

Supporting Information: ML-Metal cluster

S1 Composition of 50 TM complexes

co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_cyanide
co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_fluoride_fluoride
cr_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_misc_misc
cr_2_acetonitrile_acetonitrile_ammonia_ammonia_ammonia_ammonia
cr_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide
cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_ammonia
cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_cyanide
cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride
cr_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc
cr_2_misc_misc_misc_misc_misc_misc
cr_2_phosphine_phosphine_phosphine_phosphine_hydrogensulfide_hydrogensulfide
cr_2_phosphine_phosphine_phosphine_phosphine_phosphine_ammonia
cr_2_water_water_water_water_ammonia_ammonia
cr_2_water_water_water_water_carbonyl_carbonyl
fe_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia
fe_2_carbonyl_carbonyl_carbonyl_carbonyl_chloride_chloride
fe_2_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_cyanide
fe_2_carbonyl_carbonyl_carbonyl_carbonyl_hydrogensulfide_hydrogensulfide
fe_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_misc
fe_2_misc_misc_misc_misc_misc_acetonitrile
fe_2_misc_misc_misc_misc_misc_carbonyl
fe_2_misc_misc_misc_misc_misc_cyanide
fe_2_water_water_water_water_water_chloride
mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia
mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_carbonyl
mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_acetonitrile
mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_water
mn_3_ammonia_ammonia_ammonia_ammonia_phosphine_phosphine
mn_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride
mn_3_cyanide_cyanide_ammonia_ammonia_ammonia_ammonia
mn_3_misc_misc_misc_misc_acetonitrile_acetonitrile
mn_3_misc_misc_misc_misc_misc_misc
mn_3_phosphine_phosphine_phosphine_phosphine_ammonia_ammonia
mn_3_phosphine_phosphine_phosphine_phosphine_phosphine_chloride
mn_3_water_water_water_water_water_fluoride_fluoride
fe_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide
fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_chloride
fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_misc
fe_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_acetonitrile
fe_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_fluoride
fe_3_misc_misc_misc_misc_acetonitrile_acetonitrile
fe_3_misc_misc_misc_misc_water_water

mn_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_water_water
mn_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide
mn_2_carbonyl_carbonyl_carbonyl_carbonyl_phosphine_phosphine
mn_2_chloride_chloride_chloride_chloride_carbonyl_carbonyl
mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_carbonyl
mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_phosphine
mn_2_water_water_water_water_acetonitrile_acetonitrile
mn_2_water_water_water_water_water_water

S2 Energies of 50 TM complexes from different basis set:

S2.1 Low spin energies

Complex_index	S ²	b3lyp*/svp	b3lyp*/tzvp	b3lyp*/qzvp	b3lyp*/cbs
Complex1	0.0000	-2098.092311	-2099.100456	-2099.180400	-2099.187285
Complex2	0.0000	-2112.109926	-2113.166838	-2113.251525	-2113.258902
Complex3	0.0000	-1839.274359	-1840.321048	-1840.402078	-1840.408878
Complex4	0.0000	-1534.920480	-1535.632982	-1535.702622	-1535.710166
Complex5	0.0000	-1455.637032	-1456.280933	-1456.344628	-1456.351620
Complex6	0.0000	-1665.991695	-1666.870606	-1666.934103	-1666.939048
Complex7	0.0000	-1702.595312	-1703.515683	-1703.577655	-1703.582129
Complex8	0.0000	-1709.631143	-1710.574091	-1710.637842	-1710.642464
Complex9	0.0000	-3172.198893	-3173.193350	-3173.303218	-3173.316863
Complex10	0.0000	-1839.176642	-1840.215790	-1840.295829	-1840.302508
Complex11	0.0000	-3213.944285	-3214.853628	-3214.963223	-3214.978241
Complex12	0.0000	-2815.046182	-2815.862223	-2815.961676	-2815.975479
Complex13	0.0000	-1462.037835	-1462.689866	-1462.758913	-1462.767091
Complex14	0.0000	-1575.371094	-1576.157405	-1576.227410	-1576.234252
Complex15	0.0000	-1982.487616	-1983.475340	-1983.556462	-1983.563720
Complex16	0.0000	-2636.226646	-2637.261038	-2637.345352	-2637.352834
Complex17	0.0000	-1901.674449	-1902.602610	-1902.666665	-1902.671413
Complex18	0.0000	-2513.978576	-2514.966343	-2515.049310	-2515.056918
Complex19	0.0000	-3124.858796	-3125.893929	-3125.999934	-3126.012028
Complex20	0.0000	-2058.483062	-2059.547891	-2059.630600	-2059.637566
Complex21	0.0000	-2039.060900	-2040.109275	-2040.188997	-2040.195559
Complex22	0.0000	-2018.892901	-2019.920125	-2019.999098	-2020.005675
Complex23	0.0000	-2104.949167	-2105.755276	-2105.838439	-2105.848006
Complex24	0.0000	-1869.244374	-1870.216962	-1870.299387	-1870.307019
Complex25	0.0000	-1925.888677	-1926.928896	-1927.007742	-1927.014208
Complex26	0.0000	-1564.785206	-1565.420483	-1565.488408	-1565.496540
Complex27	0.0000	-1508.503775	-1509.080667	-1509.145926	-1509.154251
Complex28	0.0000	-2061.588656	-2062.251588	-2062.331059	-2062.341883
Complex29	0.0000	-1815.621757	-1816.571329	-1816.635499	-1816.640150
Complex30	0.0000	-1561.935573	-1562.577442	-1562.639148	-1562.645711
Complex31	0.0000	-1945.246631	-1946.295735	-1946.376599	-1946.383352
Complex32	0.0000	-1945.196557	-1946.242367	-1946.322643	-1946.329317
Complex33	0.0000	-2634.543559	-2635.316277	-2635.408794	-2635.421378
Complex34	0.0000	-3325.023509	-3325.947948	-3326.055962	-3326.070252
Complex35	0.0000	-1655.346590	-1656.133896	-1656.206151	-1656.213452
Complex36	0.5055	-2018.608359	-2019.639305	-2019.720477	-2019.727415
Complex37	0.5139	-2005.420022	-2006.081782	-2006.157837	-2006.167713
Complex38	0.5130	-1677.515223	-1678.163583	-1678.233497	-1678.241948
Complex39	0.5065	-1960.693299	-1961.679217	-1961.748764	-1961.754042

Complex40	0.5048	-1915.354040	-1916.320190	-1916.388651	-1916.393872
Complex41	0.5078	-2057.994437	-2059.058199	-2059.142199	-2059.149400
Complex42	0.5185	-1945.418018	-1946.366660	-1946.447841	-1946.455438
Complex43	0.5374	-1833.337281	-1834.281192	-1834.360084	-1834.367279
Complex44	0.5356	-1562.190183	-1562.843246	-1562.910379	-1562.918071
Complex45	0.5082	-2288.845277	-2289.775989	-2289.853203	-2289.860189
Complex46	0.5112	-3217.156794	-3218.264432	-3218.374525	-3218.386675
Complex47	0.5092	-3259.330364	-3260.325808	-3260.432289	-3260.445044
Complex48	0.6030	-3489.117956	-3490.104616	-3490.218627	-3490.233523
Complex49	0.5894	-1720.795793	-1721.626521	-1721.702656	-1721.710337
Complex50	0.8441	-1608.237360	-1608.954278	-1609.028056	-1609.036520

