	-0.316802
6	7	0	0.393478	-2.327221	0.326476
7	1	0	0.143289	-1.714620	-1.582554
8	1	0	1.392630	-2.580460	0.364964
9	1	0	0.084301	-2.028361	1.261963
10	7	0	-0.601853	2.266246	-0.370676
11	1	0	-0.252217	1.962731	1.629391
12	1	0	-1.257755	3.005455	-0.094887
13	1	0	0.129631	2.645043	-0.978503
14	1	0	3.569377	1.522554	-0.644276
15	7	0	3.373434	-0.516241	-0.297349
16	1	0	3.603917	-0.892253	-1.223962
17	1	0	4.154937	-0.673871	0.348183
18	22	0	-1.335151	0.224095	-0.367293
19	7	0	-2.983130	0.108331	0.652441
20	1	0	-3.552706	0.083868	1.501730
21	1	0	-1.561662	0.378848	-2.123033
22	7	0	-3.154849	-1.017101	-0.208461
23	1	0	-3.130466	-1.934632	0.247924
24	1	0	-3.942646	-0.950478	-0.857871

Ti(III) D7 with hydride ligands and 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2145.477119 Hartree/particle
Input spin multiplicity ($2S+1$) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.330339	-0.076969	0.375242
2	7	0	-0.031193	1.400158	0.860701
3	1	0	1.836054	-0.658727	1.973702
4	7	0	0.050371	-1.389913	-0.535214
5	7	0	2.632959	1.003979	-0.551120
6	7	0	0.599003	-2.596953	0.061292
7	1	0	-0.128099	-1.589521	-1.522582
8	1	0	1.621782	-2.641245	-0.067678
9	1	0	0.409955	-2.582746	1.068920
10	7	0	-0.073631	2.630764	0.062722
11	1	0	-0.009646	1.705114	1.837693
12	1	0	0.534431	2.474415	-0.749656
13	1	0	-1.028261	2.719217	-0.308272
14	1	0	3.209258	1.809645	-0.805589
15	7	0	3.252479	-0.270290	-0.763074
16	1	0	3.363994	-0.525740	-1.750385
17	1	0	4.140348	-0.397878	-0.265970
18	22	0	-1.416473	-0.136757	0.394512
19	1	0	-2.112284	0.166993	2.027884
20	7	0	-2.451691	0.647465	-1.039527
21	1	0	-2.702602	1.145954	-1.897987
22	7	0	-3.370776	-0.381315	-0.662824
23	1	0	-4.258157	-0.040453	-0.280526
24	1	0	-3.542650	-1.094269	-1.379285
25	1	0	-1.730297	-1.857385	1.314871
26	1	0	-1.961538	-1.238664	1.839583

Ti(III) D7 with hydride ligands and 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2146.632177 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = $S(S+1)$ = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.221401	0.461494	0.607130
2	7	0	-0.427896	-1.440538	0.413783
3	1	0	-0.658586	1.734887	1.746622
4	7	0	0.178452	1.359829	-0.698369
5	7	0	-3.149726	0.279724	0.367450
6	7	0	0.815993	2.647023	-0.403342
7	1	0	-0.257837	1.485673	-1.617269
8	1	0	0.712129	2.765521	0.611562
9	1	0	1.824189	2.563542	-0.599133
10	7	0	-1.172740	-2.290221	-0.516435
11	1	0	-0.094086	-1.999013	1.209522
12	1	0	-0.477176	-2.838225	-1.042600
13	1	0	-1.751345	-2.945765	0.023966
14	1	0	-3.983508	-0.291578	0.531456
15	7	0	-2.684494	0.232291	-0.981005
16	1	0	-2.611873	-0.711969	-1.389603
17	1	0	-3.111366	0.922913	-1.604717
18	22	0	1.268042	-0.430550	-0.380745
19	7	0	2.469737	-0.421053	1.118731
20	1	0	2.767058	-0.163682	2.061783
21	1	0	1.493679	-1.964758	-1.306976
22	7	0	3.438025	-0.180202	0.098355
23	1	0	3.902120	0.733201	0.144202
24	1	0	4.132180	-0.925784	-0.011476
25	1	0	1.729393	0.149539	-2.292386
26	1	0	1.753434	-0.659486	-2.275810
27	1	0	-1.485453	-0.293097	2.469944
28	1	0	-1.180487	0.449340	2.566270

Ti(III) D7 with hydride ligands and 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2147.778285 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = $S(S+1)$ = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.679299	0.703288	-0.137019
2	7	0	0.216282	1.492781	-0.498532
3	7	0	-2.108899	-0.927513	-1.168229
4	7	0	-0.848477	-0.258903	1.428006
5	1	0	-3.195059	1.477613	0.422800
6	7	0	-0.212111	-1.554815	1.370987
7	1	0	-0.660698	0.156771	2.346332
8	1	0	-0.111678	-1.988642	2.294745
9	1	0	-0.825405	-2.137811	0.742446
10	7	0	-0.358162	2.453652	0.426009
11	1	0	0.635724	1.949016	-1.312209
12	1	0	0.244673	2.538486	1.254965
13	1	0	-0.516560	3.371342	0.000187
14	7	0	-2.102851	-2.282840	-0.637749
15	1	0	-2.475714	-0.941304	-2.128145
16	1	0	-1.795676	-2.945854	-1.361069
17	1	0	-3.059514	-2.557271	-0.380205
18	22	0	1.205634	-0.170141	0.474282
19	7	0	2.735762	0.270160	-0.657675
20	1	0	2.902246	1.234487	-0.962909
21	1	0	1.593200	0.789914	1.934750
22	7	0	3.881471	-0.491365	-1.058051
23	1	0	3.990955	-1.270558	-0.400889
24	1	0	3.708197	-0.915010	-1.980157
25	1	0	2.533968	-1.504418	1.297072
26	1	0	2.505834	-0.859950	1.779120
27	1	0	-2.196656	1.833456	-1.832519
28	1	0	-2.650946	2.084880	-1.227355
29	1	0	0.994492	-1.691070	-1.064302
30	1	0	0.378130	-1.261406	-1.275817

Ti(III) D7 with hydride ligands and 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2148.912965 Hartree/particle
Input spin multiplicity ($2S$+1) = 3
$<S^2>$ = $S(S+1)$ = 2 (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.572924	0.602182	0.105074
2	7	0	-0.376193	1.373010	0.425958
3	7	0	3.121468	-0.467522	0.710529
4	7	0	0.426633	-0.911305	-0.887198
5	1	0	2.523545	0.907177	-1.373333
6	7	0	0.033467	-2.004120	-0.033330
7	1	0	0.749396	-1.240887	-1.799175
8	1	0	-0.151047	-2.872900	-0.549792
9	1	0	0.747396	-2.186613	0.684388
10	7	0	0.140130	2.039024	-0.749713
11	1	0	-0.693404	2.053788	1.119334
12	1	0	-0.450694	1.788181	-1.559210
13	1	0	0.243537	3.052171	-0.641145
14	7	0	4.215888	-0.940186	-0.081371
15	1	0	3.241830	-0.869247	1.645266
16	1	0	5.091837	-0.517133	0.258387
17	1	0	4.055096	-0.544436	-1.014916
18	22	0	-1.503899	-0.361722	-0.184771
19	7	0	-3.365280	0.275141	-0.137452
20	1	0	-3.720949	0.899914	-0.862033
21	1	0	-1.652411	0.362857	-1.805688
22	7	0	-4.467851	-0.006454	0.744163
23	1	0	-4.949800	-0.861188	0.432596
24	1	0	-4.095871	-0.214842	1.675568
25	1	0	-2.310920	-2.110050	-1.098471
26	1	0	-2.167078	-1.572984	-1.662061
27	1	0	2.458230	2.336695	0.699286
28	1	0	2.699228	2.177247	-0.055996
29	1	0	-1.718839	-0.559655	1.898237
30	1	0	-2.066090	-1.222007	1.642553
31	1	0	1.464168	0.544562	2.154189
32	1	0	1.086438	-0.143875	2.024246

Ti(III) D14 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2144.324868 Hartree/particle
Input spin multiplicity ($2S+1$) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	0.917784	0.283144	-0.168077
2	7	0	-0.950627	1.507520	-0.082664
3	7	0	2.827395	0.324507	0.191736
4	7	0	-0.527884	-0.999365	-1.183974
5	1	0	0.939762	0.952063	-1.828650
6	7	0	-0.984658	-2.221034	-0.561812
7	1	0	-0.513709	-1.044099	-2.204163
8	1	0	-1.600621	-2.769752	-1.169841
9	1	0	-0.198233	-2.804681	-0.240412
10	7	0	-1.341230	2.319386	-1.227787
11	1	0	-0.862822	2.167645	0.697690
12	1	0	-0.686134	2.068720	-1.978768
13	1	0	-2.285153	2.039216	-1.522137
14	7	0	2.814196	-0.621190	-0.870019
15	1	0	3.757206	0.586677	0.526722
16	1	0	3.199241	-1.542017	-0.637384
17	1	0	3.178421	-0.275933	-1.762382
18	22	0	-1.772970	-0.333819	0.305688
19	7	0	-0.169519	-0.571059	1.581036
20	1	0	0.071726	-1.410363	2.118840
21	1	0	-3.557931	-0.452844	0.627684
22	7	0	0.603106	0.561531	2.037296
23	1	0	0.037795	1.210581	2.595514
24	1	0	1.439105	0.287568	2.563164

Ti(III) D10 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2144.313886 Hartree/particle
Input spin multiplicity ($2S+1$) = 3
$\langle S^2 \rangle = S(S+1) = 2$ (formal), 2.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.588546	1.073136	0.313178
2	7	0	1.437767	-0.279566	-1.157358
3	1	0	2.774402	2.423695	0.313982
4	7	0	-0.412429	1.463063	0.158018
5	7	0	0.386335	-1.270793	1.472104
6	7	0	-1.143268	1.344409	-1.083922
7	1	0	-1.053284	1.812162	0.879489
8	1	0	-2.156671	1.485244	-0.913750
9	1	0	-0.772493	1.956791	-1.817200
10	7	0	2.277952	-1.455840	-1.365515
11	1	0	1.275858	0.092216	-2.102684
12	1	0	2.739486	-1.646801	-0.469258
13	1	0	1.646653	-2.247845	-1.557252
14	1	0	0.751645	-2.234952	1.439293
15	7	0	1.460873	-0.310705	1.687258
16	1	0	-0.297985	-1.230473	2.239643
17	1	0	1.973633	-0.524472	2.549427
18	22	0	-0.721146	-0.638262	-0.409817
19	7	0	-2.554265	-0.811166	0.281762
20	1	0	-3.080594	-1.664309	0.520119
21	1	0	-0.847073	-1.531681	-1.952330
22	7	0	-3.447402	0.335770	0.297881
23	1	0	-4.272566	0.139533	-0.284119
24	1	0	-3.802744	0.497435	1.249103

Ti(II) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2478.300739 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-2.161784	0.098766	-0.351721
2	7	0	-3.364251	1.121307	-1.530935
3	7	0	-3.841579	-0.452211	1.066045
4	7	0	-0.535710	1.201050	-0.303685
5	7	0	-1.349819	-1.825822	0.590559
6	7	0	0.570062	1.155768	0.645249
7	1	0	-0.184447	1.696968	-1.130203
8	1	0	0.899233	2.097732	0.939504
9	1	0	0.167830	0.761681	1.511626
10	7	0	-3.763349	2.520353	-1.495167
11	1	0	-3.558518	0.799147	-2.488141
12	1	0	-4.618508	2.612082	-0.930883
13	1	0	-3.032538	3.021157	-0.977135
14	1	0	-0.309581	-1.883622	0.379524
15	7	0	-1.605045	-2.056620	2.025746
16	1	0	-1.806082	-2.606251	0.101310
17	1	0	-4.282736	0.295593	1.615205
18	7	0	-4.750539	-1.103928	0.144046
19	1	0	-3.456462	-1.165012	1.708786
20	1	0	-5.639061	-1.338581	0.600993
21	1	0	-4.918398	-0.415212	-0.604589
22	1	0	-1.072284	-2.880750	2.343305
23	1	0	-1.187980	-1.248034	2.505207
24	22	0	2.356648	-0.010263	0.164677
25	7	0	1.489251	-1.837148	-0.081851
26	1	0	1.774415	-2.821324	-0.075509
27	7	0	1.459816	-1.307471	-1.431809
28	1	0	2.060363	-1.811168	-2.091571
29	1	0	0.499938	-1.216541	-1.797518
30	7	0	3.332032	1.266032	1.389285
31	1	0	4.295344	1.163573	1.740787
32	7	0	2.745391	2.468357	1.954404
33	1	0	2.763108	2.425316	2.982400
34	1	0	3.298827	3.293010	1.687908
35	7	0	4.408729	-0.513479	-0.655775
36	1	0	4.806328	-1.329849	-0.175856

37	1	0	4.959900	0.315279	-0.387533
38	7	0	4.485718	-0.784033	-2.086667
39	1	0	3.853702	-0.097622	-2.519397
40	1	0	5.435645	-0.579718	-2.429353

Ti(II) D2 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2478.319435 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.425020	0.197907	0.582549
2	7	0	2.884654	1.512956	0.588281
3	7	0	2.382692	-1.518655	-0.421150
4	7	0	0.091177	1.589857	-0.280087
5	7	0	0.647063	-1.393115	2.001621
6	7	0	0.497827	2.241507	-1.540556
7	1	0	-0.041960	2.365364	0.381046
8	1	0	1.004024	1.523117	-2.073626
9	1	0	-0.366369	2.415046	-2.080916
10	7	0	2.997867	2.909495	0.219595
11	1	0	3.630126	1.345103	1.279165
12	1	0	3.839637	3.019714	-0.364875
13	1	0	2.210905	3.082386	-0.423730
14	1	0	-0.288109	-1.006296	2.302023
15	7	0	0.436280	-2.725809	1.414012
16	1	0	1.256487	-1.523219	2.817296
17	1	0	1.594828	-1.752405	-1.084463
18	7	0	3.618511	-1.231001	-1.134933
19	1	0	2.530600	-2.350257	0.163876
20	1	0	3.508748	-1.515168	-2.115041
21	1	0	3.709644	-0.206504	-1.115381
22	1	0	-0.168198	-3.265022	2.050016
23	1	0	-0.149483	-2.538182	0.582438
24	22	0	-1.340614	0.074707	-0.155181
25	7	0	-1.994248	-0.474775	1.746949
26	1	0	-2.878916	-0.949458	1.977947
27	7	0	-2.233766	0.958340	1.687883
28	1	0	-3.227146	1.207413	1.604881
29	1	0	-1.812864	1.451276	2.480583
30	7	0	-1.110819	-1.402112	-1.519628
31	1	0	-1.947391	-1.752744	-2.014160
32	7	0	0.052488	-1.993193	-2.157775
33	1	0	-0.085230	-3.008257	-2.269114
34	1	0	0.144688	-1.618421	-3.112413
35	7	0	-3.580271	-0.036487	-0.803285
36	1	0	-4.044283	-0.838856	-0.351514

37	1	0	-3.590192	-0.199107	-1.821345
38	7	0	-4.356216	1.137241	-0.441145
39	1	0	-3.785317	1.937437	-0.751867
40	1	0	-5.233827	1.159774	-0.981383

Ti(II) D2 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2479.480022 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0003 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.362075	-0.396659	-0.242027
2	7	0	-2.507896	-1.958729	-0.526671
3	7	0	-2.280711	1.561931	0.192483
4	7	0	0.475809	-0.559610	-1.196053
5	7	0	-1.486363	-0.916873	1.938340
6	7	0	-0.236270	0.437089	-2.002087
7	1	0	0.662237	-1.393161	-1.770176
8	1	0	0.284642	1.330097	-1.814513
9	1	0	-0.220770	0.207518	-3.004219
10	7	0	-2.996919	-2.371107	-1.831407
11	1	0	-2.945023	-2.598785	0.146009
12	1	0	-3.529432	-1.601219	-2.252810
13	1	0	-2.198508	-2.556864	-2.448051
14	1	0	-0.560428	-1.383652	2.110334
15	7	0	-1.607249	0.242822	2.823944
16	1	0	-2.261210	-1.547288	2.175498
17	1	0	-1.406556	2.141546	0.319250
18	7	0	-3.172561	2.178959	-0.784524
19	1	0	-2.778339	1.519822	1.090280
20	1	0	-3.020185	3.196729	-0.775266
21	1	0	-2.853892	1.849726	-1.702314
22	1	0	-1.389050	-0.052875	3.787685
23	1	0	-0.812491	0.842998	2.541772
24	22	0	1.594330	0.161252	0.479738
25	7	0	1.361498	-1.230997	1.999139
26	1	0	1.938756	-1.298696	2.846677
27	7	0	1.993410	-1.999653	0.936476
28	1	0	2.946060	-2.307396	1.157167
29	1	0	1.429264	-2.821523	0.687893
30	7	0	1.287164	2.131448	-0.335905
31	1	0	2.165540	2.678622	-0.399073
32	7	0	0.275274	3.031325	0.212563
33	1	0	0.531467	3.312284	1.172253
34	1	0	0.245453	3.902166	-0.339151
35	7	0	3.405171	0.337971	-0.927367
36	1	0	4.182502	0.850819	-0.503541