S2.2 Intermediate spin energies

Complex_index	S ²	b3lyp*/svp	b3lyp*/tzvp	b3lyp*/qzvp	b3lyp*/cbs
Complex1	1.0142	-2098.056314	-2099.067957	-2099.145584	-2099.152035
Complex2	1.0049	-2112.108503	-2113.160137	-2113.245547	-2113.253097
Complex3	1.0076	-1839.320637	-1840.366458	-1840.447485	-1840.454290
Complex4	1.0059	-1534.974240	-1535.685602	-1535.755348	-1535.762929
Complex5	1.0031	-1455.688124	-1456.330878	-1456.387736	-1456.393254
Complex6	1.0093	-1666.037146	-1666.914535	-1666.978119	-1666.983087
Complex7	1.0144	-1702.631618	-1703.551500	-1703.613589	-1703.618084
Complex8	1.0107	-1709.669964	-1710.612190	-1710.676076	-1710.680722
Complex9	1.0085	-3172.242914	-3173.236373	-3173.346570	-3173.360318
Complex10	1.0099	-1839.216384	-1840.254954	-1840.335017	-1840.341704
Complex11	1.0096	-3213.986761	-3214.894713	-3215.004492	-3215.019590
Complex12	1.0098	-2815.095355	-2815.909910	-2816.009377	-2816.023213
Complex13	1.0636	-1462.076747	-1462.728173	-1462.806515	-1462.817225
Complex14	1.0062	-1575.403120	-1576.189217	-1576.258483	-1576.265176
Complex15	1.0045	-1982.465325	-1983.454152	-1983.535974	-1983.543355
Complex16	1.0155	-2636.191645	-2637.226118	-2637.311373	-2637.319030
Complex17	1.0124	-1901.582458	-1902.512476	-1902.577609	-1902.582515
Complex18	1.0104	-2513.940793	-2514.925678	-2515.009463	-2515.017253
Complex19	1.0108	-3124.857417	-3125.886697	-3125.993360	-3126.005691
Complex20	1.0100	-2058.429170	-2059.495089	-2059.578614	-2059.585716
Complex21	1.0114	-2038.991893	-2040.040794	-2040.121310	-2040.128005
Complex22	1.0130	-2018.825144	-2019.853402	-2019.933273	-2019.939999
Complex23	1.0644	-2104.954525	-2105.761215	-2105.845227	-2105.854994
Complex24	1.0047	-1869.304300	-1870.276295	-1870.355672	-1870.362730
Complex25	1.0052	-1925.941169	-1926.980947	-1927.060111	-1927.066635
Complex26	1.0059	-1564.863384	-1565.497323	-1565.564702	-1565.572715
Complex27	1.0060	-1508.565189	-1509.141681	-1509.207261	-1509.215679
Complex28	1.0128	-2061.667258	-2062.327881	-2062.406604	-2062.417254
Complex29	1.0072	-1815.675549	-1816.624329	-1816.688705	-1816.693391
Complex30	1.0076	-1561.989217	-1562.631614	-1562.693785	-1562.700447
Complex31	1.0077	-1945.301035	-1946.349750	-1946.430921	-1946.437731
Complex32	1.0086	-1945.249178	-1946.294151	-1946.374678	-1946.381402
Complex33	1.0236	-2634.604963	-2635.376592	-2635.469568	-2635.482306
Complex34	1.0194	-3325.072190	-3325.994257	-3326.102786	-3326.117265
Complex35	1.0393	-1655.404252	-1656.192286	-1656.265007	-1656.272400
Complex36	1.5171	-2018.604935	-2019.635431	-2019.716570	-2019.723505
Complex37	1.5187	-2005.400745	-2006.063877	-2006.140935	-2006.151066
Complex38	1.5117	-1677.498127	-1678.147260	-1678.217376	-1678.225867
Complex39	1.5096	-1960.659892	-1961.645971	-1961.716310	-1961.721712

Complex40	1.5061	-1915.357360	-1916.322126	-1916.392536	-1916.398079
Complex41	1.5111	-2057.970495	-2059.035215	-2059.119520	-2059.126769
Complex42	1.5117	-1945.413439	-1946.365173	-1946.446354	-1946.453925
Complex43	1.5040	-1833.334228	-1834.278461	-1834.357612	-1834.364854
Complex44	1.5066	-1562.194765	-1562.851047	-1562.914632	-1562.921453
Complex45	1.5177	-2288.807836	-2289.738484	-2289.816462	-2289.823593
Complex46	1.5222	-3217.138784	-3218.249771	-3218.360615	-3218.372900
Complex47	1.5150	-3259.326930	-3260.317822	-3260.424762	-3260.437699
Complex48	1.5133	-3489.131478	-3490.112997	-3490.227353	-3490.242434
Complex49	1.5038	-1720.805809	-1721.638691	-1721.714925	-1721.722605
Complex50	1.5022	-1608.255568	-1608.972756	-1609.045253	-1609.053405

S2.3 HS spin energies

Complex_index	S ²	b3lyp*/svp	b3lyp*/tzvp	b3lyp*/qzvp	b3lyp*/cbs
Complex1	2.0029	-2098.002800	-2099.012751	-2099.093909	-2099.101000
Complex2	2.0019	-2112.113430	-2113.165976	-2113.251826	-2113.259450
Complex3	2.0017	-1839.303147	-1840.349831	-1840.431371	-1840.438260
Complex4	2.0021	-1534.980803	-1535.693995	-1535.763801	-1535.771375
Complex5	2.0030	-1455.698139	-1456.344185	-1456.407518	-1456.414401
Complex6	2.0026	-1666.012559	-1666.890212	-1666.954665	-1666.959773
Complex7	2.0057	-1702.585215	-1703.506807	-1703.569899	-1703.574535
Complex8	2.0026	-1709.632226	-1710.574743	-1710.640063	-1710.644927
Complex9	2.0051	-3172.255672	-3173.246390	-3173.356663	-3173.370475
Complex10	2.0026	-1839.172706	-1840.213041	-1840.293737	-1840.300523
Complex11	2.0073	-3213.995921	-3214.899835	-3215.009958	-3215.025235
Complex12	2.0051	-2815.093459	-2815.903611	-2816.003137	-2816.017076
Complex13	2.0017	-1462.113941	-1462.768793	-1462.837702	-1462.845806
Complex14	2.0010	-1575.408625	-1576.193365	-1576.263501	-1576.270384
Complex15	2.0025	-1982.481866	-1983.470806	-1983.553378	-1983.560900
Complex16	2.0081	-2636.181678	-2637.218424	-2637.304743	-2637.312583
Complex17	2.0041	-1901.555065	-1902.486835	-1902.553000	-1902.558057
Complex18	2.0042	-2513.930463	-2514.913978	-2514.999003	-2515.007049
Complex19	2.0033	-3124.848192	-3125.875678	-3125.983267	-3125.995850
Complex20	2.0041	-2058.408834	-2059.474931	-2059.559347	-2059.566606
Complex21	4.0400	-2038.969865	-2040.016368	-2040.097934	-2040.104828
Complex22	2.0050	-2018.787752	-2019.817069	-2019.897910	-2019.904801
Complex23	2.0012	-2104.985155	-2105.792590	-2105.877083	-2105.886957
Complex24	2.0069	-1869.310934	-1870.284066	-1870.363738	-1870.370843
Complex25	2.0050	-1925.947667	-1926.989650	-1927.069365	-1927.075969
Complex26	2.0102	-1564.868251	-1565.503375	-1565.570927	-1565.578967
Complex27	2.0106	-1508.577424	-1509.156507	-1509.221974	-1509.230319
Complex28	2.0266	-2061.673058	-2062.332708	-2062.411186	-2062.421784
Complex29	2.0061	-1815.663628	-1816.611017	-1816.676633	-1816.681516
Complex30	2.0119	-1561.996662	-1562.637794	-1562.699644	-1562.706248
Complex31	2.0085	-1945.292629	-1946.341848	-1946.423030	-1946.429838
Complex32	2.0082	-1945.223020	-1946.268640	-1946.349445	-1946.356212
Complex33	2.0496	-2634.608963	-2635.376593	-2635.469174	-2635.481871
Complex34	2.0219	-3325.069257	-3325.985730	-3326.094417	-3326.109041
Complex35	2.0037	-1655.435920	-1656.226134	-1656.299255	-1656.306711
Complex36	2.5016	-2018.599528	-2019.632009	-2019.713376	-2019.720337
Complex37	2.5013	-2005.421338	-2006.084196	-2006.160774	-2006.170776
Complex38	2.5007	-1677.499828	-1678.149888	-1678.220451	-1678.229044
Complex39	2.5016	-1960.665202	-1961.651736	-1961.722536	-1961.728010

Complex40	2.5014	-1915.340553	-1916.307741	-1916.378734	-1916.384357
Complex41	2.5009	-2057.951188	-2059.016977	-2059.101705	-2059.109023
Complex42	2.5009	-1945.393063	-1946.344021	-1946.425905	-1946.433620
Complex43	2.5004	-1833.380406	-1834.324448	-1834.403778	-1834.411056
Complex44	2.5010	-1562.218049	-1562.872435	-1562.936088	-1562.942946
Complex45	2.5007	-2288.819638	-2289.745938	-2289.824297	-2289.831539
Complex46	2.5011	-3217.155648	-3218.270406	-3218.382551	-3218.395094
Complex47	2.5008	-3259.359552	-3260.344205	-3260.451879	-3260.465099
Complex48	2.5009	-3489.174744	-3490.146141	-3490.260803	-3490.276149
Complex49	2.5004	-1720.853080	-1721.684701	-1721.761073	-1721.768796
Complex50	2.5004	-1608.317719	-1609.034957	-1609.107636	-1609.115831

S3 Energies of 50 TM complexes from different functionals:

S3.1 Low spin energies

Complex_index	pbe0/tzvp	bp86/tzvp	tpssh/tzvp	m06l/tzvp	m062x/tzvp	pw9b95/qzvp	caspt2/cc
Complex1	-2098.536262	-2099.912971	-2099.727160	-2099.516190	-2099.242311	-2099.241957	-2108.215278
Complex2	-2112.614385	-2113.942833	-2113.754836	-2113.561793	-2113.304620	-2113.322426	-2122.435710
Complex3	-1839.723776	-1841.102574	-1841.010243	-1840.768176	-1840.492091	-1840.411200	-1845.150926
Complex4	-1535.229189	-1536.211497	-1536.094563	-1535.907874	-1535.748449	-1535.730105	-1540.909614
Complex5	-1455.906488	-1456.814493	-1456.674694	-1456.501711	-1456.374979	-1456.389626	-1461.706007
Complex6	-1666.397577	-1667.491686	-1667.371407	-1667.207939	-1667.004242	-1667.017425	-1672.240827
Complex7	-1703.013877	-1704.198362	-1704.040374	-1703.862131	-1703.642112	-1703.662959	-1708.842752
Complex8	-1710.077833	-1711.239348	-1711.079096	-1710.920639	-1710.697119	-1710.727450	-1715.967419
Complex9	-3172.697727	-3174.197883	-3173.935468	-3173.687419	-3173.533074	-3173.499085	-3182.206586
Complex10	-1839.619482	-1841.012071	-1840.915622	-1840.654469	-1840.367071	-1840.303335	-1845.049981
Complex11	-3214.373898	-3215.848016	-3215.589072	-3215.329492	-3215.157052	-3215.126369	-3223.622747
Complex12	-2815.409403	-2816.737828	-2816.527021	-2816.278845	-2816.099801	-2816.073450	-2823.631495
Complex13	-1462.346420	-1463.169372	-1463.042104	-1462.884871	-1462.799708	-1462.820224	-1468.261849
Complex14	-1575.744673	-1576.732930	-1576.570579	-1576.423622	-1576.273586	-1576.297233	-1581.668613
Complex15	-1982.919673	-1984.256603	-1984.110708	-1983.896664	-1983.626804	-1983.593138	-1990.992516
Complex16	-2636.752504	-2638.151689	-2637.881575	-2637.698788	-2637.474807	-2637.541207	-2647.345713
Complex17	-1902.103418	-1903.339720	-1903.128279	-1902.952032	-1902.690062	-1902.776785	-1910.504690
Complex18	-2514.459696	-2515.835877	-2515.578191	-2515.388642	-2515.143184	-2515.208101	-2524.382770
Complex19	-3125.368469	-3126.918248	-3126.634259	-3126.388644	-3126.170191	-3126.177038	-3136.636112
Complex20	-2058.943464	-2060.402446	-2060.252910	-2059.996302	-2059.669834	-2059.662415	-2066.958658
Complex21	-2039.520354	-2040.950077	-2040.789249	-2040.541149	-2040.217094	-2040.237083	-2047.608709
Complex22	-2019.338586	-2020.757778	-2020.593466	-2020.343368	-2020.022945	-2020.042845	-2027.409333
Complex23	-2105.364854	-2106.415257	-2106.182480	-2106.030613	-2105.931162	-2105.973197	-2114.962585
Complex24	-1869.665861	-1870.977992	-1870.859716	-1870.633785	-1870.367547	-1870.321301	-1876.367911
Complex25	-1926.343615	-1927.723592	-1927.597730	-1927.375994	-1927.087561	-1927.036951	-1933.047061
Complex26	-1565.060190	-1565.998968	-1565.831710	-1565.665991	-1565.497578	-1565.537983	-1572.017519
Complex27	-1508.758409	-1509.603829	-1509.440458	-1509.273672	-1509.147470	-1509.190822	-1515.787878
Complex28	-2061.879158	-2062.938220	-2062.730359	-2062.543356	-2062.376229	-2062.409368	-2069.867078
Complex29	-1816.071664	-1817.252074	-1817.082527	-1816.914195	-1816.696710	-1816.741467	-1823.173737
Complex30	-1562.211002	-1563.150538	-1562.980298	-1562.810204	-1562.660253	-1562.688588	-1569.192830
Complex31	-1945.695498	-1947.116029	-1946.997828	-1946.742352	-1946.448463	-1946.393935	-1952.336055
Complex32	-1945.641908	-1947.069857	-1946.948905	-1946.684523	-1946.386247	-1946.340908	-1952.286498
Complex33	-2634.885189	-2636.126716	-2635.922430	-2635.684265	-2635.501786	-2635.511863	-2643.833351
Complex34	-3325.457304	-3326.968499	-3326.689709	-3326.427398	-3326.221774	-3326.231829	-3335.981445
Complex35	-1655.744353	-1656.674011	-1656.501844	-1656.350856	-1656.234162	-1656.287798	-1662.986093
Complex36	-2019.060898	-2020.459432	-2020.300229	-2020.091521	-2019.793987	-2019.768301	-2027.133432

Complex37	-2005.739889	-2006.733507	-2006.516069	-2006.349965	-2006.205016	-2006.259402	-2015.199720
Complex38	-1677.800613	-1678.761748	-1678.581308	-1678.409640	-1678.228867	-1678.278438	-1686.109248
Complex39	-1961.150340	-1962.436379	-1962.245209	-1962.072810	-1961.805614	-1961.845625	-1969.506446
Complex40	-1915.832996	-1917.012812	-1916.807828	-1916.653817	-1916.428334	-1916.500437	-1924.358286
Complex41	-2058.457163	-2059.901493	-2059.762157	-2059.506015	-2059.202357	-2059.170095	-2066.462956
Complex42	-1945.842585	-1947.121887	-1946.961781	-1946.734986	-1946.493587	-1946.491977	-1954.020080
Complex43	-1833.762071	-1834.993781	-1834.861698	-1834.654635	-1834.435733	-1834.397487	-1840.569508
Complex44	-1562.486675	-1563.409859	-1563.240948	-1563.074335	-1562.942713	-1562.961103	-1569.458632
Complex45	-2289.277555	-2290.586932	-2290.379977	-2290.180362	-2289.934500	-2289.967853	-2297.287724
Complex46	-3217.768439	-3219.266434	-3218.961108	-3218.774747	-3218.624042	-3218.634489	-3229.153201
Complex47	-3259.840650	-3261.347890	-3261.043839	-3260.817155	-3260.636189	-3260.642915	-3270.615182
Complex48	-3489.627128	-3491.165768	-3490.856452	-3490.607562	-3490.454990	-3490.438264	-3500.871558
Complex49	-1721.183423	-1722.251187	-1722.092301	-1721.920646	-1721.760945	-1721.757891	-1728.167110
Complex50	-1608.590287	-1609.484804	-1609.315009	-1609.159897	-1609.077166	-1609.104880	-1615.748637