37	1	0	3.008091	0.929782	-1.674083
38	7	0	3.948489	-0.903540	-1.442365
39	1	0	3.160215	-1.557354	-1.476808
40	1	0	4.278384	-0.768603	-2.406903
41	1	0	2.789240	1.112450	1.841112
42	1	0	2.032496	1.324552	2.065388

Ti(II) D2 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2480.619950 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.794376	0.427528	0.571676
2	7	0	2.695860	2.070509	-0.043416
3	7	0	2.311456	-1.204022	-0.854527
4	7	0	-0.133247	0.864562	-0.155678
5	7	0	1.140919	-1.256383	2.032503
6	7	0	-0.131827	1.374083	-1.550292
7	1	0	-0.507793	1.651750	0.402941
8	1	0	0.810049	1.749349	-1.743915
9	1	0	-0.261253	0.525955	-2.125910
10	7	0	2.181123	3.369637	0.381783
11	1	0	3.646356	2.247070	-0.380451
12	1	0	1.225430	3.477385	0.025280
13	1	0	2.127447	3.403845	1.408050
14	1	0	0.131406	-1.083115	2.285676
15	7	0	1.256723	-2.630706	1.522331
16	1	0	1.720310	-1.209609	2.875995
17	1	0	1.401506	-1.567749	-1.248675
18	7	0	3.201666	-0.771132	-1.924736
19	1	0	2.761666	-1.996360	-0.382807
20	1	0	2.881554	-1.185207	-2.809668
21	1	0	3.074481	0.244609	-2.006666
22	1	0	0.804654	-3.266173	2.196508
23	1	0	0.637284	-2.657132	0.699124
24	22	0	-1.849638	-0.525676	0.029304
25	7	0	-1.724859	-0.950828	2.019668
26	1	0	-2.261612	-1.522035	2.681580
27	7	0	-2.120003	0.449151	2.141261
28	1	0	-3.048025	0.557238	2.566314
29	1	0	-1.446995	0.982004	2.713776
30	7	0	-1.393232	-1.415598	-1.758232
31	1	0	-2.150387	-1.757163	-2.370137
32	7	0	-0.210906	-2.230211	-2.024729
33	1	0	-0.393109	-3.213517	-1.765510
34	1	0	-0.025982	-2.251557	-3.040369
35	7	0	-2.962272	1.072819	-1.155406
36	1	0	-3.553961	0.708122	-1.907172

37	1	0	-2.127424	1.520841	-1.590300
38	7	0	-3.762728	2.025352	-0.405549
39	1	0	-3.382396	2.016538	0.546400
40	1	0	-3.612608	2.968479	-0.784083
41	1	0	-3.678893	-1.433939	-0.003235
42	1	0	-3.177657	-2.061681	-0.003283
43	1	0	3.706221	-0.261088	1.182384
44	1	0	3.474776	0.201753	1.781731

Ti(II) D2 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2481.778436 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.745940	0.246121	0.741847
2	7	0	3.051404	1.505360	-0.063751
3	7	0	2.098361	-1.236599	-0.958023
4	7	0	-0.107822	0.889493	-0.107792
5	7	0	0.873696	-1.564633	1.910937
6	7	0	-0.000166	1.353553	-1.509616
7	1	0	-0.423930	1.730082	0.398142
8	1	0	0.976080	1.644390	-1.667751
9	1	0	-0.190147	0.515612	-2.081371
10	7	0	3.323583	2.915230	0.171510
11	1	0	3.854878	1.168898	-0.608247
12	1	0	2.428110	3.411829	0.120190
13	1	0	3.654454	3.034930	1.139161
14	1	0	-0.117182	-1.294888	2.165372
15	7	0	0.854605	-2.854006	1.211169
16	1	0	1.411006	-1.714543	2.770287
17	1	0	1.157055	-1.549837	-1.305912
18	7	0	2.934990	-0.798187	-2.062739
19	1	0	2.540417	-2.075301	-0.565667
20	1	0	2.597297	-1.227006	-2.932477
21	1	0	2.789400	0.214219	-2.145169
22	1	0	0.268777	-3.507323	1.751173
23	1	0	0.319102	-2.683893	0.347328
24	22	0	-1.965354	-0.334868	0.007569
25	7	0	-1.926769	-0.857893	1.977840
26	1	0	-2.536826	-1.386644	2.610982
27	7	0	-2.145981	0.574098	2.159447
28	1	0	-3.063463	0.777372	2.572161
29	1	0	-1.425762	0.990537	2.768767
30	7	0	-1.593629	-1.234998	-1.793692
31	1	0	-2.370486	-1.458870	-2.434409
32	7	0	-0.520109	-2.189858	-2.048147
33	1	0	-0.832558	-3.147548	-1.818500
34	1	0	-0.307960	-2.215875	-3.058637
35	7	0	-2.841865	1.421891	-1.149945
36	1	0	-3.497756	1.172238	-1.895208

37	1	0	-1.950505	1.736234	-1.592029
38	7	0	-3.464035	2.482147	-0.374447
39	1	0	-3.099510	2.379645	0.578398
40	1	0	-3.144307	3.392511	-0.726669
41	1	0	-3.897939	-0.987330	-0.085481
42	1	0	-3.485637	-1.676568	-0.106745
43	1	0	3.461863	-0.831453	1.423191
44	1	0	3.335377	-0.307224	1.999226
45	1	0	1.106914	1.212565	2.368347
46	1	0	1.516505	1.796491	1.985153

Ti(II) D2 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2482.920936 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.801048	0.674766	-0.053698
2	7	0	-3.319738	0.042059	1.079868
3	7	0	-1.733308	-1.350019	-1.160664
4	7	0	-0.072338	-0.004407	1.002390
5	7	0	-0.663899	2.470101	-1.016417
6	7	0	-0.171960	-1.238767	1.814762
7	1	0	0.376646	0.673502	1.631589
8	1	0	-1.095081	-1.251881	2.270407
9	1	0	-0.206969	-2.005168	1.128605
10	7	0	-3.493218	0.122766	2.519014
11	1	0	-4.221142	-0.292613	0.722006
12	1	0	-2.559325	0.251278	2.924951
13	1	0	-4.002257	0.989157	2.754876
14	1	0	0.344990	2.255318	-0.795304
15	7	0	-0.833873	2.798891	-2.428396
16	1	0	-0.914387	3.324810	-0.508243
17	1	0	-0.760189	-1.698227	-1.010475
18	7	0	-2.712945	-2.330407	-0.710320
19	1	0	-1.857897	-1.263079	-2.173735
20	1	0	-2.268651	-3.255229	-0.683669
21	1	0	-2.949258	-2.045428	0.250290
22	1	0	0.067761	3.109693	-2.812520
23	1	0	-1.066874	1.918531	-2.900710
24	22	0	1.573353	-0.292783	-0.444405
25	7	0	2.231281	1.675191	-0.502605
26	1	0	2.537375	2.136470	-1.373130
27	7	0	2.806916	2.397318	0.630779
28	1	0	3.807391	2.576492	0.466384
29	1	0	2.368543	3.324483	0.721703
30	7	0	1.276906	-2.288140	-0.780908
31	1	0	1.372168	-3.030820	-0.073407
32	7	0	1.068119	-3.039125	-2.025697
33	1	0	0.806124	-2.342844	-2.734645
34	1	0	1.979982	-3.394381	-2.351327
35	7	0	2.657133	-0.943259	1.443454
36	1	0	3.226127	-1.773775	1.249486

37	1	0	1.826046	-1.252364	1.987857
38	7	0	3.491304	-0.020481	2.198467
39	1	0	3.177355	0.930462	1.930737
40	1	0	3.312655	-0.149786	3.200541
41	1	0	3.594090	-0.332920	-1.327566
42	1	0	3.380303	-1.066808	-1.428634
43	1	0	-3.094112	1.022398	-1.631988
44	1	0	-3.418856	1.460376	-1.054987
45	1	0	1.135872	0.030986	-2.353653
46	1	0	0.410954	0.202773	-2.002767
47	1	0	-2.353076	2.327792	1.070959
48	1	0	-1.659673	2.175111	1.418534

Ti(II) D3 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2366.581913 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.298294	-0.674826	0.344889
2	7	0	-2.017040	1.172790	0.034754
3	7	0	-3.205875	-1.509196	-0.583608
4	7	0	-0.191161	-1.832549	-0.868950
5	7	0	-0.392320	-0.236871	2.323407
6	7	0	1.153538	-1.383028	-1.152695
7	1	0	-0.398798	-2.672509	-1.427132
8	1	0	1.892802	-2.066350	-0.894233
9	1	0	1.275936	-1.193233	-2.160909
10	7	0	-1.424940	2.451358	0.483107
11	1	0	-2.688435	1.433997	-0.697324
12	1	0	-2.117144	2.930691	1.076343
13	1	0	-0.662253	2.178893	1.125001
14	1	0	-0.163215	-1.067147	2.887147
15	7	0	0.801366	0.515698	1.986737
16	1	0	-1.055939	0.325625	2.878413
17	1	0	-3.397710	-2.349382	-0.021990
18	7	0	-4.355556	-0.623332	-0.642127
19	1	0	-3.001697	-1.809885	-1.544104
20	1	0	-5.220662	-1.161615	-0.513466
21	1	0	-4.249675	0.007065	0.162663
22	1	0	1.290200	0.802651	2.846701
23	22	0	1.653132	0.323838	0.175214
24	7	0	3.475714	-0.425627	0.109006
25	1	0	4.297938	0.120213	0.408861
26	7	0	0.733941	1.590913	-1.426074
27	1	0	0.887406	1.271174	-2.390135
28	1	0	-0.272043	1.392137	-1.232921
29	7	0	3.854601	-1.783698	-0.205912
30	1	0	4.628558	-1.792799	-0.882418
31	1	0	4.192150	-2.265833	0.636311
32	7	0	0.875573	3.060585	-1.469981
33	1	0	0.082362	3.391735	-0.894542
34	1	0	1.718901	3.267031	-0.918198

Ti(II) D4 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2366.589512 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.334301	-0.181600	-0.444791
2	7	0	-0.724191	-1.794963	-1.411729
3	7	0	-3.551627	0.321145	-0.341625
4	7	0	-0.690711	1.530721	-1.225810
5	7	0	-1.570079	0.452664	1.740415
6	7	0	0.741526	1.272613	-1.309064
7	1	0	-0.952488	2.235315	-1.927424
8	1	0	1.013224	1.066294	-2.284668
9	1	0	1.327409	2.081079	-1.007630
10	7	0	0.744577	-1.945628	-1.370665
11	1	0	-1.118708	-2.558311	-1.972296
12	1	0	0.999604	-2.865990	-0.972535
13	1	0	1.135274	-1.939921	-2.326334
14	1	0	-0.681738	0.296141	2.237439
15	7	0	-1.924497	1.857723	1.653604
16	1	0	-2.340195	-0.038818	2.211764
17	1	0	-4.035688	0.468117	-1.236906
18	7	0	-4.273971	-0.623692	0.508545
19	1	0	-3.548930	1.215288	0.175007
20	1	0	-5.294729	-0.479789	0.418835
21	1	0	-4.062440	-1.556088	0.126469
22	1	0	-1.702735	2.337622	2.533061
23	1	0	-1.322978	2.239437	0.903938
24	22	0	1.652694	-0.361223	0.001630
25	7	0	3.151014	0.954669	0.020904
26	1	0	4.079668	0.655431	0.351715
27	7	0	1.430199	-1.320047	1.698451
28	1	0	1.179850	-1.508788	2.671815
29	7	0	3.166031	2.359491	-0.309541
30	1	0	3.356840	2.924334	0.527621
31	1	0	3.914073	2.567264	-0.984574
32	7	0	2.747106	-1.777444	1.356359
33	1	0	3.498371	-1.410690	1.955301
34	1	0	2.834030	-2.796588	1.280024

Ti(II) D5 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2366.590958 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.237191	-0.401936	0.728738
2	7	0	0.139608	-0.907285	2.328918
3	7	0	1.358273	1.820290	0.866859
4	7	0	0.156030	-1.568535	-0.642073
5	7	0	2.776742	-0.118476	-0.947429
6	7	0	0.550018	-1.577945	-2.048524
7	1	0	-0.039951	-2.533754	-0.335023
8	1	0	1.221493	-2.342128	-2.202204
9	1	0	-0.274536	-1.774918	-2.629367
10	7	0	-1.311391	-0.829700	2.182601
11	1	0	0.381681	-1.200826	3.282393
12	1	0	-1.759596	-1.736888	2.386738
13	1	0	-1.723941	-0.145191	2.834494
14	1	0	3.132348	0.849313	-0.950868
15	7	0	3.822519	-1.118056	-1.061162
16	1	0	2.137901	-0.256283	-1.750697
17	1	0	1.065841	2.066114	1.823959
18	7	0	2.564023	2.540506	0.467354
19	1	0	0.570204	2.071939	0.226641
20	1	0	2.443702	3.547642	0.654113
21	1	0	3.308571	2.211739	1.099528
22	1	0	4.614115	-0.737109	-1.595107
23	1	0	4.157275	-1.304742	-0.108968
24	22	0	-1.437015	-0.257724	0.015697
25	7	0	-1.034257	1.468574	-0.938441
26	1	0	-0.316739	1.492999	-1.679424
27	7	0	-3.106541	-0.969589	-0.739602
28	1	0	-3.635576	-1.114832	-1.606097
29	7	0	-2.127938	2.366018	-1.292545
30	1	0	-1.871238	3.334261	-1.060992
31	1	0	-2.277408	2.346666	-2.309232
32	7	0	-3.591192	0.149923	0.022661
33	1	0	-3.745324	1.025090	-0.501776
34	1	0	-4.363979	-0.076637	0.654013

Ti(II) D6 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2366.601942 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.603701	0.123523	-0.131081
2	7	0	1.201555	-1.245948	-1.502415
3	7	0	1.550162	-1.147177	1.679408
4	7	0	-0.077232	1.229202	-0.865644
5	7	0	-3.397874	1.650838	1.067946
6	7	0	-0.307723	2.592523	-0.381462
7	1	0	0.049967	1.261207	-1.889625
8	1	0	0.559087	3.142141	-0.469638
9	1	0	-1.000288	3.052325	-0.990753
10	7	0	-0.188951	-1.602693	-1.704466
11	1	0	1.805477	-1.807013	-2.117686
12	1	0	-0.469292	-1.478799	-2.692397
13	1	0	-0.360365	-2.594214	-1.471982
14	1	0	-3.422817	2.674614	1.143176
15	7	0	-2.048529	1.170364	1.344839
16	1	0	-3.587047	1.405521	0.086707
17	1	0	0.626693	-1.619589	1.706568
18	7	0	2.610081	-2.186923	1.698384
19	1	0	1.627747	-0.646817	2.573058
20	1	0	2.294336	-2.874654	1.001517
21	1	0	3.407502	-1.721362	1.240153
22	1	0	-1.335872	1.909255	1.168813
23	1	0	-2.024932	0.884344	2.327661
24	22	0	-1.367778	-0.365463	-0.177677
25	7	0	3.368063	0.782925	0.518381
26	1	0	4.200958	1.025039	1.063439
27	7	0	-3.114783	-0.962444	-0.870447
28	1	0	-3.800373	-1.362253	-1.518373
29	7	0	3.183044	1.625183	-0.628350
30	1	0	3.122141	2.629426	-0.412890
31	1	0	3.867706	1.482116	-1.381038
32	7	0	-3.264691	-1.426512	0.477421
33	1	0	-4.007430	-0.952362	1.005307
34	1	0	-3.335370	-2.441617	0.585488