S3.2 Intermediate spin energies

Complex_index	pbe0/tzvp	bp86/tzvp	tpssh/tzvp	m06l/tzvp	m062x/tzvp	pwpb95/qzvpp	caspt2/cc
Complex1	-2098.510686	-2099.870528	-2099.686356	-2099.483789	-2099.239968	-2099.208744	-2108.179387
Complex2	-2112.613609	-2113.930736	-2113.746174	-2113.556086	-2113.315070	-2113.315101	-2122.421938
Complex3	-1839.776554	-1841.144743	-1841.055748	-1840.825005	-1840.544281	-1840.456318	-1845.194732
Complex4	-1535.288809	-1536.269262	-1536.147846	-1535.974907	-1535.802244	-1535.780176	-1540.958665
Complex5	-1455.979053	-1456.865319	-1456.718013	-1456.565455	-1456.446383	-1456.436809	-1461.750721
Complex6	-1666.448724	-1667.557102	-1667.415260	-1667.261507	-1667.058936	-1667.061223	-1672.276796
Complex7	-1703.057406	-1704.226609	-1704.076358	-1703.916285	-1703.691990	-1703.697085	-1708.877849
Complex8	-1710.123423	-1711.269409	-1711.116885	-1710.965424	-1710.749639	-1710.765220	-1716.007099
Complex9	-3172.747793	-3174.239421	-3173.978599	-3173.742442	-3173.580547	-3173.539034	-3182.246836
Complex10	-1839.665328	-1841.046495	-1840.954854	-1840.702696	-1840.415801	-1840.340697	-1845.084704
Complex11	-3214.421904	-3215.887314	-3215.630722	-3215.382844	-3215.203155	-3215.163677	-3223.662734
Complex12	-2815.464372	-2816.796890	-2816.576037	-2816.338654	-2816.150722	-2816.119298	-2823.683283
Complex13	-1462.402554	-1463.235443	-1463.088227	-1462.946549	-1462.850899	-1462.863568	-1468.303031
Complex14	-1575.784711	-1576.752914	-1576.601802	-1576.458908	-1576.324041	-1576.332566	-1581.698499
Complex15	-1982.905536	-1984.220638	-1984.082448	-1983.870405	-1983.634275	-1983.573107	-1990.968952
Complex16	-2636.723109	-2638.094651	-2637.837961	-2637.660463	-2637.491388	-2637.504070	-2647.282109
Complex17	-1902.018680	-1903.236025	-1903.026890	-1902.875130	-1902.679021	-1902.691483	-1910.395132
Complex18	-2514.424935	-2515.774466	-2515.529173	-2515.345002	-2515.149687	-2515.164499	-2524.324028
Complex19	-3125.366794	-3126.897278	-3126.620005	-3126.379068	-3126.190314	-3126.166623	-3136.615683
Complex20	-2058.896190	-2060.327456	-2060.191436	-2059.940920	-2059.665241	-2059.606479	-2066.881560
Complex21	-2039.456147	-2040.857417	-2040.711747	-2040.471503	-2040.204252	-2040.162514	-2047.515537
Complex22	-2019.275137	-2020.666342	-2020.517000	-2020.275172	-2020.013140	-2019.967926	-2027.312823
Complex23	-2105.377026	-2106.418354	-2106.189568	-2106.033827	-2105.950852	-2105.978204	-2114.968040
Complex24	-1869.734228	-1871.031620	-1870.915121	-1870.702240	-1870.433438	-1870.378604	-1876.425066
Complex25	-1926.404974	-1927.767979	-1927.648998	-1927.435429	-1927.149430	-1927.091808	-1933.101151
Complex26	-1565.144962	-1566.063543	-1565.912119	-1565.746275	-1565.579465	-1565.598094	-1572.073746
Complex27	-1508.827647	-1509.663895	-1509.501592	-1509.349542	-1509.212927	-1509.250507	-1515.844781
Complex28	-2061.963870	-2063.003641	-2062.810709	-2062.623096	-2062.457268	-2062.473802	-2069.925538
Complex29	-1816.131988	-1817.306181	-1817.134998	-1816.982889	-1816.758563	-1816.792783	-1823.226616
Complex30	-1562.275108	-1563.198800	-1563.033263	-1562.870783	-1562.725599	-1562.745360	-1569.249629
Complex31	-1945.758252	-1947.161966	-1947.051351	-1946.806372	-1946.513275	-1946.449465	-1952.387957
Complex32	-1945.702386	-1947.112605	-1947.000275	-1946.745008	-1946.449127	-1946.393663	-1952.335247
Complex33	-2634.953321	-2636.210833	-2635.983695	-2635.759125	-2635.568513	-2635.567748	-2643.889429
Complex34	-3325.511723	-3327.015222	-3326.736027	-3326.482913	-3326.280286	-3326.274352	-3336.029857
Complex35	-1655.810602	-1656.742230	-1656.560089	-1656.419226	-1656.297111	-1656.349026	-1663.040904
Complex36	-2019.065593	-2020.431555	-2020.291974	-2020.084975	-2019.825454	-2019.758359	-2027.119468

Complex37	-2005.735628	-2006.712745	-2006.492722	-2006.342034	-2006.220724	-2006.247156	-2015.188368
Complex38	-1677.792388	-1678.736040	-1678.561597	-1678.396650	-1678.240076	-1678.260995	-1686.088537
Complex39	-1961.123897	-1962.380076	-1962.203148	-1962.041306	-1961.819926	-1961.815007	-1969.464488
Complex40	-1915.842855	-1916.993488	-1916.803920	-1916.657784	-1916.474557	-1916.509111	-1924.356518
Complex41	-2058.440557	-2059.862435	-2059.730714	-2059.489869	-2059.216750	-2059.147696	-2066.435063
Complex42	-1945.847558	-1947.109221	-1946.951009	-1946.739320	-1946.520412	-1946.490932	-1954.016990
Complex43	-1833.768286	-1834.977866	-1834.850492	-1834.657904	-1834.465547	-1834.401232	-1840.573460
Complex44	-1562.498344	-1563.405437	-1563.243848	-1563.087355	-1562.979118	-1562.967843	-1569.466787
Complex45	-2289.246337	-2290.520013	-2290.330056	-2290.144058	-2289.958349	-2289.931450	-2297.237027
Complex46	-3217.762967	-3219.235920	-3218.940437	-3218.765245	-3218.650066	-3218.622753	-3229.133012
Complex47	-3259.843198	-3261.321296	-3261.030045	-3260.813676	-3260.673356	-3260.642111	-3270.604973
Complex48	-3489.643600	-3491.161733	-3490.857725	-3490.624723	-3490.493900	-3490.453017	-3500.883900
Complex49	-1721.205865	-1722.254719	-1722.101580	-1721.936376	-1721.798075	-1721.774547	-1728.184965
Complex50	-1608.617927	-1609.499931	-1609.325308	-1609.186178	-1609.112171	-1609.125321	-1615.774956

S3.3 High spin energies

Complex_index	pbe0/tzvp	bp86/tzvp	tpssh/tzvp	m06l/tzvp	m062x/tzvp	pw95/qzvpp	caspt2/cc
Complex1	-2098.461068	-2099.820041	-2099.634359	-2099.439365	-2099.212769	-2099.168629	-2108.134001
Complex2	-2112.627767	-2113.927206	-2113.749974	-2113.570144	-2113.346065	-2113.323053	-2122.433415
Complex3	-1839.771391	-1841.107749	-1841.032866	-1840.815819	-1840.574102	-1840.449270	-1845.194751
Complex4	-1535.309043	-1536.266382	-1536.152144	-1535.993936	-1535.841341	-1535.795109	-1540.977706
Complex5	-1456.001922	-1456.869401	-1456.734818	-1456.591064	-1456.487572	-1456.453417	-1461.769738
Complex6	-1666.435102	-1667.506693	-1667.382666	-1667.242427	-1667.091593	-1667.048357	-1672.260389
Complex7	-1703.023144	-1704.151617	-1704.021921	-1703.876839	-1703.714780	-1703.661878	-1708.830215
Complex8	-1710.096273	-1711.203262	-1711.069469	-1710.930196	-1710.774130	-1710.739120	-1715.977891
Complex9	-3172.769465	-3174.234268	-3173.984622	-3173.764204	-3173.628066	-3173.556115	-3182.263756
Complex10	-1839.633998	-1840.978687	-1840.906056	-1840.671124	-1840.433871	-1840.308313	-1845.045010
Complex11	-3214.438366	-3215.875738	-3215.632329	-3215.401122	-3215.248130	-3215.174445	-3223.672172
Complex12	-2815.469048	-2816.772593	-2816.565544	-2816.346904	-2816.188751	-2816.118213	-2823.679169
Complex13	-1462.442898	-1463.264892	-1463.119047	-1462.991060	-1462.900679	-1462.897461	-1468.342202
Complex14	-1575.801024	-1576.738799	-1576.599809	-1576.467229	-1576.368242	-1576.348447	-1581.716952
Complex15	-1982.936003	-1984.222731	-1984.098029	-1983.895943	-1983.682234	-1983.602330	-1991.002297
Complex16	-2636.728852	-2638.059852	-2637.824995	-2637.661130	-2637.546139	-2637.511628	-2647.294301
Complex17	-1902.005279	-1903.177279	-1902.994283	-1902.834415	-1902.708952	-1902.682495	-1910.382116
Complex18	-2514.428899	-2515.732448	-2515.514094	-2515.338762	-2515.201305	-2515.172169	-2524.327173
Complex19	-3125.371149	-3126.863113	-3126.607674	-3126.376415	-3126.230278	-3126.171600	-3136.621145
Complex20	-2058.890797	-2060.279239	-2060.168362	-2059.930524	-2059.706090	-2059.603413	-2066.877444
Complex21	-2039.446835	-2040.801941	-2040.683345	-2040.454661	-2040.248381	-2040.158224	-2047.503709
Complex22	-2019.253586	-2020.608461	-2020.477115	-2020.247516	-2020.042580	-2019.953973	-2027.291854
Complex23	-2105.421389	-2106.440442	-2106.217142	-2106.073974	-2106.006225	-2106.018589	-2115.015884
Complex24	-1869.750601	-1871.025979	-1870.916690	-1870.722332	-1870.469473	-1870.389978	-1876.436564
Complex25	-1926.421479	-1927.760271	-1927.650272	-1927.452945	-1927.190344	-1927.105252	-1933.113003
Complex26	-1565.162189	-1566.059301	-1565.914966	-1565.769500	-1565.615467	-1565.609907	-1572.083445
Complex27	-1508.853863	-1509.670709	-1509.513292	-1509.382037	-1509.254470	-1509.269693	-1515.860256
Complex28	-2061.980302	-2062.996823	-2062.812544	-2062.646152	-2062.496386	-2062.480790	-2069.936028
Complex29	-1816.130332	-1817.268083	-1817.115109	-1816.981385	-1816.797925	-1816.791570	-1823.224082
Complex30	-1562.291991	-1563.194263	-1563.037315	-1562.896221	-1562.762782	-1562.753936	-1569.264780
Complex31	-1945.758932	-1947.136166	-1947.036939	-1946.809687	-1946.542391	-1946.445681	-1952.375820
Complex32	-1945.684823	-1947.065413	-1946.968280	-1946.730334	-1946.468934	-1946.372586	-1952.306283
Complex33	-2634.967364	-2636.194024	-2635.980478	-2635.778694	-2635.614920	-2635.570654	-2643.894087
Complex34	-3325.515639	-3326.988492	-3326.723727	-3326.493452	-3326.318984	-3326.266633	-3336.021693
Complex35	-1655.855393	-1656.769143	-1656.590287	-1656.469625	-1656.353903	-1656.388865	-1663.082219
Complex36	-2019.070988	-2020.415088	-2020.286019	-2020.095665	-2019.850449	-2019.761275	-2027.125942

Complex37 -2005.758442 -2006.717531 -2006.509785 -2006.374772 -2006.259040 -2006.268308 -2015.212151
 Complex38 -1677.808326 -1678.724150 -1678.563538 -1678.418497 -1678.280029 -1678.276441 -1686.112138
 Complex39 -1961.140746 -1962.369081 -1962.207520 -1962.066754 -1961.862054 -1961.830130 -1969.483529
 Complex40 -1915.839345 -1916.959931 -1916.782565 -1916.656060 -1916.501383 -1916.504643 -1924.366041
 Complex41 -2058.434822 -2059.826373 -2059.712763 -2059.493488 -2059.241103 -2059.142668 -2066.432635
 Complex42 -1945.838306 -1947.070989 -1946.930717 -1946.739846 -1946.542061 -1946.483051 -1954.013328
 Complex43 -1833.829540 -1835.011037 -1834.895835 -1834.723807 -1834.538730 -1834.459393 -1840.644223
 Complex44 -1562.533989 -1563.410251 -1563.264062 -1563.126903 -1563.037031 -1563.002305 -1569.510663
 Complex45 -2289.270583 -2290.501479 -2290.335833 -2290.167729 -2290.021316 -2289.959474 -2297.267058
 Complex46 -3217.803883 -3219.225820 -3218.957603 -3218.795349 -3218.733750 -3218.669349 -3229.188035
 Complex47 -3259.887109 -3261.323923 -3261.054913 -3260.855788 -3260.747697 -3260.688092 -3270.658629
 Complex48 -3489.693144 -3491.176547 -3490.890885 -3490.676525 -3490.566397 -3490.501723 -3500.941330
 Complex49 -1721.267011 -1722.287909 -1722.146903 -1722.002207 -1721.871523 -1721.832760 -1728.256424
 Complex50 -1608.694415 -1609.554251 -1609.387851 -1609.270296 -1609.194986 -1609.197171 -1615.860630

S4 Optimized geometries of 50 TM complexes

S4.1 Low spin geometries

Complex1: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_cyanide_s_1.xyz

Co 0.0026197922 0.0029795147 0.0030260334
 C 0.0007069991 3.0644007788 0.0012168812
 N 0.0025223423 1.9123993474 0.0031855984
 C -0.0028756818 4.5199195035 -0.0029639885
 H -0.2799789657 4.8869862434 -0.9961138516
 H 0.9942925120 4.8915697513 0.2527744399
 H -0.7202214485 4.8900785414 0.7361623528
 C 3.0640409663 -0.0021125949 0.0000695078
 N 1.9120455176 0.0019310917 0.0016517246
 C 4.5194889491 -0.0102118740 -0.0018388004
 H 4.8942695447 1.0181238811 -0.0020940356
 H 4.8856125416 -0.5238308122 -0.8963325119
 H 4.8879733704 -0.5242892904 0.8914217911
 C -0.0020307318 -3.0585536354 0.0005260122
 N 0.0017035872 -1.9065568057 0.0018325283
 C -0.0096356373 -4.5139999565 -0.0010757175
 H 1.0188385968 -4.8883846807 0.0039590078
 H -0.5187462397 -4.8805329940 -0.8979752924
 H -0.5280433633 -4.8824331228 0.8896949822
 C -3.0589102464 0.0007878357 0.0002735498
 N -1.9069111775 0.0028399001 0.0030692104
 C -4.5144172839 -0.0031380552 -0.0055004073
 H -4.8850244564 -0.7421868595 0.7116911976
 H -4.8802246466 -0.2513560310 -1.0067431344
 H -4.8868444080 0.9858781496 0.2790733211
 C 0.0037986035 0.0012504822 1.9354442755
 N 0.0046208887 -0.0008814715 3.1010584607
 C 0.0007607147 0.0039474672 -1.9296236778
 N -0.0015475112 0.0045354229 -3.0952467873

 Complex2: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_fluoride_fluoride_s_1.xyz

Co 0.0016768886 0.0023290872 0.0011049839
C 0.4284747956 3.0064920403 0.4991202667
N 0.2693638351 1.8798773890 0.3203477026
C 0.6280359501 4.4318748622 0.7213851035
H 0.5975347553 4.9632919485 -0.2347224035
H 1.5997470278 4.6010655342 1.1953172887
H -0.1586516949 4.8188484817 1.3762595884
C 3.0058111815 -0.4905055932 0.4357014994
N 1.8812174879 -0.3051579104 0.2698851352
C 4.4273567741 -0.7271570585 0.6455494842
H 4.9100379203 0.1934485472 0.9876218172
H 4.8924478344 -1.0477276978 -0.2916987364
H 4.5656505374 -1.5042352385 1.4035264573
C -0.4286666530 -3.0005614811 -0.5024109520
N -0.2663710592 -1.8751187699 -0.3191348921
C -0.6353708832 -4.4236247271 -0.7328414291
H 0.3254509573 -4.9466402772 -0.7054567982
H -1.0971641941 -4.5775671728 -1.7128955292
H -1.2875524696 -4.8339549012 0.0441998907
C -3.0026811693 0.4888142974 -0.4394330417
N -1.8779166860 0.3090401657 -0.2687039168
C -4.4245438715 0.7142865782 -0.6591924885
H -5.0054044470 -0.0685704256 -0.1619578340
H -4.6401974734 0.6993462492 -1.7319387004
H -4.7141883512 1.6863241119 -0.2483412856
F -0.2798878721 -0.2707278989 1.7378999328
F 0.2830178200 0.2752354534 -1.7358731235

Complex3: cr_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_misc_misc_s_1.xyz

Cr 0.0004489396 -0.0014034206 0.0003014702
C -0.4507083156 3.1447726414 -0.5066993564
N -0.2673143657 2.0118406596 -0.3503021270
C -0.6792846063 4.5693836280 -0.7039327380
H -0.9172644061 4.7732900705 -1.7527934511
H 0.2160758579 5.1335950360 -0.4230274050
H -1.5147906352 4.9004138470 -0.0780003454
C 3.1378381667 0.5299079103 0.4770476057
N 2.0017621888 0.3573752130 0.3314449676
C 4.5656471569 0.7518947210 0.6590705466
H 4.7893142254 1.8197639292 0.5654944705
H 5.1277372643 0.2063065383 -0.1061421885
H 4.8803433607 0.4063667745 1.6488874955
C 0.4460521135 -3.1481590889 0.5069732857
N 0.2671667971 -2.0144750052 0.3508410895
C 0.6674456545 -4.5734537531 0.7071294601
H 1.7300925176 -4.7630433783 0.8912726085
H 0.3525074820 -5.1338474089 -0.1789121275
H 0.0928604156 -4.9203722530 1.5724831620
C -3.1364325323 -0.5338837411 -0.4786444284
N -2.0007305981 -0.3602286214 -0.3314862378
C -4.5637865618 -0.7545129214 -0.6657858412

H -4.9408940746 -1.4496184595 0.0911656175
H -4.7506744532 -1.1714866133 -1.6608110742
H -5.1004239495 0.1957069499 -0.5746182809
C -0.2320134798 0.2088504902 2.0438727593
N -0.3659078129 0.3339163052 3.1937664988
C -0.5285264375 0.4871885960 4.6047431286
H 0.1466190694 -0.1996252617 5.1214338967
H -1.5620517998 0.2589333886 4.8767555592
H -0.2921865155 1.5160541722 4.8872071018
C 0.2341948305 -0.2110027458 -2.0431748867
N 0.3707541907 -0.3340551767 -3.1929861937
C 0.5384471751 -0.4828218988 -4.6038513237
H 0.1003409755 -1.4314562708 -4.9237116744
H 1.6045799317 -0.4701689914 -4.8437088970
H 0.0386632491 0.3438374267 -5.1150679154