Ti(II) D6 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2367.757704 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.439627	-0.319986	0.077952
2	7	0	1.097967	0.606161	1.799496
3	7	0	1.354492	1.420505	-1.254178
4	7	0	-0.193183	-1.588198	0.629681
5	7	0	-3.679488	-1.482973	-1.295697
6	7	0	-0.487079	-2.764704	-0.180748
7	1	0	0.024375	-1.897007	1.589864
8	1	0	0.373021	-3.309113	-0.333852
9	1	0	-1.135302	-3.378138	0.333841
10	7	0	-0.271322	0.739585	2.308209
11	1	0	1.754592	1.022545	2.474017
12	1	0	-0.379292	0.252845	3.210044
13	1	0	-0.515966	1.727427	2.467481
14	1	0	-3.656311	-2.396834	-1.766334
15	7	0	-2.330240	-0.925840	-1.271720
16	1	0	-3.926344	-1.664300	-0.315944
17	1	0	0.499407	2.015108	-1.082141
18	7	0	2.536628	2.301625	-1.106391
19	1	0	1.325923	1.166271	-2.247098
20	1	0	2.335815	2.860478	-0.268259
21	1	0	3.289504	1.662475	-0.810366
22	1	0	-1.609928	-1.678546	-1.335311
23	1	0	-2.252621	-0.305109	-2.081760
24	22	0	-1.550551	0.158372	0.539115
25	7	0	3.124092	-0.826528	-0.868085
26	1	0	3.929636	-0.916555	-1.494174
27	7	0	-1.975258	2.050184	-0.000497
28	1	0	-2.875767	2.529399	0.120858
29	7	0	2.977041	-1.943079	0.019759
30	1	0	2.862925	-2.848794	-0.453819
31	1	0	3.710661	-2.023314	0.734536
32	7	0	-1.064126	2.944702	-0.700194
33	1	0	-1.485202	3.251537	-1.589182
34	1	0	-0.922577	3.805299	-0.151595
35	1	0	-3.372992	0.361504	1.319455
36	1	0	-3.159892	-0.401753	1.546837

Ti(II) D6 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2368.899950 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.384578	-0.642619	0.117174
2	7	0	1.325585	0.594393	1.781105
3	7	0	1.959024	1.280992	-1.008136
4	7	0	-0.442156	-1.416293	0.999331
5	7	0	-3.908860	-0.920098	-0.952928
6	7	0	-1.029194	-2.644618	0.492480
7	1	0	-0.248323	-1.528079	2.003078
8	1	0	-0.310053	-3.378373	0.458011
9	1	0	-1.763143	-2.963597	1.138811
10	7	0	0.014454	1.105491	2.167073
11	1	0	1.971948	0.665050	2.577665
12	1	0	-0.280743	0.756953	3.091147
13	1	0	0.021478	2.132866	2.228650
14	1	0	-4.140022	-1.895292	-1.181143
15	7	0	-2.461128	-0.744759	-1.017396
16	1	0	-4.167054	-0.780676	0.030564
17	1	0	1.060239	1.726710	-1.309721
18	7	0	2.754076	2.235641	-0.255712
19	1	0	2.490354	1.015495	-1.841562
20	1	0	2.452172	3.183797	-0.515300
21	1	0	2.444624	2.073083	0.717251
22	1	0	-1.958470	-1.647305	-0.862701
23	1	0	-2.245719	-0.386181	-1.951542
24	22	0	-1.364848	0.534569	0.473543
25	7	0	2.337586	-1.453670	-1.427264
26	1	0	3.194292	-1.615957	-1.963585
27	7	0	-1.504598	2.291148	-0.487102
28	1	0	-2.332319	2.900442	-0.494115
29	7	0	1.729457	-2.655834	-0.956961
30	1	0	1.110221	-3.098551	-1.645373
31	1	0	2.386679	-3.352573	-0.586900
32	7	0	-0.540867	2.807127	-1.448562
33	1	0	-0.945886	2.783917	-2.395573
34	1	0	-0.354146	3.801056	-1.253339
35	1	0	2.553807	-1.899136	1.440019
36	1	0	3.028291	-1.298728	1.231598

37	1	0	-3.015313	1.299081	1.303118
38	1	0	-3.020624	0.526438	1.583660

Ti(II) D6 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2370.044406 Hartree/particle
Input spin multiplicity (2*S*+1) = 5
$\langle S^2 \rangle$ = *S*(*S*+1) = 6 (formal), 6.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.601307	-0.775201	-0.102903
2	7	0	1.024488	-0.526327	1.806935
3	7	0	3.600876	0.193720	0.500665
4	7	0	-0.529059	-1.292887	-0.429969
5	7	0	-4.598353	-1.285992	-0.118838
6	7	0	-1.024413	-1.700323	-1.771791
7	1	0	-0.689697	-2.127859	0.155219
8	1	0	-0.777455	-0.915301	-2.386534
9	1	0	-0.427837	-2.472838	-2.109332
10	7	0	-0.308349	-0.109063	2.224138
11	1	0	1.630085	-0.542703	2.639432
12	1	0	-0.680602	-0.736927	2.952738
13	1	0	-0.271744	0.829076	2.649810
14	1	0	-4.824896	-2.152898	-0.621514
15	7	0	-3.423814	-0.675736	-0.728738
16	1	0	-4.316296	-1.554195	0.832377
17	1	0	3.595403	0.389858	1.511275
18	7	0	4.870367	-0.337566	0.053405
19	1	0	3.427676	1.093325	-0.005362
20	1	0	5.643787	0.092488	0.576356
21	1	0	4.872909	-1.339736	0.271110
22	1	0	-2.864750	-1.343709	-1.308083
23	1	0	-3.766095	0.058271	-1.356764
24	22	0	-1.774189	0.167246	0.551566
25	7	0	1.465036	0.845562	-1.286488
26	1	0	0.864939	0.904386	-2.121041
27	7	0	-1.419797	1.932828	-0.122075
28	1	0	-0.470060	1.920547	-0.532095
29	7	0	2.315675	2.015056	-1.211396
30	1	0	2.786717	2.181430	-2.109193
31	1	0	1.763564	2.857321	-1.001844
32	7	0	-1.898310	3.293255	-0.155264
33	1	0	-2.730823	3.328391	-0.755897

34	1	0	-2.228068	3.535089	0.786527
35	1	0	1.935127	-2.776618	0.297935
36	1	0	2.629552	-2.455016	0.551978
37	1	0	2.663619	-1.640132	-1.680323
38	1	0	1.944165	-1.933921	-1.853273
39	1	0	-3.194280	0.504115	1.914834
40	1	0	-3.231963	1.204858	1.506989

Ti(II) D6 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2371.187181 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = $S(S+1)$ = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.380810	-0.527473	-0.017156
2	7	0	1.038647	-0.207332	2.017873
3	7	0	3.668935	-0.434525	0.182184
4	7	0	-0.468940	-1.141269	-0.784417
5	7	0	-4.026493	-1.964082	-0.117166
6	7	0	-0.995641	-0.721259	-2.112099
7	1	0	-0.781054	-2.116741	-0.696358
8	1	0	-0.710136	0.264564	-2.188540
9	1	0	-0.452911	-1.209778	-2.839825
10	7	0	0.114278	0.931703	2.007286
11	1	0	1.840261	0.024000	2.632046
12	1	0	-0.114188	1.231923	2.964486
13	1	0	0.582824	1.714059	1.500202
14	1	0	-4.234186	-2.501383	-0.968148
15	7	0	-3.339218	-0.732377	-0.469811
16	1	0	-3.362361	-2.518426	0.435094
17	1	0	3.925621	-0.446461	1.178831
18	7	0	4.528880	-1.276917	-0.617317
19	1	0	3.745222	0.551552	-0.169463
20	1	0	5.489606	-1.261425	-0.255706
21	1	0	4.180173	-2.237046	-0.539921
22	1	0	-2.831258	-0.806399	-1.379207
23	1	0	-4.060615	-0.012069	-0.567148
24	22	0	-1.524059	0.030623	0.745956
25	7	0	1.551205	1.519243	-0.408207
26	1	0	0.778849	2.065826	-0.814113
27	7	0	-1.863481	1.813856	-0.024080
28	1	0	-1.277645	2.603162	0.273063
29	7	0	2.823998	2.061903	-0.850377
30	1	0	2.867528	2.135967	-1.878228
31	1	0	2.952570	3.013151	-0.485017
32	7	0	-2.743560	2.356165	-1.038412
33	1	0	-2.793939	1.693962	-1.821293
34	1	0	-3.696762	2.443326	-0.662767
35	1	0	1.715543	-2.575544	0.247138
36	1	0	1.521498	-2.371168	0.990506

37	1	0	-1.504602	-1.784415	1.867703
38	1	0	-0.842494	-1.428592	2.133226
39	1	0	-2.614259	0.370205	2.549067
40	1	0	-3.155444	0.033262	2.094999
41	1	0	2.090415	-1.060134	-1.992154
42	1	0	1.872974	-0.320421	-2.140276

Ti(II) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2366.592431 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.384880	0.235584	-0.361275
2	7	0	0.314653	-1.617031	-0.574651
3	7	0	3.180092	-1.018801	-0.937614
4	7	0	-0.305273	1.550129	-0.009840
5	7	0	2.295042	1.147377	1.142748
6	7	0	-0.764921	2.539693	-1.008418
7	1	0	0.048234	2.053601	0.823012
8	1	0	-1.038459	3.397588	-0.510142
9	1	0	0.036596	2.794084	-1.602142
10	7	0	0.988890	-2.657077	0.259757
11	1	0	0.322887	-2.009161	-1.524336
12	1	0	1.026151	-2.250126	1.204888
13	1	0	0.338229	-3.451260	0.358472
14	1	0	3.150194	0.740337	1.550463
15	7	0	1.753514	2.166076	2.011894
16	1	0	3.170381	-1.151371	-1.961165
17	7	0	4.479805	-0.616051	-0.448535
18	1	0	2.918274	-1.923599	-0.505175
19	1	0	5.224554	-1.027453	-1.022326
20	1	0	4.528427	0.402787	-0.547727
21	1	0	1.670955	1.812220	2.973596
22	1	0	2.390298	2.971345	2.045912
23	22	0	-1.234421	-0.312163	0.029598
24	7	0	-2.773809	0.593130	-1.314554
25	1	0	-3.033947	0.119096	-2.182774
26	1	0	-2.206246	1.450857	-1.540718
27	7	0	-2.425726	-0.965822	1.448321
28	1	0	-2.502580	-0.898646	2.464725
29	7	0	-4.009888	0.908870	-0.607537
30	1	0	-3.787924	0.833236	0.394403
31	1	0	-4.272125	1.882273	-0.798276
32	7	0	-3.364676	-1.983498	1.006046
33	1	0	-3.993224	-1.597554	0.293751
34	1	0	-2.874672	-2.792485	0.609134

V(II) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2667.367132 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0008 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	2.122730	0.420532	-0.113530
2	7	0	3.748277	1.419271	0.260103
3	7	0	3.486642	-1.143078	-0.966714
4	7	0	0.474330	1.434350	-0.101211
5	7	0	1.040071	-1.504441	0.295141
6	7	0	-0.712770	1.341352	0.749930
7	1	0	0.253815	2.137191	-0.813936
8	1	0	-0.412723	1.049323	1.692653
9	1	0	-1.165447	2.270213	0.810457
10	7	0	4.919534	1.726068	-0.542855
11	1	0	3.767364	2.090267	1.033884
12	1	0	5.591281	0.947428	-0.504348
13	1	0	4.634923	1.831370	-1.521487
14	1	0	0.150716	-1.420265	0.837238
15	7	0	0.758394	-2.197294	-0.961807
16	1	0	1.701721	-2.098288	0.809559
17	1	0	4.117402	-0.761463	-1.683048
18	7	0	4.202710	-1.726900	0.151095
19	1	0	2.887633	-1.869754	-1.383952
20	1	0	5.059197	-2.197660	-0.167625
21	1	0	4.465034	-0.924769	0.742536
22	1	0	0.092789	-2.963283	-0.780143
23	1	0	0.243502	-1.508297	-1.529474
24	23	0	-2.240414	0.014514	0.116394
25	7	0	-1.742464	-1.229288	1.594683
26	1	0	-2.265099	-2.092370	1.811852
27	7	0	-1.118511	-0.736425	2.816498
28	1	0	-1.839868	-0.508734	3.512028
29	1	0	-0.533830	-1.467894	3.241046
30	7	0	-3.332639	1.500899	-0.483512
31	1	0	-4.306256	1.422601	-0.807590
32	7	0	-3.011779	2.883716	-0.190135
33	1	0	-2.996831	3.425881	-1.062898
34	1	0	-3.744183	3.301638	0.397962
35	7	0	-3.744785	-1.444193	-0.672551
36	1	0	-4.426548	-1.653272	0.065712

37	1	0	-3.238145	-2.317008	-0.875977
38	7	0	-4.499106	-0.979597	-1.822849
39	1	0	-3.873120	-0.344672	-2.331140
40	1	0	-4.731927	-1.765336	-2.439885

V(II) D2 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2667.378141 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0008 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.309512	-0.066276	-0.280907
2	7	0	-2.604467	1.371288	-0.248082
3	7	0	-2.483331	-1.439403	1.051261
4	7	0	0.178915	0.893679	-1.382499
5	7	0	-0.676530	-1.937387	-1.315104
6	7	0	0.232857	2.311679	-1.770688
7	1	0	0.361009	0.390600	-2.262909
8	1	0	-0.708857	2.574807	-2.100502
9	1	0	0.353120	2.816871	-0.873230
10	7	0	-3.912143	1.425907	0.370007
11	1	0	-2.433383	2.236712	-0.780546
12	1	0	-3.932174	2.159463	1.092373
13	1	0	-4.618042	1.691483	-0.329739
14	1	0	0.201736	-1.722081	-1.838816
15	7	0	-0.410312	-3.034883	-0.383451
16	1	0	-1.408857	-2.264169	-1.952443
17	1	0	-2.275399	-1.224880	2.036815
18	7	0	-3.915889	-1.493940	0.797144
19	1	0	-2.088007	-2.368445	0.845680
20	1	0	-4.392940	-1.901328	1.612041
21	1	0	-4.200507	-0.496642	0.726911
22	1	0	0.066072	-3.796613	-0.887787
23	1	0	0.291658	-2.636924	0.260134
24	23	0	1.671941	0.262097	-0.050737
25	7	0	2.099200	-1.267320	-1.465267
26	1	0	2.748646	-2.050076	-1.299089
27	7	0	2.923457	-0.080095	-1.700547
28	1	0	3.932278	-0.259917	-1.688429
29	1	0	2.687393	0.371163	-2.591484
30	7	0	1.407226	1.668818	1.247218
31	1	0	1.751376	1.573772	2.212718
32	7	0	0.525877	2.809004	1.144660
33	1	0	-0.417784	2.543829	1.464028
34	1	0	0.860082	3.569618	1.746745
35	7	0	3.110872	-0.637928	1.437956
36	1	0	3.957783	-0.071836	1.558219

37	1	0	3.392612	-1.539720	1.027727
38	7	0	2.539595	-0.806135	2.764410
39	1	0	1.528411	-0.920911	2.616502
40	1	0	2.900635	-1.661646	3.203775

V(II) D2 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2668.535595 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0012 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.313128	0.082399	-0.320705
2	7	0	2.340472	-1.471792	-0.906867
3	7	0	2.870963	0.905692	1.040594
4	7	0	-0.570420	-0.391537	-1.095441
5	7	0	0.882509	2.209209	-0.747793
6	7	0	-1.021436	-1.655334	-1.711451
7	1	0	-0.982718	0.345130	-1.684232
8	1	0	-0.469167	-1.801923	-2.568010
9	1	0	-0.711549	-2.387929	-1.041345
10	7	0	3.741711	-1.753426	-0.653682
11	1	0	1.975971	-2.138123	-1.602986
12	1	0	3.845659	-2.677069	-0.209745
13	1	0	4.250419	-1.806737	-1.546344
14	1	0	-0.028268	2.299077	-1.245370
15	7	0	0.859339	3.031413	0.465456
16	1	0	1.634777	2.575148	-1.339671
17	1	0	2.808530	0.427980	1.950589
18	7	0	4.232212	0.928086	0.526041
19	1	0	2.559463	1.878637	1.181511
20	1	0	4.892203	1.053150	1.305042
21	1	0	4.371231	-0.026437	0.140898
22	1	0	0.556082	3.986678	0.223403
23	1	0	0.091464	2.612783	1.016411
24	23	0	-1.412137	-0.108356	0.785615
25	7	0	-2.150051	1.714371	0.287462
26	1	0	-2.669352	2.305164	0.949312
27	7	0	-2.056100	2.410530	-0.990080
28	1	0	-2.870042	2.188602	-1.583068
29	1	0	-2.105183	3.426461	-0.840593
30	7	0	-0.743018	-1.778622	1.529432
31	1	0	-0.609525	-1.905457	2.541050
32	7	0	-0.105662	-2.855848	0.810732
33	1	0	0.888058	-2.614215	0.638934
34	1	0	-0.145059	-3.724185	1.354726
35	7	0	-3.275341	-1.120442	-0.001490
36	1	0	-3.545615	-1.917638	0.579812

37	1	0	-2.836040	-1.486634	-0.873527
38	7	0	-4.451700	-0.313115	-0.244117
39	1	0	-4.103881	0.655448	-0.202875
40	1	0	-4.801531	-0.490904	-1.191544
41	1	0	-2.164205	0.241943	2.574640
42	1	0	-1.428870	0.563776	2.618499