Complex4: cr_2_acetonitrile_acetonitrile_ammonia_ammonia_ammonia_ammonia_s_1.xyz

Cr 0.0652482084 -0.0992963227 0.0005043054
C -0.3494446123 3.0920184442 0.4576167020
N -0.1868208761 1.9563767350 0.2734866075
C -0.5445966523 4.5177636112 0.6872926108
H -1.1622061404 4.9474418409 -0.1084732882
H 0.4233731504 5.0296153404 0.7052888204
H -1.0465437656 4.6752668350 1.6480957167
C 3.2478014780 0.4086442905 -0.4169770485
N 2.1139291963 0.2272806299 -0.2385644818
C 4.6685873603 0.6453321729 -0.6371840487
H 4.8829143692 1.7172475430 -0.5702160617
H 4.9569594934 0.2883803358 -1.6318662238
H 5.2612707855 0.1142374120 0.1151446657
N 0.3111903182 -2.2460740898 -0.3217655581
H 1.2822120798 -2.4554762019 -0.5673035819
H 0.1310751699 -2.8062657266 0.5143196982
H -0.2541736473 -2.6698682258 -1.0613770966
N -2.0727881276 -0.4093054510 0.2375948759
H -2.3752272978 -1.3857234144 0.2203473819
H -2.4070681687 -0.0447866990 1.1335739622
H -2.6391017149 0.0714722127 -0.4652370740
N 0.4190529752 -0.4176955606 2.1374284830
H 0.1698032412 0.4150828698 2.6764614183
H -0.0231763908 -1.2035839293 2.6199141917
H 1.4249693798 -0.5268720958 2.2786555158
N -0.2887744758 0.2274511257 -2.1302021478
H -0.4629766295 1.2226706477 -2.2817165157
H 0.5505586105 0.0231787898 -2.6780386761
H -1.0505786905 -0.2723580172 -2.5944402002

Complex5: cr_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_1.xyz

Cr 0.0007187662 0.0003712808 -0.0019986812

```

N -0.2587679007 2.1442629071 0.3687192536
H -1.2322992829 2.3252508032 0.6099964367
H 0.3120305586 2.5430268934 1.1136154271
H -0.0869238649 2.6429106358 -0.5041825996
N 2.1755548241 0.2762445412 -0.0897519433
H 2.3911858579 1.2729198457 -0.1003948409
H 2.6043567651 -0.1089641806 0.7515201703
H 2.6378311471 -0.1136308934 -0.9118540445
N 0.2596991829 -2.1438010164 -0.3724305048
H 1.2357154469 -2.3284493547 -0.6004884145
H 0.0738368744 -2.6441440207 0.4966190734
H -0.3027180017 -2.5380159390 -1.1260988696
N -2.1746971542 -0.2757887127 0.0832133130
H -2.3899595531 -1.2725985576 0.0862799026
H -2.6394435774 0.1083828839 0.9066175428
H -2.6013903213 0.1144745251 -0.7568013356
C 0.3840324627 -0.3333629602 2.0169180436
N 0.6992490208 -0.5421522642 3.1292130685
C -0.3841515468 0.3328363708 -2.0207422816
N -0.7038424040 0.5402210236 -3.1320488710

```

Complex6: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_ammonia_s_1.xyz

```

Cr -0.1095522433 0.1256494793 -0.0654596607
C 0.2810403517 2.1620934965 -0.3234400406
O 0.4889776596 3.2619797704 -0.4571666800
C 1.9047941379 0.0639728616 0.3023666677
O 3.0164291596 0.0303562344 0.4961269296
C -0.6045921373 -1.8407915715 0.2093930774
O -0.8768643928 -2.9275116899 0.3483720799
C -2.1646929156 0.3234792790 -0.3971711368
O -3.2721479052 0.4378699403 -0.5733404283
C -0.1919045213 0.1395827600 2.0273935002
O -0.2478533496 0.1656269888 3.1524779936
N 0.3757397720 -0.4106379843 -2.0679130185
H -0.4392488419 -0.7270754326 -2.6061808984
H 0.7788849390 0.3684367490 -2.6025426715
H 1.0612560253 -1.1713756353 -2.1573127665

```

Complex7: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_s_1.xyz

```

Cr -0.0003921070 -0.0003977354 0.0420315290
C 0.1208134786 2.0049788468 -0.0213692592
O 0.1933092148 3.1325443864 -0.1009323060
C 2.0049920156 0.1206973958 -0.0214130085
O 3.1325597403 0.1931279449 -0.1010046310
C -0.1216829879 -2.0053747670 -0.0258348548
O -0.1942730097 -3.1327640490 -0.1078860317
C -2.0053790632 -0.1215732939 -0.0257971797
O -3.1327743883 -0.1940929643 -0.1078268583
C -0.0017626717 -0.0018050696 2.1631288447

```

O -0.0021390192 -0.0022023460 3.2933301838
C 0.0022922205 0.0023406122 -1.8921795453
N 0.0044378386 0.0045214443 -3.0705672767

Complex8: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_1.xyz
Cr -0.0486216514 -0.0485123657 -0.0189696943
C -0.1946639450 1.9537029289 -0.3259858823
O -0.2923698952 3.0622649952 -0.5330753693
C 1.9528694514 -0.2029158178 -0.3255435241
O 3.0609891482 -0.3056647604 -0.5325666923
C 0.0986060537 -2.0473834539 0.2993825564
O 0.1841234935 -3.1663373814 0.4481957616
C -2.0467999629 0.1069728954 0.2984688704
O -3.1654316714 0.1975108142 0.4467662789
C 0.2947020739 0.2941288007 2.0433852674
O 0.4809524980 0.4799944622 3.1438946841
F -0.3243528077 -0.3237643102 -1.7293554291

Complex9: cr_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_s_1
Cr 0.2372616223 0.0837030184 -0.0022140841
S 0.7224280659 2.5011593675 -0.6344345707
H 0.8826789829 3.1999817160 0.5091419656
H -0.4602121519 3.0729415196 -0.9448380716
S 2.7600419967 -0.1699687272 -0.2358115864
H 3.0401562264 -1.4804149525 -0.0679069417
H 2.9847745252 -0.1781734959 -1.5666948593
S -0.0174503489 -2.4005446091 0.4072145762
H 0.0407286908 -2.6774657857 1.7279951593
H -1.3106371291 -2.7549817013 0.2614360758
S -2.2248535357 0.5606080844 0.3588954296
H -2.7797443533 -0.3894440890 1.1415572599
H -2.9193352228 0.2199033251 -0.7466417140
S 0.7202532560 0.3584747784 2.5064357391
H -0.2700178727 1.1102350186 3.0355808378
H 1.6684208347 1.3069682150 2.6698851206
C -0.1800778790 -0.1256780504 -1.9887040795
N -0.3702975757 -0.2733292472 -3.1276827479
C -0.5891847461 -0.4566687135 -4.5331606952
H -1.6631755259 -0.4345714345 -4.7342657157
H -0.1762651428 -1.4241140960 -4.8310865109
H -0.0890250022 0.3469746833 -5.0794551582

Complex10: cr_2_misc_misc_misc_misc_misc_misc_s_1.xyz
Cr 0.0015815547 -0.0010737124 0.0007571986
C 0.4037883499 2.0012652140 0.1976369316
N 0.6137227522 3.1387534979 0.3297107488
C 0.8686653562 4.5357600042 0.4893290351

H 1.5111787739 4.8765914704 -0.3267609804
 H 1.3685438675 4.7055953575 1.4460868817
 H -0.0783048449 5.0805068840 0.4628676227
 C 2.0262712161 -0.2293497179 -0.2356893709
 N 3.1712941907 -0.3746416705 -0.3883130770
 C 4.5768237148 -0.5543436241 -0.5734338368
 H 4.7517153923 -1.0101762774 -1.5514638573
 H 4.9657020860 -1.2072112460 0.2117741511
 H 5.0739455282 0.4178939731 -0.5286846987
 C -0.4025754524 -2.0028955341 -0.1969649497
 N -0.6161991181 -3.1393709010 -0.3317534905
 C -0.8804115550 -4.5340075879 -0.4970065563
 H -1.6655210982 -4.6687524941 -1.2448828473
 H -1.2047934283 -4.9523163114 0.4593433454
 H 0.0336686804 -5.0358698203 -0.8243991410
 C -2.0232436907 0.2255920565 0.2381446354
 N -3.1683763079 0.3678500682 0.3927922388
 C -4.5741551890 0.5397877956 0.5833518776
 H -4.7555046130 1.5113488426 1.0501363559
 H -4.9535902326 -0.2568253476 1.2278268530
 H -5.0751928798 0.5016025795 -0.3873220394
 C 0.3486037001 -0.4194254359 1.9782014113
 N 0.5287726279 -0.6344341731 3.1081580888
 C 0.7496835681 -0.8977834939 4.4952180847
 H 1.1901462750 -1.8922868415 4.6043276884
 H -0.2055706457 -0.8603823643 5.0248146770
 H 1.4301324868 -0.1464561762 4.9032425207
 C -0.3456138175 0.4189955628 -1.9762212223
 N -0.5257620495 0.6363027853 -3.1057418283
 C -0.7469020191 0.9046600576 -4.4918035212
 H -1.4474793946 0.1702397145 -4.8964904911
 H 0.2046226573 0.8438193534 -5.0259272371
 H -1.1631134796 1.9097653178 -4.5989747584