V(II) D2 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2669.680202 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$<S^2>$ = *S*(*S*+1) = 12 (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.912062	0.545573	0.390082
2	7	0	2.187087	2.466742	0.413684
3	7	0	2.252560	-1.109242	-1.050859
4	7	0	-0.127595	0.797141	-0.118622
5	7	0	1.524276	-1.072341	1.851372
6	7	0	-0.175756	1.199986	-1.547638
7	1	0	-0.403183	1.657211	0.381227
8	1	0	0.745297	1.583863	-1.812632
9	1	0	-0.304518	0.291124	-2.037819
10	7	0	1.370112	3.647634	0.182750
11	1	0	3.135303	2.838160	0.534778
12	1	0	0.642181	3.405749	-0.497495
13	1	0	0.878459	3.885497	1.054436
14	1	0	0.516510	-0.933797	2.176443
15	7	0	1.645181	-2.466975	1.401622
16	1	0	2.158505	-0.980947	2.650796
17	1	0	1.337022	-1.587835	-1.230312
18	7	0	2.932128	-0.756792	-2.288319
19	1	0	2.835356	-1.811281	-0.578695
20	1	0	2.531539	-1.302789	-3.060496
21	1	0	2.710418	0.227074	-2.475010
22	1	0	1.273965	-3.072878	2.147610
23	1	0	0.959392	-2.552743	0.636264
24	23	0	-1.813296	-0.505614	0.176284
25	7	0	-1.226229	-1.062406	2.105605
26	1	0	-1.717117	-1.794559	2.633885
27	7	0	-2.002247	0.173705	2.245789
28	1	0	-2.854636	0.054072	2.802136
29	1	0	-1.437421	0.898113	2.708213
30	7	0	-1.286738	-1.507330	-1.573116
31	1	0	-2.094889	-1.863352	-2.108069
32	7	0	-0.318385	-2.598146	-1.477696
33	1	0	-0.708473	-3.392550	-0.940589
34	1	0	-0.132658	-2.976982	-2.418503
35	7	0	-2.916680	0.874851	-1.200238
36	1	0	-3.376229	0.390903	-1.977986

37	1	0	-2.089557	1.381304	-1.588161
38	7	0	-3.906762	1.763250	-0.614185
39	1	0	-3.646371	1.866979	0.371459
40	1	0	-3.829947	2.692670	-1.044464
41	1	0	-3.591454	-1.280467	0.456970
42	1	0	-3.133214	-1.929638	0.352453
43	1	0	3.907348	0.450626	0.375626
44	1	0	3.760095	0.486871	1.150484

V(II) D2 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2670.832137 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.847432	-0.011055	-0.713101
2	7	0	-2.840615	1.723974	-0.132648
3	7	0	-1.836865	-0.821608	1.294521
4	7	0	0.027718	0.910932	-0.291250
5	7	0	-1.038528	-1.994749	-1.377389
6	7	0	-0.134490	1.730318	0.939288
7	1	0	0.214766	1.618859	-1.017196
8	1	0	-1.144921	1.972852	0.984085
9	1	0	-0.001156	1.036949	1.693354
10	7	0	-2.643732	3.052715	-0.699239
11	1	0	-3.845096	1.688114	0.071164
12	1	0	-1.783503	3.450803	-0.304588
13	1	0	-2.470355	2.984446	-1.713153
14	1	0	-0.054307	-1.806996	-1.734001
15	7	0	-0.999109	-3.075415	-0.382131
16	1	0	-1.608310	-2.349150	-2.151501
17	1	0	-0.823104	-0.781379	1.589893
18	7	0	-2.718259	-0.167040	2.246318
19	1	0	-2.098950	-1.814401	1.247440
20	1	0	-2.250438	-0.128774	3.159421
21	1	0	-2.812495	0.801680	1.902289
22	1	0	-0.598571	-3.908085	-0.836575
23	1	0	-0.279557	-2.800009	0.322334
24	23	0	1.876043	-0.166451	-0.026859
25	7	0	1.664143	-1.416221	-1.688117
26	1	0	2.339442	-2.165457	-1.884798
27	7	0	2.243621	-0.161990	-2.175956
28	1	0	3.170599	-0.282026	-2.597133
29	1	0	1.638351	0.253022	-2.895988
30	7	0	1.112252	-0.899398	1.791385
31	1	0	1.643587	-0.605400	2.628627
32	7	0	0.978584	-2.358342	1.847810
33	1	0	1.903791	-2.812339	1.790946
34	1	0	0.583029	-2.639280	2.756274
35	7	0	2.625419	1.693921	0.975135
36	1	0	3.053843	1.548148	1.894899

37	1	0	1.701437	2.165977	1.112432
38	7	0	3.562815	2.504722	0.210693
39	1	0	3.418448	2.250064	-0.771902
40	1	0	3.308577	3.495713	0.304157
41	1	0	3.771574	-0.629518	0.098930
42	1	0	3.435602	-1.294605	0.392431
43	1	0	-3.529189	-1.117083	-0.867116
44	1	0	-3.753792	-0.392813	-1.077183
45	1	0	-1.593814	0.416490	-2.602255
46	1	0	-2.214231	0.874095	-2.385152

V(II) D2 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2671.965310 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.761562	0.793924	0.233594
2	7	0	-3.235198	-0.312504	1.209567
3	7	0	-1.707103	-0.713118	-1.371261
4	7	0	0.084809	0.008260	0.880696
5	7	0	-0.620490	2.507155	-0.681797
6	7	0	-0.053340	-1.222531	1.687457
7	1	0	0.580949	0.666117	1.502224
8	1	0	-0.807915	-1.078019	2.373516
9	1	0	-0.433336	-1.915220	1.028702
10	7	0	-3.267055	-0.942610	2.512316
11	1	0	-4.190331	0.040741	1.083640
12	1	0	-2.848854	-1.876940	2.452285
13	1	0	-2.722267	-0.410867	3.206750
14	1	0	0.425488	2.280465	-0.527640
15	7	0	-0.843368	2.882775	-2.076616
16	1	0	-0.828686	3.360312	-0.151719
17	1	0	-0.814497	-1.279699	-1.193053
18	7	0	-2.880839	-1.583805	-1.383172
19	1	0	-1.628045	-0.338483	-2.323693
20	1	0	-2.550926	-2.549593	-1.505422
21	1	0	-3.250046	-1.494121	-0.413032
22	1	0	0.065781	3.083621	-2.512069
23	1	0	-1.224217	2.062325	-2.556602
24	23	0	1.698254	-0.334212	-0.525673
25	7	0	2.102294	1.754574	-0.366446
26	1	0	2.640786	2.206451	-1.120433
27	7	0	2.595986	2.261329	0.911721
28	1	0	3.625166	2.297951	0.906538
29	1	0	2.286761	3.233015	1.053655
30	7	0	0.785784	-2.155558	-1.026620
31	1	0	0.827156	-2.925705	-0.347309
32	7	0	0.992811	-2.825193	-2.309153
33	1	0	0.278020	-2.500007	-2.971074
34	1	0	1.896357	-2.539222	-2.711468
35	7	0	2.686952	-1.207845	1.189528
36	1	0	3.273105	-2.003273	0.919907

37	1	0	1.826076	-1.562016	1.668358
38	7	0	3.476347	-0.361310	2.072188
39	1	0	3.056771	0.580949	2.001292
40	1	0	3.346776	-0.683642	3.039035
41	1	0	3.467875	-0.245828	-1.283950
42	1	0	3.227995	-0.945108	-1.593483
43	1	0	-3.360768	1.319253	-0.902952
44	1	0	-3.409849	1.842740	-0.322010
45	1	0	1.121101	0.004723	-2.421012
46	1	0	0.659223	0.526587	-2.062279
47	1	0	-2.294503	1.620491	1.870919
48	1	0	-1.608202	2.021274	1.791327

V(II) D3 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2555.624692 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.396234	-0.163899	-0.702333
2	7	0	2.553995	1.297469	-0.185763
3	7	0	3.190932	-1.437872	-0.076717
4	7	0	-0.083215	0.591753	-1.747475
5	7	0	0.406544	-1.984117	0.163057
6	7	0	-1.321866	1.150974	-1.205253
7	1	0	0.167220	1.132112	-2.587258
8	1	0	-1.125383	2.068750	-0.750249
9	1	0	-2.005798	1.290600	-1.962353
10	7	0	3.959380	1.607908	-0.306814
11	1	0	2.095417	2.180599	0.059133
12	1	0	4.506876	1.163026	0.441881
13	1	0	4.314661	1.276828	-1.208868
14	1	0	0.989975	-2.307559	0.951197
15	7	0	-0.985902	-1.884398	0.555570
16	1	0	0.508728	-2.679927	-0.593950
17	1	0	3.990369	-0.927776	-0.478961
18	7	0	3.246132	-1.489707	1.375760
19	1	0	3.233112	-2.401106	-0.421881
20	1	0	4.214461	-1.610541	1.700072
21	1	0	2.923133	-0.562171	1.682940
22	1	0	-1.362169	-2.830718	0.695521
23	23	0	-1.752518	-0.079489	0.490667
24	7	0	-1.234633	1.423358	1.606254
25	1	0	-1.277181	1.414619	2.633692
26	7	0	-3.541105	-0.975265	-0.459868
27	1	0	-3.299560	-0.999658	-1.461547
28	1	0	-3.659757	-1.953226	-0.174125
29	7	0	-0.686648	2.679315	1.138076
30	1	0	-1.210241	3.466922	1.541379
31	1	0	0.287226	2.781400	1.455204
32	7	0	-4.813395	-0.307889	-0.229019
33	1	0	-4.580911	0.650733	0.056790
34	1	0	-5.347157	-0.255675	-1.104984

V(II) D5 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2555.660573 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.295435	-0.336685	0.198723
2	7	0	-0.298570	-2.020257	-0.166150
3	7	0	-3.206103	-1.039987	-0.688099
4	7	0	0.337937	0.401561	1.316997
5	7	0	-2.388594	1.545999	0.602456
6	7	0	0.198466	1.719185	1.947434
7	1	0	0.582282	-0.291570	2.040532
8	1	0	-0.219009	1.589202	2.878819
9	1	0	1.137714	2.106761	2.108311
10	7	0	1.145023	-1.920308	-0.303479
11	1	0	-0.591270	-2.978970	-0.390783
12	1	0	1.673593	-2.469907	0.391222
13	1	0	1.459741	-2.256652	-1.224640
14	1	0	-1.634258	2.140621	0.996891
15	7	0	-3.057438	2.134202	-0.558995
16	1	0	-3.112743	1.423854	1.318249
17	1	0	-2.959816	-1.476887	-1.586306
18	7	0	-4.033041	-1.910167	0.140903
19	1	0	-3.755728	-0.195318	-0.894450
20	1	0	-4.591738	-2.538999	-0.449423
21	1	0	-3.387501	-2.488945	0.687908
22	1	0	-3.199324	3.146251	-0.413310
23	1	0	-2.387204	2.027526	-1.334377
24	23	0	1.659530	0.165907	-0.214594
25	7	0	3.470757	-0.134746	0.362708
26	1	0	4.198759	0.578856	0.505043
27	7	0	1.431610	0.938722	-1.986055
28	1	0	0.578807	1.079667	-2.539845
29	7	0	4.016447	-1.466292	0.442053
30	1	0	4.764253	-1.591958	-0.252721
31	1	0	4.443453	-1.619314	1.364322
32	7	0	1.701445	2.093630	-1.157567
33	1	0	2.501533	2.635975	-1.500161
34	1	0	0.898692	2.716895	-1.005706

V(II) D5 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2556.818879 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.368622	-0.415343	0.645260
2	7	0	-0.426940	-2.167683	0.092252
3	7	0	-2.746109	-0.839691	-1.043819
4	7	0	0.371152	0.293103	1.611339
5	7	0	-1.999688	1.695645	0.328497
6	7	0	0.305094	1.637756	2.191872
7	1	0	0.746848	-0.354957	2.320889
8	1	0	-0.190573	1.583524	3.092460
9	1	0	1.258412	1.964185	2.402390
10	7	0	1.014587	-1.999536	0.009728
11	1	0	-0.620556	-3.115411	0.439521
12	1	0	1.521620	-2.375463	0.828207
13	1	0	1.422902	-2.498983	-0.792281
14	1	0	-1.333683	2.235718	0.910625
15	7	0	-1.967611	2.069981	-1.082559
16	1	0	-2.950569	1.862977	0.669506
17	1	0	-2.152489	-1.518075	-1.545776
18	7	0	-4.105196	-1.309628	-0.837440
19	1	0	-2.794749	0.045840	-1.568513
20	1	0	-4.415103	-1.857672	-1.650048
21	1	0	-4.072123	-1.953095	-0.039731
22	1	0	-2.085226	3.088652	-1.169391
23	1	0	-0.997111	1.837971	-1.408655
24	23	0	1.453326	0.099021	-0.147751
25	7	0	3.360010	-0.251879	-0.291794
26	1	0	4.113002	0.453112	-0.279465
27	7	0	0.811695	1.313448	-1.619449
28	1	0	1.235645	1.202840	-2.551185
29	7	0	3.907363	-1.585522	-0.360599
30	1	0	4.446729	-1.702807	-1.227889
31	1	0	4.566919	-1.740509	0.412914
32	7	0	1.714612	2.113688	-0.799667
33	1	0	2.585875	2.379181	-1.271283
34	1	0	1.247851	2.956256	-0.450021
35	1	0	-2.523662	-1.391821	1.917270
36	1	0	-2.630932	-0.613852	2.129235

V(II) D5 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2557.966793 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0003 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.115931	0.831571	-0.742246
2	7	0	0.732368	-0.790267	-2.016005
3	7	0	2.710569	-0.487475	0.055189
4	7	0	-0.919539	1.289732	-0.829860
5	7	0	1.218292	2.174217	1.035975
6	7	0	-1.407436	2.522151	-0.213862
7	1	0	-1.379433	1.162549	-1.742925
8	1	0	-1.304888	3.291828	-0.888005
9	1	0	-2.414864	2.427138	-0.020221
10	7	0	-0.186297	-1.629750	-1.192380
11	1	0	0.185471	-0.568303	-2.859336
12	1	0	-0.784582	-2.208477	-1.802990
13	1	0	0.417325	-2.294075	-0.688459
14	1	0	0.277952	2.616078	0.966239
15	7	0	1.398600	1.439368	2.285076
16	1	0	1.931860	2.908445	1.017816
17	1	0	2.192718	-1.156688	0.661117
18	7	0	3.435619	-1.181980	-0.998956
19	1	0	3.389966	0.005380	0.641747
20	1	0	3.717205	-2.110278	-0.657854
21	1	0	2.712508	-1.320148	-1.731662
22	1	0	0.980789	1.977116	3.056745
23	1	0	0.826386	0.579828	2.179548
24	23	0	-1.217812	-0.485096	0.262159
25	7	0	-0.289415	-1.350017	1.796310
26	1	0	-0.764688	-1.437479	2.704563
27	7	0	-2.996884	-0.975285	-0.356164
28	1	0	-3.252407	-1.761632	-0.971223
29	7	0	0.838848	-2.259713	1.745514
30	1	0	1.417760	-2.147711	2.589412
31	1	0	0.510902	-3.235606	1.767194
32	7	0	-4.111179	-0.081405	-0.154626
33	1	0	-4.481509	0.252351	-1.054595
34	1	0	-4.882965	-0.572639	0.315370
35	1	0	-2.495819	0.517954	1.538025
36	1	0	-1.802507	0.716404	1.830495

37	1	0	1.857307	2.051685	-2.063710
38	1	0	2.523958	1.650330	-1.838757

V(II) D5 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2559.096523 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = S(S+1) = 12 (formal), 12.0003 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.502867	-0.283489	-0.566429
2	7	0	-0.670391	1.363268	-1.509742
3	7	0	-2.983633	1.170438	0.375213
4	7	0	0.242077	-1.324265	-0.844849
5	7	0	-2.122886	-2.002041	0.723005
6	7	0	0.359692	-2.730607	-0.455928
7	1	0	0.750411	-1.189840	-1.729865
8	1	0	0.068687	-3.311709	-1.255670
9	1	0	1.377533	-2.899618	-0.334460
10	7	0	0.743137	1.462049	-1.139152
11	1	0	-0.731538	1.514310	-2.524889
12	1	0	1.374830	1.253195	-1.924419
13	1	0	0.990608	2.398256	-0.765036
14	1	0	-1.262938	-2.586844	0.579726
15	7	0	-2.393355	-1.732496	2.132725
16	1	0	-2.933130	-2.522224	0.373777
17	1	0	-2.620717	1.418278	1.306514
18	7	0	-3.155883	2.339761	-0.469254
19	1	0	-3.904644	0.751833	0.532595
20	1	0	-3.344189	3.163469	0.113930
21	1	0	-2.215228	2.444553	-0.911315
22	1	0	-2.162431	-2.567724	2.688807
23	1	0	-1.711242	-1.016301	2.406558
24	23	0	1.290194	0.109170	0.399958
25	7	0	2.309096	1.655152	1.246406
26	1	0	2.966633	1.590800	2.033471
27	7	0	2.954027	-0.554618	-0.489289
28	1	0	3.789457	0.002497	-0.269360
29	7	0	2.082414	3.031223	0.883620
30	1	0	1.686095	3.566244	1.669428
31	1	0	2.969503	3.489385	0.639689
32	7	0	3.268551	-1.964892	-0.522321
33	1	0	3.781389	-2.185259	-1.385233
34	1	0	3.892560	-2.229359	0.254800
35	1	0	1.986895	-1.018287	1.862351
36	1	0	1.230712	-1.254537	1.823881

37	1	0	-2.436199	-1.033385	-2.090387
38	1	0	-2.964109	-0.469001	-1.868493
39	1	0	-0.369647	0.650519	1.363264
40	1	0	0.252240	1.059269	1.726141

V(II) D5 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2560.227127 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = S(S+1) = 12 (formal), 12.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.451363	-0.900894	-0.352510
2	7	0	-0.031607	-1.973337	0.650459
3	7	0	-2.353082	-0.659003	1.619753
4	7	0	-0.290462	0.768906	-0.048894
5	7	0	-4.100113	0.802232	-1.029850
6	7	0	-0.826565	2.079120	-0.446054
7	1	0	0.035549	0.864724	0.932062
8	1	0	-1.431000	2.423505	0.315822
9	1	0	-0.019957	2.728628	-0.427071
10	7	0	1.313339	-1.418023	0.749754
11	1	0	0.050682	-2.994874	0.675317
12	1	0	1.533016	-1.191911	1.730167
13	1	0	2.052832	-2.072334	0.424745
14	1	0	-4.559811	1.488898	-1.642801
15	7	0	-2.781102	0.467838	-1.541655
16	1	0	-4.663837	-0.053608	-1.060992
17	1	0	-1.711526	0.007445	2.074326
18	7	0	-3.748762	-0.312684	1.797131
19	1	0	-2.168286	-1.566847	2.063195
20	1	0	-3.890336	0.109842	2.721781
21	1	0	-3.963743	0.394816	1.079546
22	1	0	-2.821481	0.275027	-2.552001
23	1	0	-2.154755	1.310306	-1.402817
24	23	0	1.860486	0.306998	-0.424837
25	7	0	3.742880	-0.465621	-0.162715
26	1	0	4.615397	0.045675	-0.345181
27	7	0	2.086352	1.559198	1.158492
28	1	0	3.015138	1.471939	1.595491
29	7	0	3.957133	-1.888018	-0.323504
30	1	0	4.285985	-2.129953	-1.272611
31	1	0	4.685902	-2.210964	0.324584
32	7	0	1.794061	2.958783	0.884188
33	1	0	1.609795	3.451847	1.767543
34	1	0	2.603621	3.437233	0.458417
35	1	0	-1.000952	-1.453195	-2.217758
36	1	0	-0.379692	-0.988689	-2.055845

37	1	0	-2.817034	-2.333213	-0.517671
38	1	0	-2.139895	-2.748620	-0.538214
39	1	0	1.509691	-0.687540	-2.123656
40	1	0	2.300205	-0.746024	-2.000914
41	1	0	1.953865	1.745555	-1.735998
42	1	0	2.726304	1.646226	-1.540206

V(II) D6 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2555.665801 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0005 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.448152	-0.064241	0.116259
2	7	0	-0.870387	-1.954004	0.196182
3	7	0	-3.407526	-0.626198	-0.717518
4	7	0	0.224455	0.449609	1.355333
5	7	0	3.638840	1.907209	-0.455216
6	7	0	0.383400	1.866512	1.698522
7	1	0	-0.031717	-0.066017	2.211389
8	1	0	-0.546757	2.265063	1.888514
9	1	0	0.928895	1.941040	2.566279
10	7	0	0.527552	-2.291929	0.438238
11	1	0	-1.380393	-2.815338	-0.041889
12	1	0	0.649012	-2.726309	1.364769
13	1	0	0.866683	-2.983690	-0.244429
14	1	0	3.775251	2.904079	-0.243084
15	7	0	2.216271	1.596224	-0.498592
16	1	0	4.008436	1.374354	0.339278
17	1	0	-3.299543	-1.150053	-1.596443
18	7	0	-4.335169	-1.267772	0.191738
19	1	0	-3.754298	0.332845	-0.940196
20	1	0	-5.078905	-1.745081	-0.331030
21	1	0	-3.809695	-1.978163	0.709914
22	1	0	1.645667	2.139658	0.185736
23	1	0	1.891803	1.820604	-1.444863
24	23	0	1.593632	-0.425242	0.079032
25	7	0	-1.922356	1.783741	-0.341388
26	1	0	-1.281826	2.587416	-0.292189
27	7	0	3.378823	-1.379361	0.041964
28	1	0	4.329904	-1.014743	0.184434
29	7	0	-3.170944	2.185327	-0.963045
30	1	0	-3.660940	2.864605	-0.367341
31	1	0	-2.992375	2.656010	-1.859456
32	7	0	3.018368	-1.207777	-1.353173
33	1	0	3.563630	-0.493114	-1.851524
34	1	0	3.061864	-2.086127	-1.880868

V(II) D6 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2556.811895 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = S(S+1) = 12 (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.425817	0.074109	-0.289554
2	7	0	0.931427	-1.833578	-0.456659
3	7	0	3.467620	-0.467296	0.337609
4	7	0	-0.448511	0.605471	-1.182078
5	7	0	-4.202046	1.496420	-0.231178
6	7	0	-0.753697	2.045328	-1.238395
7	1	0	-0.257662	0.292744	-2.145923
8	1	0	0.138799	2.560273	-1.245669
9	1	0	-1.221296	2.259190	-2.128995
10	7	0	-0.447161	-2.288062	-0.614400
11	1	0	1.524338	-2.662092	-0.313906
12	1	0	-0.560108	-2.772370	-1.515705
13	1	0	-0.710698	-2.953964	0.129992
14	1	0	-4.201477	2.473765	-0.546796
15	7	0	-2.910354	1.189520	0.367472
16	1	0	-4.277194	0.917184	-1.072302
17	1	0	3.466532	-1.186356	1.074469
18	7	0	4.410773	-0.781490	-0.719658
19	1	0	3.733111	0.446204	0.765115
20	1	0	5.207256	-1.309609	-0.342638
21	1	0	3.922197	-1.386443	-1.386697
22	1	0	-2.166584	1.843672	0.019425
23	1	0	-3.032276	1.322420	1.377294
24	23	0	-1.834519	-0.657191	-0.154461
25	7	0	1.739867	1.814410	0.568488
26	1	0	1.011772	2.505462	0.793722
27	7	0	-2.110641	-1.731094	1.582427
28	1	0	-2.889239	-1.518700	2.220130
29	7	0	2.988784	2.197290	1.203773
30	1	0	3.375700	3.030929	0.744116
31	1	0	2.834463	2.449432	2.188494
32	7	0	-1.082794	-0.719800	1.799886
33	1	0	-1.279475	-0.021221	2.526337
34	1	0	-0.161301	-1.135344	1.983726
35	1	0	-2.880868	-1.014922	-1.725272
36	1	0	-3.258705	-1.419219	-1.107596

V(II) D6 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2557.957441 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = $S(S+1)$ = 12 (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.481546	0.151180	-0.514044
2	7	0	0.957312	-1.772732	-0.088200
3	7	0	3.492949	-0.336980	0.268410
4	7	0	-0.494130	0.642758	-1.222375
5	7	0	-4.300909	1.338358	-0.296059
6	7	0	-0.837486	2.084877	-1.147766
7	1	0	-0.443479	0.408756	-2.221874
8	1	0	0.045911	2.612102	-1.087228
9	1	0	-1.280813	2.371529	-2.029708
10	7	0	-0.339796	-2.250030	-0.556081
11	1	0	1.625959	-2.552327	-0.169968
12	1	0	-0.286177	-2.606345	-1.523956
13	1	0	-0.674138	-3.015410	0.048690
14	1	0	-4.342201	2.322078	-0.588389
15	7	0	-3.017828	1.084400	0.343912
16	1	0	-4.313524	0.776784	-1.152725
17	1	0	3.432708	-1.206452	0.817864
18	7	0	4.655539	-0.319069	-0.595266
19	1	0	3.560818	0.461533	0.937530
20	1	0	5.444976	-0.793511	-0.140881
21	1	0	4.420585	-0.855661	-1.434765
22	1	0	-2.295443	1.783300	0.043002
23	1	0	-3.182849	1.177904	1.352134
24	23	0	-1.829729	-0.688579	-0.166441
25	7	0	1.434990	1.558120	0.844024
26	1	0	0.601764	2.109463	1.086223
27	7	0	-2.058395	-1.735799	1.597000
28	1	0	-2.843581	-1.473933	2.209534
29	7	0	2.537359	1.898711	1.718354
30	1	0	2.842457	2.865545	1.549289
31	1	0	2.252842	1.845368	2.704788
32	7	0	-1.044050	-0.700958	1.751520
33	1	0	-1.185914	-0.031727	2.515408
34	1	0	-0.095539	-1.103176	1.787463
35	1	0	2.075230	0.173070	-2.319828
36	1	0	1.856909	-0.619709	-2.285221

37	1	0	-3.223437	-1.565037	-1.062317
38	1	0	-2.883762	-1.165546	-1.706214

V(II) D6 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2559.100280 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = $S(S+1)$ = 12 (formal), 12.0003 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.623075	-0.429072	-0.306171
2	7	0	1.002399	-1.058260	1.559158
3	7	0	3.761742	-0.315834	0.299636
4	7	0	-0.400266	-0.546366	-0.936815
5	7	0	-3.947119	-1.862097	-1.026658
6	7	0	-0.921309	0.323074	-2.015277
7	1	0	-0.558482	-1.497070	-1.299700
8	1	0	-1.091076	1.219254	-1.519861
9	1	0	-0.161818	0.484636	-2.690792
10	7	0	-0.011804	-0.123733	2.065795
11	1	0	1.716577	-1.163707	2.298840
12	1	0	-0.270225	-0.375490	3.030225
13	1	0	0.354141	0.842851	2.101012
14	1	0	-4.048290	-2.014112	-2.037106
15	7	0	-3.310333	-0.575782	-0.796983
16	1	0	-3.297523	-2.577173	-0.684981
17	1	0	3.876500	-0.492380	1.308810
18	7	0	4.773695	-0.993657	-0.484763
19	1	0	3.856201	0.712618	0.136678
20	1	0	5.669812	-1.002266	0.017112
21	1	0	4.476718	-1.966876	-0.595925
22	1	0	-2.734128	-0.263017	-1.613631
23	1	0	-4.063680	0.105624	-0.660158
24	23	0	-1.715574	-0.311724	0.713054
25	7	0	1.735702	1.482616	-0.629566
26	1	0	0.930054	2.076616	-0.864874
27	7	0	-1.851587	1.696386	0.397697
28	1	0	-1.208061	2.269505	0.957005
29	7	0	2.913500	2.292693	-0.396720
30	1	0	3.209500	2.741497	-1.272376
31	1	0	2.709887	3.050754	0.267427
32	7	0	-3.067091	2.479373	0.318743
33	1	0	-3.408651	2.474522	-0.647834
34	1	0	-3.815001	2.074411	0.901972
35	1	0	1.911143	-2.189777	-1.135567
36	1	0	1.720092	-2.439693	-0.398170

37	1	0	-1.646217	-2.318070	1.089731
38	1	0	-0.869828	-2.157128	1.129793
39	1	0	-2.817445	0.307810	2.199566
40	1	0	-3.055450	-0.453936	2.144749

V(II) D6 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2560.252258 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = S(S+1) = 12 (formal), 12.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.608936	-0.580223	-0.266276
2	7	0	0.981270	-0.653832	1.703655
3	7	0	3.731921	-0.292295	0.329184
4	7	0	-0.440376	-0.810309	-0.784372
5	7	0	-3.970739	-2.080471	-0.397102
6	7	0	-0.986980	-0.248938	-2.037914
7	1	0	-0.650458	-1.815871	-0.859275
8	1	0	-1.117155	0.753666	-1.800087
9	1	0	-0.269183	-0.306783	-2.772702
10	7	0	0.058733	0.474529	1.893483
11	1	0	1.724455	-0.561464	2.417237
12	1	0	-0.087796	0.654647	2.894553
13	1	0	0.509672	1.306530	1.444612
14	1	0	-4.059857	-2.524512	-1.318345
15	7	0	-3.352818	-0.773509	-0.549466
16	1	0	-3.317820	-2.652934	0.147135
17	1	0	3.856966	-0.420271	1.344268
18	7	0	4.794780	-0.915931	-0.431840
19	1	0	3.743386	0.737632	0.126831
20	1	0	5.696031	-0.796904	0.046356
21	1	0	4.600191	-1.920595	-0.467005
22	1	0	-2.804199	-0.693847	-1.436318
23	1	0	-4.114955	-0.089377	-0.587715
24	23	0	-1.708600	-0.090582	0.778463
25	7	0	1.528205	1.469338	-0.308233
26	1	0	0.770904	1.907491	-0.852583
27	7	0	-1.863736	1.745534	-0.102089
28	1	0	-1.252697	2.465163	0.301638
29	7	0	2.757282	2.223811	-0.478428
30	1	0	2.938456	2.441734	-1.469130
31	1	0	2.686157	3.125158	0.008143
32	7	0	-3.089697	2.445764	-0.428537
33	1	0	-3.412804	2.142052	-1.352881
34	1	0	-3.842844	2.218534	0.239121
35	1	0	1.844882	-2.557848	-0.466296
36	1	0	1.686366	-2.504848	0.309319

37	1	0	-1.627665	-1.902818	1.706432
38	1	0	-0.847094	-1.736505	1.700918
39	1	0	-2.767807	0.945168	2.035882
40	1	0	-2.978710	0.201955	2.244039
41	1	0	2.134114	-0.932233	-2.139394
42	1	0	2.216812	-0.140222	-2.083453

V(II) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2555.653910 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.450475	0.015909	0.151934
2	7	0	-0.047104	1.565559	0.047380
3	7	0	-3.069674	1.411915	-0.626024
4	7	0	0.140189	-1.122016	0.998276
5	7	0	-2.537902	-1.417621	-0.773728
6	7	0	-0.067985	-2.581795	0.877059
7	1	0	0.051536	-0.955221	2.009931
8	1	0	-0.001474	-2.782956	-0.128060
9	1	0	0.723733	-3.076357	1.317160
10	7	0	-0.293402	2.248248	1.328962
11	1	0	-0.007414	2.308384	-0.657351
12	1	0	-1.285273	2.152237	1.610823
13	1	0	0.270195	1.783480	2.048640
14	1	0	-2.141672	-2.299882	-1.122993
15	7	0	-2.782212	-1.547005	0.645779
16	1	0	-2.615039	1.826948	-1.451757
17	7	0	-4.308585	0.735061	-0.961316
18	1	0	-3.302669	2.188565	0.000684
19	1	0	-4.753743	1.198366	-1.760815
20	1	0	-3.987564	-0.213189	-1.250141
21	1	0	-3.779361	-1.529752	0.876434
22	1	0	-2.288143	-2.339296	1.083230
23	23	0	1.431026	0.113635	-0.126470
24	7	0	2.693383	-1.669219	-0.694543
25	1	0	2.450503	-1.997191	-1.635722
26	1	0	2.401355	-2.404323	-0.036563
27	7	0	3.001879	1.212525	-0.413331
28	1	0	3.721463	1.072781	-1.129710
29	7	0	4.132859	-1.469748	-0.674123
30	1	0	4.279784	-0.668819	-0.044700
31	1	0	4.598638	-2.294544	-0.282853
32	7	0	3.170142	2.572437	0.063708
33	1	0	2.233266	2.935741	0.272827
34	1	0	3.658076	2.547139	0.968578

V(II) D8 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2555.661472 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$\langle S^2 \rangle = S(S+1) = 12$ (formal), 12.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.467235	-0.341014	-0.198601
2	7	0	0.372180	1.250831	0.474470
3	7	0	2.815568	0.608881	-1.201238
4	7	0	-0.106210	-1.545817	-0.777772
5	7	0	2.233934	-1.688815	0.919630
6	7	0	-0.477765	-2.863287	-0.214234
7	1	0	-0.282882	-1.622506	-1.786497
8	1	0	0.084509	-3.585189	-0.688305
9	1	0	-0.108821	-2.835900	0.745925
10	7	0	0.412058	2.592843	-0.141158
11	1	0	0.423591	1.417458	1.486557
12	1	0	1.418874	2.775574	-0.333490
13	1	0	0.017088	2.455134	-1.081494
14	1	0	2.154227	-2.703234	0.794344
15	7	0	3.319066	-1.473359	1.851342
16	1	0	3.479013	0.102951	-1.802910
17	7	0	3.165881	2.008632	-1.120846
18	1	0	4.081817	2.118591	-0.665544
19	1	0	3.261814	2.400735	-2.067140
20	1	0	3.979561	-0.820829	1.412042
21	1	0	2.946401	-0.986532	2.674632
22	23	0	-1.257284	0.036757	0.014812
23	7	0	-2.939068	-1.402711	0.064901
24	1	0	-3.358543	-1.496717	0.995702
25	1	0	-2.392142	-2.275109	-0.115570
26	7	0	-2.740251	1.649976	0.492947
27	1	0	-3.165664	1.915778	-0.408069
28	1	0	-3.498252	1.241484	1.050638
29	7	0	-4.048058	-1.198257	-0.863931
30	1	0	-3.626240	-0.803439	-1.712827
31	1	0	-4.450320	-2.108171	-1.126995
32	7	0	-2.241036	2.801041	1.226812
33	1	0	-1.307102	3.019732	0.830182
34	1	0	-2.849904	3.608385	1.049507