Complex11: cr_2_phosphine_phosphine_phosphine_phosphine_hydrogensulfide_hydrogensulfide_s_1.xyz
 Cr -0.0031564234 0.0051175937 0.0355054049
 P 0.4784501334 2.4528462599 -0.3938414990
 H -0.3557496293 3.3657179869 0.2869153582
 H 1.7298358708 3.0307228278 -0.0923378469
 H 0.3099478863 2.9414851292 -1.7069965126
 P 2.4725703797 -0.2538556936 0.5101974583
 H 2.9281468018 -0.0701223187 1.8327938058
 H 3.0453555134 -1.5191086007 0.2576263930
 H 3.4093203526 0.5534352098 -0.1691198910
 P -0.4846849194 -2.4426082178 0.4648317792
 H -0.3164604623 -2.9310908173 1.7780685321
 H -1.7359127644 -3.0206608890 0.1630356288
 H 0.3498145149 -3.3554348129 -0.2156161141
 P -2.4788700063 0.2641476973 -0.4393204992
 H -2.9342225151 0.0803864818 -1.7619983693
 H -3.4157645463 -0.5430996804 0.2398399962

H -3.0516662052 1.5294348054 -0.1869139605
S -0.3144391059 0.3351609058 2.5194145615
H -0.0691261981 1.6182646339 2.8607923362
H -1.6270108461 0.3809578879 2.8331278142
S 0.3081571173 -0.3249368565 -2.4484323200
H 0.0636622231 -1.6082354119 -2.7896572632
H 1.6207407731 -0.3699060812 -2.7622264880

Complex12: cr_2_phosphine_phosphine_phosphine_phosphine_phosphine_ammonia_s_1.xyz

Cr -0.0110530662 -0.0308283609 -0.0489107642
P 0.4616665075 2.4245307428 -0.3962319785
H -0.3332341358 3.3806692009 0.2720595365
H 1.7355494017 2.9591913812 -0.1094801752
H 0.3144383330 2.9170334611 -1.7127113735
P 2.4615735068 -0.3835979685 -0.4401124466
H 3.3860860193 0.6797958790 -0.3708070826
H 3.1238658806 -1.3039897014 0.4006759791
H 2.8412019104 -0.9301968063 -1.6863687467
P -0.4094146346 -2.4932805696 0.3600109892
H 0.5472436442 -3.1794562270 1.1390368142
H -1.5814326057 -2.9601802149 0.9910380811
H -0.4071299050 -3.3484332875 -0.7652500430
P -2.4754422618 0.2751606656 0.4066171930
H -3.2693890366 -0.7741325281 0.9155534176
H -2.8865397475 1.3065240289 1.2780067665
H -3.2735562693 0.6229817484 -0.7071348546
P 0.3575862161 0.4119057616 2.4681033328
H 1.6521029518 0.7147203674 2.9409013426
H -0.3426600763 1.5043723263 3.0224266874
H 0.0000072538 -0.5801710552 3.4056081299
N -0.4152453190 -0.2425373946 -2.1683881508
H -1.2052648969 0.3283242894 -2.4825486701
H 0.3664523589 0.0163599373 -2.7747978607
H -0.6615095939 -1.2013768438 -2.4267882609

Complex13: cr_2_water_water_water_water_ammonia_ammonia_s_1.xyz

Cr 0.0008141154 -0.0009484194 0.0011704034
O 0.2234643394 2.0877263672 -0.1024623969
H 0.8185282177 2.6824439614 0.3864750250
H -0.1380694383 2.6074022621 -0.8418667134
O 2.0253761512 -0.4481674079 0.4957586297
H 2.5686948382 -1.0091972815 -0.0849898300
H 2.6510482348 0.1392371102 0.9545547755
O -0.2291481607 -2.0872040346 0.1052015971
H 0.1451827678 -2.6099725044 0.8359504841
H -0.8139752625 -2.6859927392 -0.3910056569
O -2.0241112836 0.4457404885 -0.4982712845
H -2.5587889950 1.0309803944 0.0664103190
H -2.6571775857 -0.1535854294 -0.9307090901

N -0.2908354606 0.2212462307 2.1380050224
H -0.4192092089 1.1909396970 2.4383212082
H -1.1200547350 -0.2725920574 2.4817718525
H 0.4846479744 -0.1430330522 2.6978446887
N 0.2905501820 -0.2215142045 -2.1367208023
H -0.4922277201 0.1391148380 -2.6887097915
H 1.1138689191 0.2774502176 -2.4871635929
H 0.4214651465 -1.1900673423 -2.4395661036

Complex14: cr_2_water_water_water_water_carbonyl_carbonyl_s_1.xyz

Cr 0.0001571938 -0.0000856475 0.0001360238
O -0.2721326226 1.9756942868 0.3370503598
H -0.3300797565 2.6552085401 -0.3593455594
H -0.4268642158 2.4148184646 1.1934842228
O 1.9721283129 0.3196816735 -0.3252153539
H 2.4347795677 0.3958783783 -1.1798094726
H 2.6253735293 0.4776939076 0.3806876170
O 0.2721992077 -1.9757945297 -0.3369669305
H 0.4279914622 -2.4144768008 -1.1934325944
H 0.3296601175 -2.6556237300 0.3591724149
O -1.9719186232 -0.3196585689 0.3252496588
H -2.4347356836 -0.3952251836 1.1798115803
H -2.6250219725 -0.4782420097 -0.3806547272
C 0.3201000743 -0.2666988004 1.9778652108
O 0.5083448788 -0.4240213177 3.0844206550
C -0.3204806514 0.2667958862 -1.9780206241
O -0.5095023021 0.4240466953 -3.0844345459

Complex15: fe_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_1.xyz

Fe -0.0749960090 -0.0654768850 -0.0085243025
C 0.3777204579 3.0086577331 -0.4619460906
N 0.2066618449 1.8745352551 -0.3117190413
C 0.5944926240 4.4385497486 -0.6461175544
H 0.2488549066 4.7468299832 -1.6380893791
H 1.6605266268 4.6696213105 -0.5532592324
H 0.0412034296 5.0004122185 0.1133148100
C 2.9893906726 -0.5702303789 -0.4597854458
N 1.8573979251 -0.3846693979 -0.3099741901
C 4.4162405684 -0.8044814190 -0.6455486108
H 4.9300423410 0.1434012696 -0.8352670272
H 4.5792122314 -1.4738291369 -1.4964569217
H 4.8384107055 -1.2641673056 0.2539331646
C -0.5245416541 -3.1341069408 0.4722366340
N -0.3600344890 -2.0056777660 0.2768333584
C -0.7304573455 -4.5553584925 0.7230669460
H 0.2246109566 -5.0873931953 0.6667682340
H -1.4151936076 -4.9732641465 -0.0219562984
H -1.1596440972 -4.6989211136 1.7199543345
C -3.1395501851 0.4286288450 0.4681425205

N -2.0132727411 0.2481736779 0.2749618685
C -4.5579752589 0.6554258423 0.7169569790
H -4.8863191395 0.0572387596 1.5730903857
H -5.1444695955 0.3688351630 -0.1619721889
H -4.7354776928 1.7138066627 0.9332823343
C 0.4391571962 0.3576343237 3.0783915772
N 0.2501151783 0.1971797455 1.9488939886
C 0.6782963454 0.5598571738 4.5025564654
H -0.2495089865 0.4090160705 5.0634664783
H 1.0396514749 1.5777432359 4.6804063754
H 1.4296000144 -0.1513020067 4.8604484229
N -0.4059089706 -0.2873979445 -1.9949637512
H -1.2620982100 0.1806591020 -2.2948718434
H 0.3575916089 0.0952464924 -2.5538190735
H -0.4985932522 -1.2719647425 -2.2469567766

Complex16: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_chloride_chloride_s_1.xyz

Fe -0.0000003020 0.0000002779 -0.0027207263
C -0.0000261641 1.8777725283 -0.0027102991
O -0.0000421991 3.0137192633 -0.0027787034
C 1.8777716817 0.0000203714 -0.0027377911
O 3.0137185219 0.0000311416 -0.0028166980
C 0.0000257143 -1.8777704123 -0.0034872853
O 0.0000421508 -3.0137169161 -0.0039531767
C -1.8777711013 -0.0000199751 -0.0034518742
O -3.0137177553 -0.0000306585 -0.0038995444
Cl -0.0008847950 -0.0009875014 2.3407415688
Cl 0.0008841011 0.0009819238 -2.3464513866