V(II) D8 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2556.811883 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$<S^2>$ = *S*(*S*+1) = 12 (formal), 12.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.551870	-0.225100	-0.384564
2	7	0	0.095707	0.828863	0.601959
3	7	0	2.819740	1.198790	-0.715244
4	7	0	0.013209	-1.622366	-0.899361
5	7	0	2.560122	-1.651910	0.437673
6	7	0	-0.223978	-2.693908	0.084896
7	1	0	0.160249	-2.049939	-1.821466
8	1	0	-0.457839	-3.563377	-0.408338
9	1	0	0.673798	-2.840534	0.575077
10	7	0	0.098366	2.303268	0.638561
11	1	0	-0.011004	0.543437	1.583564
12	1	0	1.092082	2.591887	0.757118
13	1	0	-0.087420	2.567159	-0.340145
14	1	0	2.753761	-2.519837	-0.077054
15	7	0	3.640799	-1.471709	1.378032
16	1	0	3.582752	1.055838	-1.392323
17	7	0	2.950904	2.500846	-0.093608
18	1	0	3.824302	2.541533	0.448555
19	1	0	3.027970	3.229920	-0.815818
20	1	0	4.040133	-0.540539	1.205969
21	1	0	3.240834	-1.435508	2.322807
22	23	0	-1.289982	0.015552	-0.744420
23	7	0	-2.462742	-1.051903	0.775668
24	1	0	-2.521396	-0.429722	1.591834
25	1	0	-1.847485	-1.876568	0.952597
26	7	0	-2.895961	1.525307	-0.241793
27	1	0	-3.026123	2.308930	-0.894766
28	1	0	-3.742732	0.940415	-0.277708
29	7	0	-3.827434	-1.385323	0.405219
30	1	0	-3.769327	-1.832674	-0.516189
31	1	0	-4.212174	-2.084021	1.056309
32	7	0	-2.761014	1.974977	1.136099
33	1	0	-1.794043	2.350993	1.216658
34	1	0	-3.421149	2.739787	1.319927
35	1	0	-2.106079	-0.296100	-2.464335
36	1	0	-1.476553	0.234008	-2.612330

V(II) D8 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2557.964649 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0005 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	1.560525	-0.350009	-0.551899
2	7	0	0.190279	0.672796	0.598177
3	7	0	2.846085	1.067997	-0.871773
4	7	0	-0.120979	-1.687296	-0.843016
5	7	0	2.325183	-1.624135	0.753719
6	7	0	-0.353529	-2.613335	0.284003
7	1	0	-0.072032	-2.234670	-1.709089
8	1	0	-0.561851	-3.546705	-0.089085
9	1	0	0.572002	-2.664837	0.762635
10	7	0	0.287682	2.134167	0.755611
11	1	0	0.073978	0.307239	1.552264
12	1	0	1.287562	2.342912	0.944584
13	1	0	0.179274	2.481078	-0.208941
14	1	0	2.981166	-2.353604	0.455909
15	7	0	2.844896	-1.125070	2.011805
16	1	0	3.518647	1.018218	-1.649063
17	7	0	3.132593	2.225978	-0.052663
18	1	0	4.068427	2.130849	0.363028
19	1	0	3.167809	3.071996	-0.638373
20	1	0	3.177814	-0.161325	1.875057
21	1	0	2.064780	-1.060614	2.675115
22	23	0	-1.261186	0.052390	-0.778296
23	7	0	-2.570315	-0.863246	0.725209
24	1	0	-2.616042	-0.186861	1.499407
25	1	0	-1.998508	-1.703119	0.972020
26	7	0	-2.704602	1.742337	-0.302113
27	1	0	-2.701440	2.558466	-0.927237
28	1	0	-3.613952	1.272585	-0.405670
29	7	0	-3.938792	-1.146147	0.333070
30	1	0	-3.882678	-1.633835	-0.567276
31	1	0	-4.370991	-1.799207	1.001181
32	7	0	-2.592984	2.122430	1.099115
33	1	0	-1.590780	2.367800	1.245536
34	1	0	-3.163800	2.955837	1.283489
35	1	0	2.166198	-1.111781	-2.321142
36	1	0	2.751578	-1.378419	-1.870806

37	1	0	-2.199500	-0.314710	-2.438561
38	1	0	-1.541074	0.142598	-2.648502

V(II) D8 with 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2559.103694 Hartree/particle
Input spin multiplicity ($2S$+1) = 7
$<S^2>$ = S(S+1) = 12 (formal), 12.0004 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.058409	-0.647555	0.679463
2	7	0	-0.481166	0.334522	-1.104486
3	7	0	-2.980396	-0.339490	0.605442
4	7	0	0.909912	0.133817	1.413311
5	7	0	-0.068640	-2.337138	-0.020058
6	7	0	1.870010	-0.801561	2.003563
7	1	0	0.622339	0.799466	2.145620
8	1	0	2.491591	-0.301308	2.652174
9	1	0	1.358487	-1.491522	2.569846
10	7	0	-1.325607	1.266271	-1.870528
11	1	0	-0.333720	-0.446156	-1.760329
12	1	0	-2.300577	0.948441	-1.689739
13	1	0	-1.276667	2.160968	-1.366284
14	1	0	0.393729	-2.967399	0.645051
15	7	0	-0.937569	-3.216244	-0.806653
16	1	0	-3.614643	-0.628267	1.362577
17	7	0	-3.753830	0.164017	-0.509485
18	1	0	-4.352481	-0.584673	-0.884256
19	1	0	-4.387488	0.910687	-0.192839
20	1	0	-1.917005	-3.042572	-0.534964
21	1	0	-0.875544	-2.921490	-1.787703
22	23	0	1.379724	0.941148	-0.442339
23	7	0	0.665151	2.940437	0.361963
24	1	0	0.919950	3.707701	-0.268104
25	1	0	1.207668	3.083128	1.226237
26	7	0	2.098431	-0.974318	-1.147273
27	1	0	1.266910	-1.619436	-0.869213
28	1	0	2.235506	-0.990480	-2.163301
29	7	0	-0.763458	3.066379	0.605618
30	1	0	-1.107349	2.131587	0.897381
31	1	0	-0.934875	3.719614	1.379312
32	7	0	3.342191	-1.470568	-0.554467
33	1	0	3.143094	-1.410392	0.460366
34	1	0	3.392554	-2.480738	-0.752044
35	1	0	-1.390162	-1.066965	2.576416
36	1	0	-1.399624	-1.796835	2.252154

37	1	0	3.090603	1.370864	0.546616
38	1	0	3.303169	1.409419	-0.214034
39	1	0	1.154580	1.582636	-2.338947
40	1	0	1.894500	1.808213	-2.184451

V(II) D8 with 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2560.258571 Hartree/particle
Input spin multiplicity (2*S*+1) = 7
$\langle S^2 \rangle$ = *S*(*S*+1) = 12 (formal), 12.0002 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.106675	1.506897	0.001806
2	7	0	0.041699	0.028921	-1.509754
3	7	0	2.021754	1.648347	0.307368
4	7	0	0.059928	-0.152004	1.332204
5	7	0	-2.208605	1.241071	-0.139056
6	7	0	-0.919934	-0.329146	2.404489
7	1	0	0.972701	0.103900	1.758377
8	1	0	-0.471278	-0.826665	3.185317
9	1	0	-1.174537	0.595912	2.777684
10	7	0	0.981943	0.035680	-2.635126
11	1	0	-0.884416	0.019692	-1.958684
12	1	0	1.104047	1.014049	-2.933728
13	1	0	1.897307	-0.237355	-2.244284
14	1	0	-2.725030	1.203131	0.748266
15	7	0	-3.069157	2.058546	-0.999400
16	1	0	2.500634	2.455881	-0.118953
17	7	0	2.435423	1.559931	1.708116
18	1	0	3.459317	1.484533	1.772198
19	1	0	2.182657	2.414962	2.228095
20	1	0	-2.671001	3.005497	-1.087305
21	1	0	-3.028722	1.662741	-1.944861
22	23	0	0.081142	-1.572241	-0.177931
23	7	0	2.310429	-1.770255	0.006375
24	1	0	2.586777	-2.680494	-0.377240
25	1	0	2.518619	-1.804968	1.016244
26	7	0	-2.086211	-1.551522	-0.317804
27	1	0	-2.277964	-0.488476	-0.417835
28	1	0	-2.435353	-2.051924	-1.141754
29	7	0	3.111852	-0.756659	-0.662510
30	1	0	2.739602	0.197594	-0.315831
31	1	0	4.092871	-0.851253	-0.368418
32	7	0	-2.817855	-2.087083	0.831540
33	1	0	-2.377603	-1.595852	1.631305
34	1	0	-3.776746	-1.712596	0.785483
35	1	0	-0.113648	2.857704	1.462994
36	1	0	-0.881413	2.750788	1.265923

37	1	0	0.321499	3.076425	-1.074438
38	1	0	-0.334638	2.832737	-1.454092
39	1	0	0.237647	-2.341613	-2.052728
40	1	0	0.170336	-2.996789	-1.624010
41	1	0	0.081882	-2.795476	1.417515
42	1	0	-0.155166	-3.269958	0.830540

Cr(II) D1 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2868.297909 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0005 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	2.081933	-0.095814	-0.043832
2	7	0	3.599804	-1.227532	0.568858
3	7	0	3.622329	1.148763	-1.023754
4	7	0	0.803571	-1.266885	0.909681
5	7	0	0.636936	1.398188	-0.746884
6	7	0	-0.606983	-1.577984	0.730782
7	1	0	1.258166	-2.147913	1.178046
8	1	0	-0.774144	-2.360513	0.059371
9	1	0	-0.975232	-1.911456	1.635530
10	7	0	3.811948	-1.286058	2.012967
11	1	0	3.578416	-2.210409	0.269953
12	1	0	4.426491	-0.506453	2.267081
13	1	0	2.917569	-1.115957	2.498414
14	1	0	-0.179556	1.463748	-0.061575
15	7	0	1.170883	2.734645	-1.020369
16	1	0	0.264192	1.055295	-1.641227
17	1	0	3.982615	1.839157	-0.348265
18	7	0	4.674809	0.303159	-1.548002
19	1	0	3.196489	1.689673	-1.784828
20	1	0	5.553343	0.832337	-1.593134
21	1	0	4.753606	-0.433269	-0.809068
22	1	0	0.382120	3.379377	-1.169272
23	1	0	1.600433	3.038780	-0.139573
24	24	0	-2.095674	-0.248626	0.086199
25	7	0	-1.405020	1.282441	1.250244
26	1	0	-0.742949	1.030179	1.997597
27	7	0	-2.377871	2.242779	1.754652
28	1	0	-2.729670	1.959327	2.679249
29	1	0	-1.939097	3.162050	1.885502
30	7	0	-2.827455	-1.664370	-1.101489
31	1	0	-3.419970	-1.475887	-1.919398
32	7	0	-2.168963	-2.942287	-1.247866
33	1	0	-2.840978	-3.710071	-1.130201
34	1	0	-1.760974	-3.047640	-2.185320
35	7	0	-3.706955	1.043060	-0.421115
36	1	0	-3.642581	1.545499	-1.312408

37	1	0	-3.575753	1.746756	0.346240
38	7	0	-5.030584	0.420809	-0.393069
39	1	0	-4.852713	-0.583292	-0.247053
40	1	0	-5.525168	0.766155	0.435075

Cr(II) D1 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2869.433071 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$<S^2>$ = $S(S+1)$ = 20 (formal), 20.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.935531	-0.310917	0.599177
2	7	0	-3.802695	-0.705745	0.117401
3	7	0	-2.128310	2.950616	0.374686
4	7	0	-1.138682	-1.171195	-1.038617
5	7	0	-0.038733	0.459787	1.332940
6	7	0	0.205174	-1.751921	-1.087554
7	1	0	-1.779478	-1.906613	-1.369132
8	1	0	0.348863	-2.519705	-0.393623
9	1	0	0.347191	-2.160780	-2.022206
10	7	0	-4.307922	-1.333857	-1.075903
11	1	0	-4.440871	-1.000273	0.863090
12	1	0	-3.964101	-0.797911	-1.878054
13	1	0	-3.916241	-2.284510	-1.186535
14	1	0	0.346561	0.832804	0.431150
15	7	0	0.068480	1.601461	2.267373
16	1	0	0.669171	-0.234223	1.633053
17	1	0	-2.287565	3.788579	-0.199644
18	7	0	-1.958455	1.773334	-0.449080
19	1	0	-2.983299	2.799806	0.919725
20	1	0	-2.658380	1.709495	-1.199187
21	1	0	-1.010307	1.789016	-0.871173
22	1	0	-0.557234	2.317247	1.859997
23	1	0	-0.406203	1.300281	3.127329
24	24	0	1.878156	-0.529220	-0.693865
25	7	0	0.951698	1.107790	-1.508775
26	1	0	0.276674	0.862224	-2.248465
27	7	0	1.785937	2.225360	-1.931210
28	1	0	2.106429	2.107931	-2.901444
29	1	0	1.253502	3.103016	-1.904119
30	7	0	2.402779	-1.795276	0.776569
31	1	0	3.381997	-1.869226	1.087266
32	7	0	1.763762	-3.090997	0.909182
33	1	0	2.359068	-3.841922	0.536048
34	1	0	1.604081	-3.309280	1.899627
35	7	0	3.410918	0.820861	-0.121181
36	1	0	3.121759	1.666386	-0.670932

37	1	0	4.385753	0.628548	-0.374911
38	7	0	3.437052	1.168445	1.313096
39	1	0	2.644917	1.807970	1.465087
40	1	0	3.138495	0.303424	1.788095
41	1	0	-2.482959	-0.761692	2.350875
42	1	0	-2.677844	0.022034	2.378101

Cr(II) D2 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2868.301642 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$<S^2>$ = $S(S+1)$ = 20 (formal), 20.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.616100	-0.176484	0.185857
2	7	0	2.825556	1.321113	0.685316
3	7	0	3.200850	-0.774274	-1.255291
4	7	0	-0.065173	0.276426	1.226183
5	7	0	0.799136	-2.192997	-0.157847
6	7	0	-0.215297	1.538825	1.960557
7	1	0	-0.264813	-0.467263	1.921338
8	1	0	0.708419	1.783917	2.340407
9	1	0	-0.422581	2.253274	1.239886
10	7	0	2.550224	2.709939	0.347082
11	1	0	3.114849	1.344089	1.671125
12	1	0	2.875939	2.869043	-0.611343
13	1	0	1.533312	2.879410	0.344531
14	1	0	-0.221041	-2.244167	0.185629
15	7	0	0.887980	-2.660060	-1.540795
16	1	0	1.370132	-2.843638	0.393947
17	1	0	3.088220	-0.229518	-2.122766
18	7	0	4.501600	-0.579808	-0.648941
19	1	0	3.074473	-1.761285	-1.510202
20	1	0	5.207529	-0.423187	-1.377468
21	1	0	4.363961	0.302593	-0.106440
22	1	0	0.304144	-3.502302	-1.643138
23	1	0	0.419034	-1.937297	-2.099695
24	24	0	-1.710416	-0.006545	0.011974
25	7	0	-1.828929	-1.925196	0.783549
26	1	0	-2.658786	-2.493893	0.552076
27	7	0	-1.506963	-2.107915	2.191103
28	1	0	-2.276440	-1.792732	2.794751
29	1	0	-1.353164	-3.101192	2.400928
30	7	0	-1.730887	1.735323	-1.010216
31	1	0	-1.802466	1.672863	-2.038351
32	7	0	-0.895846	2.866473	-0.666592
33	1	0	-0.066880	2.914854	-1.273469
34	1	0	-1.415097	3.741563	-0.809329
35	7	0	-3.610036	-0.349952	-1.044734
36	1	0	-4.074518	-1.160753	-0.623232

37	1	0	-3.467130	-0.565437	-2.041879
38	7	0	-4.464225	0.807093	-0.846157
39	1	0	-3.792507	1.601177	-0.864967
40	1	0	-5.116929	0.897655	-1.632807

Cr(II) D2 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2869.445499 Hartree/particle
Input spin multiplicity (2*S*+1) = 9
$<S^2>$ = *S*(*S*+1) = 20 (formal), 20.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.390631	0.084695	-0.537151
2	7	0	2.536524	-1.512659	-0.919746
3	7	0	3.015699	0.875279	0.696514
4	7	0	-0.492847	-0.574577	-0.818242
5	7	0	0.701794	2.189621	-0.903957
6	7	0	-0.740543	-2.009801	-0.632091
7	1	0	-1.017079	-0.280794	-1.661015
8	1	0	0.059091	-2.504057	-1.084211
9	1	0	-0.576575	-2.171641	0.379041
10	7	0	1.980396	-2.702561	-1.531153
11	1	0	3.361750	-1.223672	-1.469256
12	1	0	2.024638	-2.650878	-2.557246
13	1	0	2.530201	-3.524754	-1.253604
14	1	0	-0.352603	2.183502	-1.054786
15	7	0	1.032078	3.124802	0.171230
16	1	0	1.171473	2.543978	-1.744150
17	1	0	2.491923	0.829531	1.585707
18	7	0	4.244853	0.112984	0.732828
19	1	0	3.226259	1.862477	0.514232
20	1	0	4.624402	0.109604	1.685812
21	1	0	3.951974	-0.850880	0.490054
22	1	0	0.489588	3.990122	0.034729
23	1	0	0.629505	2.690693	1.014050
24	24	0	-1.399350	0.498513	0.679299
25	7	0	-2.145138	1.760255	-0.761934
26	1	0	-2.886082	2.424293	-0.490885
27	7	0	-2.531459	1.109007	-2.008598
28	1	0	-3.369913	0.526781	-1.871223
29	1	0	-2.743980	1.813778	-2.723076
30	7	0	-0.013560	-0.155475	2.038779
31	1	0	0.232671	0.367972	2.891031
32	7	0	-0.020614	-1.580531	2.331827
33	1	0	0.943072	-1.929555	2.414353
34	1	0	-0.485625	-1.777790	3.227725
35	7	0	-3.307939	-0.978400	0.906031
36	1	0	-4.130565	-0.458071	1.223581

37	1	0	-3.119390	-1.710701	1.606256
38	7	0	-3.623200	-1.537274	-0.397927
39	1	0	-2.707659	-1.903320	-0.743815
40	1	0	-4.244772	-2.348648	-0.286319
41	1	0	-1.965293	1.365622	2.327762
42	1	0	-2.380087	1.784722	1.808764

Cr(II) D2 with 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2870.589949 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.673322	-0.618735	0.655425
2	7	0	-2.583666	-1.653304	-0.774110
3	7	0	-2.477039	1.264759	-0.133785
4	7	0	0.154093	-0.631208	-0.377996
5	7	0	-0.717471	0.339857	2.366952
6	7	0	0.000683	-0.736218	-1.843662
7	1	0	0.650865	-1.489893	-0.094509
8	1	0	-0.990629	-0.986870	-2.006788
9	1	0	0.117149	0.241774	-2.166832
10	7	0	-2.210048	-3.042541	-0.952644
11	1	0	-3.610536	-1.660222	-0.729582
12	1	0	-1.330966	-3.061337	-1.480955
13	1	0	-1.998292	-3.481055	-0.042758
14	1	0	0.306139	0.021974	2.326424
15	7	0	-0.770000	1.803734	2.354065
16	1	0	-1.139348	0.052837	3.255772
17	1	0	-1.640740	1.812464	-0.456137
18	7	0	-3.442998	1.115304	-1.209216
19	1	0	-2.923857	1.809457	0.611188
20	1	0	-3.299783	1.869604	-1.890694
21	1	0	-3.194296	0.228176	-1.672636
22	1	0	-0.083173	2.152837	3.038763
23	1	0	-0.367903	2.065772	1.438363
24	24	0	1.646923	0.757205	0.014195
25	7	0	2.029206	-0.178735	1.798884
26	1	0	2.605822	0.299697	2.505136
27	7	0	2.425465	-1.581308	1.746541
28	1	0	3.446771	-1.667688	1.833680
29	1	0	2.030325	-2.088560	2.549081
30	7	0	1.021191	2.006084	-1.468140
31	1	0	1.714966	2.552814	-1.997718
32	7	0	-0.156320	2.833601	-1.253605
33	1	0	0.080592	3.709637	-0.762761
34	1	0	-0.535322	3.126330	-2.165249
35	7	0	2.896197	-0.488482	-1.552485
36	1	0	3.565118	0.019016	-2.138034

37	1	0	2.058555	-0.710267	-2.123845
38	7	0	3.552873	-1.697657	-1.090349
39	1	0	3.046750	-1.977307	-0.236668
40	1	0	3.418381	-2.445671	-1.781242
41	1	0	3.169685	1.796177	0.628508
42	1	0	2.674156	2.355543	0.374771
43	1	0	-2.924341	-1.438194	1.891815
44	1	0	-2.267654	-1.907521	1.948871

Cr(II) D3 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.557512 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0015 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.669341	-0.249978	-0.451211
2	7	0	-3.024857	1.197500	-0.289331
3	7	0	-2.970937	-1.466054	0.884302
4	7	0	-0.422240	0.978785	-1.413668
5	7	0	-0.308562	-1.948508	-0.515088
6	7	0	0.855129	0.511777	-1.956546
7	1	0	-0.888931	1.541547	-2.138136
8	1	0	0.715128	-0.143468	-2.741176
9	1	0	1.358471	1.311950	-2.363318
10	7	0	-2.612997	2.535444	0.113218
11	1	0	-3.608990	1.344333	-1.122388
12	1	0	-2.676251	2.587955	1.135118
13	1	0	-1.618858	2.667043	-0.125469
14	1	0	-0.029576	-2.245073	-1.465699
15	7	0	0.875026	-1.620869	0.296927
16	1	0	-0.766132	-2.778381	-0.110790
17	1	0	-2.499311	-1.451694	1.800747
18	7	0	-4.324809	-0.948002	0.952254
19	1	0	-3.037865	-2.452726	0.611815
20	1	0	-4.676164	-1.027985	1.911965
21	1	0	-4.195183	0.062764	0.699420
22	1	0	1.364934	-2.509704	0.474836
23	24	0	2.218581	-0.291793	-0.439413
24	7	0	4.046526	-0.271446	0.043440
25	1	0	4.785159	-0.769421	-0.461952
26	7	0	1.268806	1.417723	0.954374
27	1	0	1.772693	2.250016	1.271084
28	1	0	0.565045	1.694165	0.237133
29	7	0	4.706442	0.396749	1.138043
30	1	0	4.007269	1.012837	1.564437
31	1	0	4.933375	-0.297635	1.864963
32	7	0	0.639084	0.813373	2.111730
33	1	0	-0.299064	1.213891	2.243128
34	1	0	0.526233	-0.183200	1.851705

Cr(II) D4 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.562595 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0007 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.803132	-0.131634	0.223148
2	7	0	-0.565067	-1.641503	0.205267
3	7	0	-3.213803	-1.562293	-0.697479
4	7	0	-0.618912	1.413244	0.646339
5	7	0	-3.468159	1.344550	0.180546
6	7	0	0.621462	1.439046	-0.152807
7	1	0	-0.284291	1.424782	1.619067
8	1	0	0.322558	1.524258	-1.131722
9	1	0	1.168759	2.313343	0.026080
10	7	0	0.828817	-1.588434	0.592559
11	1	0	-0.935096	-2.557285	0.504295
12	1	0	0.924465	-1.673574	1.615372
13	1	0	1.379192	-2.378972	0.188293
14	1	0	-3.806670	1.490091	1.143412
15	7	0	-2.998037	2.576609	-0.423909
16	1	0	-4.265552	0.986654	-0.357757
17	1	0	-2.800062	-2.506849	-0.656741
18	7	0	-4.603146	-1.526034	-0.277725
19	1	0	-3.196613	-1.290326	-1.687586
20	1	0	-5.114988	-2.330459	-0.661689
21	1	0	-4.601947	-1.630629	0.741557
22	1	0	-3.549413	3.367600	-0.071359
23	1	0	-2.024125	2.647182	-0.052925
24	24	0	2.158347	-0.017393	-0.003896
25	7	0	3.364181	1.458842	-0.500963
26	1	0	4.372417	1.312117	-0.632948
27	7	0	3.562724	-1.399629	0.088056
28	1	0	4.554941	-1.181343	-0.064980
29	7	0	3.094153	2.814687	-0.084397
30	1	0	3.617133	3.068332	0.765827
31	1	0	3.379670	3.479304	-0.814594
32	7	0	3.278330	-2.770816	-0.264898
33	1	0	3.542823	-2.980014	-1.238110
34	1	0	3.813853	-3.415464	0.330335

Cr(II) D5 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.578180 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.376076	0.255444	-0.604150
2	7	0	1.235863	-1.515923	-1.458118
3	7	0	3.130721	-0.402329	0.492560
4	7	0	-0.410265	0.911377	-1.323524
5	7	0	1.169239	1.700816	0.952372
6	7	0	-0.775847	2.280876	-0.968160
7	1	0	-0.542284	0.765061	-2.334068
8	1	0	-0.514480	2.918425	-1.728612
9	1	0	-1.812170	2.306444	-0.832261
10	7	0	-0.148425	-1.966638	-1.389057
11	1	0	1.682716	-1.903687	-2.295299
12	1	0	-0.519161	-2.206764	-2.317112
13	1	0	-0.234407	-2.798090	-0.785651
14	1	0	0.315899	2.220189	0.622400
15	7	0	1.039911	1.003880	2.226308
16	1	0	1.955260	2.353126	1.036831
17	1	0	3.183341	-1.412722	0.298664
18	7	0	4.388330	0.296658	0.320117
19	1	0	2.830956	-0.260546	1.470017
20	1	0	5.164525	-0.279586	0.666843
21	1	0	4.526013	0.420204	-0.686820
22	1	0	0.637657	1.647020	2.920141
23	1	0	0.335322	0.248239	2.086619
24	24	0	-1.510011	-0.615660	-0.309554
25	7	0	-2.985449	0.443489	0.443878
26	1	0	-3.753030	-0.062660	0.903729
27	7	0	-1.694972	-2.077173	1.033625
28	1	0	-2.614754	-2.421363	1.346072
29	7	0	-3.482960	1.655687	-0.163744
30	1	0	-4.258135	1.464993	-0.813599
31	1	0	-3.853242	2.288992	0.556820
32	7	0	-1.035936	-1.421001	2.163504
33	1	0	-1.711259	-0.881678	2.724305
34	1	0	-0.615825	-2.128461	2.781540

Cr(II) D6 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.588006 Hartree/particle
Input spin multiplicity ($2S+1$) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0005 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.479787	0.065221	-0.023980
2	7	0	0.655353	-1.806071	-0.383266
3	7	0	3.192919	-0.974112	0.720808
4	7	0	-0.100121	0.977304	-1.044098
5	7	0	-3.693808	1.893075	0.008116
6	7	0	-0.237690	2.406177	-0.764589
7	1	0	0.190686	0.866865	-2.030343
8	1	0	0.712108	2.808948	-0.777301
9	1	0	-0.760466	2.849629	-1.530291
10	7	0	-0.482463	-1.823902	-1.336563
11	1	0	0.225619	-2.185313	0.474320
12	1	0	-0.076097	-1.655097	-2.263472
13	1	0	-0.875723	-2.773894	-1.379126
14	1	0	-3.791267	2.840624	0.391252
15	7	0	-2.547951	1.245993	0.617359
16	1	0	-3.487751	1.993935	-0.989962
17	1	0	3.076782	-1.266822	1.700731
18	7	0	3.575141	-2.066107	-0.147158
19	1	0	3.894163	-0.203534	0.695022
20	1	0	4.130910	-2.752499	0.373976
21	1	0	2.677464	-2.497660	-0.430632
22	1	0	-1.786410	1.917271	0.812474
23	1	0	-2.887064	0.729960	1.454029
24	24	0	-1.628072	-0.318055	-0.450051
25	7	0	2.411806	1.762398	0.450558
26	1	0	1.945795	2.578650	0.864688
27	7	0	-2.677593	-1.649139	0.566702
28	1	0	-3.096008	-2.489278	0.145482
29	7	0	3.822050	1.778021	0.779119
30	1	0	4.323513	2.439304	0.173262
31	1	0	3.976833	2.093916	1.745108
32	7	0	-3.485558	-1.200407	1.680183
33	1	0	-4.485984	-1.190435	1.441610
34	1	0	-3.372871	-1.839161	2.475745

Cr(II) D6 with 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2757.717364 Hartree/particle
Input spin multiplicity (2*S*+1) = 9
$<S^2>$ = *S*(*S*+1) = 20 (formal), 20.0005 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.128005	0.090990	-0.036414
2	7	0	0.133475	1.626561	0.608893
3	7	0	-2.853127	1.201454	0.590245
4	7	0	0.497516	-0.781026	-1.088425
5	7	0	2.413576	2.439287	-0.944497
6	7	0	0.205249	-2.168862	-1.430161
7	1	0	0.545473	-0.232926	-1.964281
8	1	0	-0.669911	-2.174700	-1.975150
9	1	0	0.953335	-2.545526	-2.024462
10	7	0	1.241867	1.089321	1.404043
11	1	0	-0.330125	2.332491	1.203856
12	1	0	1.879389	1.842868	1.694485
13	1	0	0.920255	0.586207	2.243538
14	1	0	2.372468	2.984527	-1.812602
15	7	0	2.892854	1.097703	-1.236431
16	1	0	1.434191	2.324451	-0.566923
17	1	0	-2.960920	1.200673	1.613859
18	7	0	-2.995681	2.531579	0.034811
19	1	0	-3.586408	0.573089	0.168827
20	1	0	-3.626831	3.095294	0.615057
21	1	0	-2.073747	2.976719	0.051301
22	1	0	2.612421	0.781136	-2.175793
23	1	0	3.917461	1.134631	-1.238781
24	24	0	2.114449	-0.454904	0.159664
25	7	0	-2.463969	-1.282743	-0.688515
26	1	0	-2.274080	-2.291517	-0.702573
27	7	0	1.489455	-1.737956	1.511308
28	1	0	1.820742	-2.704885	1.367604
29	7	0	-3.891022	-1.058723	-0.609195
30	1	0	-4.332471	-1.185524	-1.528555
31	1	0	-4.347183	-1.721130	0.031540
32	7	0	0.038680	-1.746109	1.547011
33	1	0	-0.324857	-2.372394	0.810499
34	1	0	-0.283802	-2.100069	2.455487
35	1	0	3.913710	-0.883386	0.764472
36	1	0	3.804121	-1.359490	0.116988

Cr(II) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.580417 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0006 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	-1.458068	-0.117347	-0.290868
2	7	0	0.167302	-1.441632	-0.499220
3	7	0	-2.742050	-1.602448	0.553200
4	7	0	-0.021721	1.174478	-1.052672
5	7	0	-2.807934	1.302645	-0.122796
6	7	0	-0.296312	2.607321	-0.954791
7	1	0	-0.016309	0.986016	-2.065064
8	1	0	-0.919990	2.724910	-0.145131
9	1	0	0.574405	3.105432	-0.731522
10	7	0	0.285185	-2.099359	-1.815987
11	1	0	0.264666	-2.210529	0.172510
12	1	0	-0.492619	-1.777202	-2.403866
13	1	0	1.142810	-1.768407	-2.275778
14	1	0	-2.813936	2.067933	-0.808980
15	7	0	-4.126408	1.122882	0.441179
16	1	0	-2.316214	-2.534180	0.627383
17	7	0	-3.320352	-1.304686	1.886757
18	1	0	-3.564020	-1.746731	-0.046020
19	1	0	-2.508179	-1.054938	2.466376
20	1	0	-3.794789	-0.394186	1.693690
21	1	0	-4.379338	1.945814	1.002442
22	1	0	-4.842260	1.051119	-0.295215
23	24	0	1.505057	0.077631	-0.079335
24	7	0	2.720311	1.839737	0.409287
25	1	0	2.140618	2.603067	0.775386
26	1	0	3.105191	2.167503	-0.488523
27	7	0	2.909521	-1.038647	0.799634
28	1	0	2.775305	-1.312640	1.780607
29	7	0	3.756110	1.563561	1.387114
30	1	0	3.918991	0.534887	1.267315
31	1	0	4.605344	2.084311	1.146067
32	7	0	3.375300	-2.247284	0.134625
33	1	0	2.611086	-2.680391	-0.403484
34	1	0	4.088844	-1.974590	-0.547608

Cr(II) D8 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2756.572223 Hartree/particle
Input spin multiplicity ($2S$+1) = 9
$\langle S^2 \rangle = S(S+1) = 20$ (formal), 20.0008 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	24	0	1.533874	-0.194963	-0.134227
2	7	0	0.132797	1.365969	-0.009740
3	7	0	3.140366	0.875893	-0.071313
4	7	0	-0.198043	-1.202922	-0.979563
5	7	0	2.354470	-1.995367	0.176056
6	7	0	-0.290236	-2.625478	-0.630730
7	1	0	-0.062261	-1.103746	-1.991660
8	1	0	-0.380013	-3.178230	-1.491033
9	1	0	0.666923	-2.825317	-0.224426
10	7	0	0.169144	2.550347	-0.895814
11	1	0	0.164435	1.785216	0.930202
12	1	0	1.167495	2.849508	-0.849739
13	1	0	0.049211	2.182827	-1.847417
14	1	0	3.021794	-2.345634	-0.522202
15	7	0	3.035578	-2.187323	1.457640
16	1	0	4.090740	0.518814	0.081818
17	7	0	3.137879	2.311909	-0.214221
18	1	0	3.489246	2.762052	0.642922
19	1	0	3.780585	2.591425	-0.967030
20	1	0	3.389525	-1.277550	1.788975
21	1	0	2.321702	-2.466926	2.138371
22	24	0	-1.418699	0.091490	-0.024098
23	7	0	-2.636539	-1.620827	0.457205
24	1	0	-2.883135	-1.730238	1.445801
25	1	0	-1.889099	-2.336577	0.206364
26	7	0	-2.815328	1.608061	0.692091
27	1	0	-3.595626	1.589753	0.019126
28	1	0	-3.220110	1.348519	1.599183
29	7	0	-3.873903	-1.786540	-0.295538
30	1	0	-3.690181	-1.400422	-1.228522
31	1	0	-4.050322	-2.790686	-0.431535
32	7	0	-2.247743	2.937153	0.842614
33	1	0	-1.517040	3.053836	0.111653
34	1	0	-2.977159	3.640605	0.688148

Ti(II) D2 with hydride ligands and no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2257.133001 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.134894	0.624654	-0.128348
2	7	0	3.044130	-0.209361	-1.150107
3	7	0	-0.308481	1.901842	0.665953
4	7	0	1.446203	-1.352878	0.912435
5	7	0	-0.186597	3.016908	-0.250145
6	1	0	-0.350292	2.293300	1.610078
7	1	0	0.805098	3.144503	-0.517127
8	1	0	-0.777027	2.838505	-1.067737
9	1	0	0.651662	-1.482642	1.568126
10	7	0	1.525985	-2.470293	-0.021959
11	1	0	2.351916	-1.306327	1.395690
12	1	0	3.304926	0.253830	-2.028118
13	7	0	4.081879	-0.122242	-0.137034
14	1	0	2.874085	-1.208393	-1.328161
15	1	0	5.012866	-0.179770	-0.567137
16	1	0	3.952447	0.820307	0.268895
17	1	0	1.435862	-3.355173	0.495424
18	1	0	0.681126	-2.378389	-0.605520
19	22	0	-1.441886	0.221601	0.190263
20	7	0	-1.520523	-1.298741	1.540479
21	1	0	-2.152596	-2.083230	1.730697
22	7	0	-1.919531	-0.128436	2.293588
23	1	0	-2.909633	-0.090954	2.558977
24	1	0	-1.338578	0.041767	3.120189
25	7	0	-2.086446	-0.916806	-1.680697
26	1	0	-1.905785	-1.923378	-1.629601
27	1	0	-1.425854	-0.523058	-2.370312
28	7	0	-3.486227	-0.734668	-2.036563
29	1	0	-3.693639	0.213899	-1.682173
30	1	0	-3.582288	-0.722427	-3.058902
31	1	0	-2.706128	1.322057	-0.544131
32	1	0	2.392910	1.910688	0.337059

Ti(II) D2 with hydride ligands 1 H_2 molecule bound
Sum of electronic and thermal Enthalpies= -2258.297042 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = S(S+1) = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.184074	0.655805	0.122851
2	7	0	2.787123	-0.783668	0.762846
3	7	0	0.689219	-0.855663	-1.269541
4	7	0	-0.062826	2.549679	-0.115287
5	7	0	1.270361	-2.203336	-1.142299
6	1	0	0.669521	-0.599430	-2.263541
7	1	0	0.479678	-2.863575	-1.112472
8	1	0	1.814081	-2.408858	-1.989387
9	1	0	-0.941064	2.240973	-0.584554
10	7	0	-0.358292	3.321899	1.082736
11	1	0	0.483646	3.151601	-0.739580
12	1	0	2.370863	-1.627361	0.302805
13	7	0	4.115502	-0.483086	0.235163
14	1	0	2.891871	-0.962351	1.764621
15	1	0	4.464906	-1.309649	-0.263715
16	1	0	3.954576	0.257242	-0.463877
17	1	0	-1.298041	3.725633	0.994909
18	1	0	-0.395157	2.648205	1.857193
19	22	0	-1.182873	-0.572621	-0.322132
20	7	0	-2.429910	0.905952	-0.898571
21	1	0	-3.415451	1.170070	-0.803741
22	7	0	-2.182164	0.205428	-2.137260
23	1	0	-2.973542	-0.343067	-2.491176
24	1	0	-1.827792	0.812047	-2.883974
25	7	0	-1.792119	-0.893040	1.835709
26	1	0	-2.302630	-0.098378	2.233697
27	1	0	-0.862078	-0.909185	2.286540
28	7	0	-2.582247	-2.092515	2.068614
29	1	0	-2.329691	-2.714990	1.285891
30	1	0	-2.283156	-2.535278	2.944924
31	1	0	2.372467	1.990029	1.040069
32	1	0	2.423892	1.508278	-0.914616
33	1	0	1.984945	1.717578	1.688883
34	1	0	-1.490807	-2.381125	-0.459501

Ti(II) D2 with hydride ligands and 2 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2259.450239 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$<S^2>$ = S(S+1) = 6 (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.424316	-0.267005	0.073777
2	7	0	-3.150872	1.225347	0.196942
3	7	0	-0.148331	-0.491319	-1.580126
4	7	0	-0.242597	-2.030687	0.966743
5	7	0	-1.296242	0.238347	-2.069166
6	1	0	0.014854	-1.319080	-2.164143
7	1	0	-1.917566	-0.352784	-2.632639
8	1	0	-1.003235	1.064176	-2.606276
9	1	0	0.666158	-2.034959	0.460827
10	7	0	-0.004633	-2.104318	2.398189
11	1	0	-0.788965	-2.858553	0.710214
12	1	0	-2.993315	1.815428	-0.628551
13	7	0	-4.461557	0.586945	0.190080
14	1	0	-3.107484	1.838281	1.016655
15	1	0	-5.095656	1.088597	-0.441794
16	1	0	-4.277669	-0.355724	-0.190541
17	1	0	0.929170	-2.499470	2.559599
18	1	0	0.020077	-1.133611	2.734820
19	22	0	1.503153	0.424083	-0.602759
20	7	0	2.535216	-1.199000	-0.041794
21	1	0	3.386122	-1.430125	0.482110
22	7	0	2.763610	-1.187460	-1.463914
23	1	0	3.699151	-0.877899	-1.744793
24	1	0	2.541051	-2.079365	-1.920327
25	7	0	1.660762	1.464560	1.393482
26	1	0	1.907426	0.818977	2.152652
27	1	0	0.680549	1.748016	1.563581
28	7	0	2.594404	2.585105	1.462807
29	1	0	2.853763	2.765188	0.482607
30	1	0	2.104538	3.409618	1.826451
31	1	0	-2.460194	-0.833702	1.697306
32	1	0	-2.693501	-1.497525	-0.409752
33	1	0	-1.991070	-0.278860	2.047323
34	1	0	2.715071	1.628949	-1.230023
35	1	0	1.000272	2.212609	-1.371518
36	1	0	0.327731	2.093437	-0.928899

Ti(II) D2 with hydride ligands and 3 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2260.598996 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.435265	-0.218914	0.223465
2	7	0	-3.219660	1.116052	-0.285324
3	7	0	-0.160108	-1.063263	-1.186096
4	7	0	-0.086321	-1.300178	1.718077
5	7	0	-1.371160	-0.782167	-1.917232
6	1	0	0.144827	-2.039058	-1.287658
7	1	0	-1.920651	-1.628022	-2.103339
8	1	0	-1.170480	-0.283180	-2.793676
9	1	0	0.819824	-1.338974	1.191231
10	7	0	0.126520	-0.793919	3.061725
11	1	0	-0.477365	-2.242265	1.813370
12	1	0	-3.108590	1.265124	-1.295347
13	7	0	-4.505525	0.519583	0.053782
14	1	0	-3.177383	2.036186	0.162844
15	1	0	-5.178461	0.675319	-0.704994
16	1	0	-4.303549	-0.490197	0.125894
17	1	0	1.115296	-0.908844	3.313432
18	1	0	-0.067833	0.213922	3.033915
19	22	0	1.389643	0.385969	-0.948745
20	7	0	2.447112	-0.964789	0.105169
21	1	0	3.218751	-0.690500	0.733881
22	7	0	2.655151	-2.309175	-0.402293
23	1	0	3.508912	-2.340703	-0.975277
24	1	0	2.810303	-2.964633	0.375329
25	7	0	1.664129	1.825506	0.788283
26	1	0	1.910092	1.338494	1.658212
27	1	0	0.711395	2.200958	0.932065
28	7	0	2.666992	2.860683	0.570078
29	1	0	2.782433	2.904662	-0.451366
30	1	0	2.305893	3.763296	0.896455
31	1	0	-2.466012	-0.195320	1.920839
32	1	0	-2.658795	-1.560068	0.419852
33	1	0	-2.068588	0.500998	2.033983
34	1	0	2.347471	1.580032	-1.956566
35	1	0	0.535265	1.964981	-1.853415
36	1	0	-0.105293	1.734889	-1.401317

37	1	0	2.079568	-0.099368	-2.802107
38	1	0	1.896755	-0.831281	-2.573285

Ti(II) D2 with hydride ligands and 4 H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2261.743088 Hartree/particle
Input spin multiplicity ($2S$+1) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	2.223797	-0.015717	-0.477881
2	7	0	1.187648	-1.547600	0.951213
3	7	0	0.314949	0.223923	-1.489711
4	7	0	1.436208	1.588052	0.901623
5	7	0	1.035356	-0.916310	-2.039710
6	1	0	0.577286	1.035218	-2.062467
7	1	0	1.265854	-0.800121	-3.031420
8	1	0	0.427949	-1.737601	-1.917248
9	1	0	0.398671	1.511423	0.790786
10	7	0	1.802610	1.628008	2.309661
11	1	0	1.719472	2.483413	0.492163
12	1	0	0.273078	-1.705576	0.457716
13	7	0	1.864168	-2.805978	1.237495
14	1	0	0.941480	-1.146347	1.863084
15	1	0	1.204878	-3.581194	1.094172
16	1	0	2.597030	-2.898390	0.524727
17	1	0	0.949921	1.684615	2.877376
18	1	0	2.260465	0.735612	2.527457
19	22	0	-1.686789	0.052534	-0.705924
20	7	0	-1.582097	1.690570	0.479251
21	1	0	-2.105866	1.816740	1.360931
22	7	0	-1.283766	2.992609	-0.098839
23	1	0	-2.159066	3.484450	-0.319852
24	1	0	-0.790145	3.582856	0.584875
25	7	0	-3.085197	-0.686458	0.969404
26	1	0	-3.896652	-0.061197	0.995202
27	1	0	-2.569939	-0.556225	1.851694
28	7	0	-3.572887	-2.037708	0.808626
29	1	0	-2.793656	-2.538060	0.358487
30	1	0	-3.750636	-2.464689	1.724887
31	1	0	3.893770	0.820421	0.090302
32	1	0	2.933779	1.206593	-1.643185
33	1	0	3.830838	0.293597	0.712873
34	1	0	-3.248585	-0.716613	-1.758359
35	1	0	3.689577	-1.170401	-1.165613
36	1	0	3.711782	-0.457809	-1.592249

37	1	0	-2.443612	1.320996	-2.144728
38	1	0	-1.753996	1.131592	-2.479122
39	1	0	-1.115961	-1.732270	-0.426567
40	1	0	-2.680819	-1.254768	-1.925303

Ti(II) D3 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2145.390222 Hartree/particle
Input spin multiplicity ($2S+1$) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.390816	-1.124714	-0.590097
2	7	0	-2.399965	0.055391	-0.652054
3	7	0	1.368864	-1.940762	-1.061105
4	7	0	-0.585475	-0.845799	1.667149
5	7	0	2.423284	-1.100345	-0.544287
6	1	0	1.746119	-2.769314	-1.532355
7	1	0	3.033029	-1.599956	0.120622
8	1	0	3.031742	-0.728195	-1.287926
9	1	0	-0.478722	-1.763918	2.120329
10	7	0	0.465641	0.072504	2.034166
11	1	0	-1.529396	-0.485275	1.882748
12	1	0	-2.807151	-0.081841	-1.586290
13	7	0	-3.275848	-0.418983	0.407718
14	1	0	-2.234859	1.064200	-0.529035
15	1	0	-4.255575	-0.200124	0.189978
16	1	0	-3.150774	-1.444698	0.380959
17	1	0	0.515337	0.218651	3.048408
18	22	0	1.326978	0.623829	0.367696
19	7	0	0.416891	2.632111	-0.092027
20	1	0	0.093752	3.039645	0.791135
21	1	0	1.242756	3.162958	-0.401559
22	7	0	-0.687522	2.682616	-1.036579
23	1	0	-0.712707	3.602717	-1.497239
24	1	0	-0.467794	1.972826	-1.755975
25	1	0	-1.601053	-2.473033	-0.275898
26	1	0	2.898649	1.547700	0.164059

Ti(II) D6 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2145.398063 Hartree/particle
Input spin multiplicity ($2S+1$) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	1.276825	0.188714	0.444996
2	7	0	1.239710	2.156553	0.478343
3	7	0	2.667974	-0.773685	-1.067553
4	7	0	-0.638836	-0.156219	1.320326
5	7	0	-3.727599	-0.952540	-0.492505
6	7	0	-0.925200	-1.552416	1.669427
7	1	0	-0.686738	0.427708	2.167054
8	1	0	-0.049452	-1.971971	2.015220
9	1	0	-1.588010	-1.568738	2.454669
10	7	0	0.036770	2.564148	-0.208579
11	1	0	1.790230	2.956074	0.809104
12	1	0	-0.559653	3.169907	0.373807
13	1	0	0.241894	3.084350	-1.075362
14	1	0	-3.863787	-1.231626	0.484243
15	7	0	-2.327255	-1.234254	-0.840990
16	1	0	-3.809717	0.075395	-0.526245
17	1	0	3.441018	-0.107735	-1.215230
18	7	0	3.133161	-2.093235	-0.674241
19	1	0	2.174688	-0.862526	-1.962398
20	1	0	4.101974	-2.230844	-0.982460
21	1	0	3.102530	-2.077991	0.357049
22	1	0	-1.890494	-1.803958	-0.085354
23	1	0	-2.349483	-1.800672	-1.692578
24	22	0	-1.089416	0.606286	-0.580977
25	1	0	-2.475187	1.727647	-1.044310
26	1	0	2.086124	-0.983483	1.624780

Ti(II) D7 with no H_2 molecules bound
Sum of electronic and thermal Enthalpies= -2145.398388 Hartree/particle
Input spin multiplicity ($2S+1$) = 5
$\langle S^2 \rangle = S(S+1) = 6$ (formal), 6.0001 (found)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-1.150088	-0.336356	0.079410
2	7	0	-0.589923	1.743074	-0.185741
3	7	0	-3.199944	-0.099713	-0.922945
4	7	0	0.644166	-0.707238	1.244142
5	7	0	1.129897	-2.086238	1.076189
6	1	0	0.467772	-0.529991	2.243027
7	1	0	1.733880	-2.332229	1.870150
8	1	0	0.304811	-2.704243	1.112345
9	7	0	-0.200629	2.583176	0.934142
10	1	0	-0.918045	2.374807	-0.922490
11	1	0	-0.416569	2.124605	1.822492
12	1	0	0.792430	2.883066	0.888022
13	1	0	-3.096312	-0.452873	-1.885163
14	7	0	-4.208578	-0.824459	-0.169964
15	1	0	-3.504502	0.877319	-0.987266
16	1	0	-4.922341	-1.196523	-0.806712
17	1	0	-3.688708	-1.612452	0.250923
18	22	0	1.215992	0.758609	-0.109246
19	7	0	2.407103	-0.783887	-1.153313
20	1	0	2.328233	-0.985790	-2.153347
21	1	0	2.051432	-1.607543	-0.617444
22	7	0	3.829987	-0.578220	-0.861951
23	1	0	3.901151	0.373439	-0.467775
24	1	0	4.093709	-1.232669	-0.118483
25	1	0	2.577480	1.997990	0.076136
26	1	0	-1.838843	-1.991953	0.628067