Complex17: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_cyanide_s_1.xyz

Fe 0.0000000546 0.0000003715 0.0000006449
C -0.0000371957 1.8577842479 0.0000288659
O -0.0000606652 2.9940305798 0.0000457912
C 1.8577845090 0.0000293011 -0.0000145585
O 2.9940308524 0.0000440954 -0.0000245069
C 0.0000363474 -1.8577838141 -0.0000277642
O 0.0000590941 -2.9940302555 -0.0000447127
C -1.8577837561 -0.0000304122 0.0000144892
O -2.9940301443 -0.0000473087 0.0000228421
C 0.0000142468 -0.0000285368 1.9475021061
N 0.0000236158 -0.0000469342 3.1135221584
C -0.0000141057 0.0000298869 -1.9475024755
N -0.0000232791 0.0000491370 -3.1135225922

Complex18: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_hydrogensulfide_hydrogensulfide_s_1.xyz

Fe 0.1052629933 0.0772635825 0.0174780649
C 0.3839040407 1.9471441469 -0.3537223149

O 0.5477616810 3.0405547556 -0.5793508971
C 1.9923361610 -0.2304022548 -0.2155962295
O 3.0983618308 -0.4106362404 -0.3475147883
C -0.1613003063 -1.7827983200 0.3501854616
O -0.3207969899 -2.8853610115 0.5374707273
C -1.7567079599 0.4036048887 0.2798633468
O -2.8554540281 0.6034890020 0.4501569558
S 0.5490839402 0.4804570628 2.4045522960
H -0.3725401238 -0.2950692618 3.0225975175
H -0.1199615947 1.6324447126 2.6455793292
S -0.2528533674 -0.2637426966 -2.3931221527
H -1.3881764552 -1.0001829339 -2.4292577336
H 0.5510914122 -1.3167506324 -2.6718649186

Complex19: fe_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_misc_s_1.xyz

Fe 0.4952720067 -0.0822612531 -0.0282622028
S 0.7399916070 2.3069664139 0.3713198469
H 1.7546491285 2.3953422883 1.2587213054
H 1.4830123383 2.7660937468 -0.6584487834
S 2.8663733205 -0.3695257282 0.3452473602
H 3.0139473625 -1.5079799750 1.0565752426
H 3.3806031311 -0.8976079704 -0.7863982258
S 0.0476106460 -2.4250391179 -0.4270855327
H 0.4420061218 -3.0936601061 0.6779701307
H 1.0604365632 -2.8915795669 -1.1888799361
S -1.8604373121 0.4214552920 -0.4198623251
H -2.5003459592 0.0886637871 0.7217271021
H -2.3293919754 -0.6482063869 -1.0994735156
C 0.1846994350 -0.3176563402 1.8798979955
N -0.0093786153 -0.4420242465 3.0201490211
C -0.2521531228 -0.5773444265 4.4282742148
H 0.1685460926 -1.5245813005 4.7744053932
H -1.3300967933 -0.5614951473 4.6071635423
H 0.2240182874 0.2553233888 4.9518625531
C 0.7765859957 0.1805822351 -1.9385847248
N 0.9248582799 0.3526230333 -3.0793206961
C 1.0906759061 0.5740049459 -4.4877055978
H 0.4654593607 -0.1359670958 -5.0347261812
H 2.1408775975 0.4262296232 -4.7508991891
H 0.7870631090 1.5967376362 -4.7246449367

Complex20: fe_2_misc_misc_misc_misc_misc_acetonitrile_s_1.xyz

Fe 0.0006446929 0.0024885894 0.0345130645
C 0.0021947608 1.9373581326 0.0219750200
N 0.0043120957 3.0992555522 0.0087288223
C 0.0086575544 4.5294715265 -0.0058578268
H 0.8448878795 4.8804029558 -0.6153229073
H 0.1178938250 4.8983790070 1.0168361986
H -0.9327189637 4.8883978299 -0.4287656095

C 1.9355516514 0.0006540000 0.0219975383
 N 3.0974653866 -0.0015408293 0.0103815802
 C 4.5277163806 -0.0057231351 -0.0008400116
 H 4.8802289397 -0.8412296514 -0.6103796417
 H 4.8940967327 -0.1160858798 1.0226462591
 H 4.8875723534 0.9361825350 -0.4217671046
 C -0.0011458161 -1.9324260038 0.0198904439
 N -0.0036846552 -3.0943117836 0.0059003474
 C -0.0087144798 -4.5245299524 -0.0088183806
 H -0.8448936113 -4.8750052495 -0.6186128748
 H -0.1185623861 -4.8934102146 1.0138266555
 H 0.9326538019 -4.8838960559 -0.4313579512
 C -1.9342516152 0.0027324418 0.0220750616
 N -3.0961676802 0.0015609727 0.0104818695
 C -4.5263703093 -0.0014715470 -0.0010662191
 H -4.8910407468 0.9875683186 0.2864291354
 H -4.8899423010 -0.7493960598 0.7077102653
 H -4.8770964067 -0.2458184580 -1.0066386187
 C 0.0005841466 0.0010844284 1.9345284737
 N 0.0001276454 -0.0006960477 3.0970432822
 C -0.0017277989 -0.0047047211 4.5272543254
 H 0.6046059489 -0.8401856347 4.8854695447
 H -1.0282582646 -0.1142775094 4.8852531824
 H 0.4169214928 0.9368754912 4.8907582051
 C 0.0006229716 0.0040173671 -3.1284572604
 N 0.0006306588 0.0036872236 -1.9731052684
 C 0.0004633042 0.0039439962 -4.5862160952
 H 1.0235336925 -0.1045635193 -4.9603730771
 H -0.4172809619 0.9441107827 -4.9603714078
 H -0.6049814348 -0.8280386594 -4.9599370944

Complex21: fe_2_misc_misc_misc_misc_misc_carbonyl_s_1.xyz

Fe 0.0017002992 0.0032667222 -0.0100229458
 C 0.0018077138 1.9398573193 0.0019321169
 N 0.0026593984 3.1000993123 -0.0049646521
 C 0.0051463165 4.5321618525 -0.0265937882
 H 0.8409201855 4.8773022031 -0.6399233010
 H 0.1140314057 4.9048784951 0.9945822393
 H -0.9372813446 4.8839373386 -0.4530206253
 C 1.9383197979 0.0022234077 0.0013720904
 N 3.0985610858 0.0003893898 -0.0044366685
 C 4.5306560986 -0.0031546528 -0.0236600314
 H 4.8762240175 -0.8384421929 -0.6374080899
 H 4.9014552044 -0.1135453733 0.9980582111
 H 4.8839151836 0.9395315473 -0.4482706629
 C 0.0010217013 -1.9334842531 -0.0003874675
 N -0.0009771844 -3.0937197069 -0.0079134659
 C -0.0053280359 -4.5257859819 -0.0294863462
 H -0.8418216017 -4.8698454258 -0.6424438553
 H -0.1143118441 -4.8982469909 0.9917807059
 H 0.9364883705 -4.8788549617 -0.4561790451

C -1.9349556385 0.0028002079 0.0018048109
 N -3.0952035703 0.0011517455 -0.0037962214
 C -4.5272491239 -0.0024261679 -0.0235861238
 H -4.8909763728 0.9872252340 0.2626157265
 H -4.8924424241 -0.7516345357 0.6827906979
 H -4.8680592214 -0.2455857792 -1.0328957725
 C 0.0015306485 0.0014420540 1.9283533585
 N 0.0007877426 -0.0007857514 3.0887220187
 C -0.0011601335 -0.0049123721 4.5207320307
 H 0.6065729863 -0.8403453527 4.8763156269
 H -1.0283642064 -0.1157703660 4.8760303084
 H 0.4167030845 0.9378514459 4.8817096967
 C 0.0010015302 0.0041743545 -1.8727032395
 O 0.0003412589 0.0046078695 -3.0083367917

Complex22: fe_2_misc_misc_misc_misc_misc_cyanide_s_1.xyz

Fe 0.0401660554 0.0396832330 0.3151295428
 C -0.2625520581 1.9107219900 0.4758318008
 N -0.4377078712 3.0616911235 0.5121753770
 C -0.6358079829 4.4709381153 0.4592092540
 H 0.2577273060 4.9468413154 0.0467861181
 H -0.8241306959 4.8551610259 1.4649944966
 H -1.4920064623 4.6924528411 -0.1833201917
 C 1.9066649220 0.3331051752 0.5276453573
 N 3.0538245328 0.5247286898 0.5910585937
 C 4.4547913062 0.7791228336 0.5665900460
 H 4.9522156748 0.0098024478 -0.0298064317
 H 4.8510713820 0.7658228854 1.5850959667
 H 4.6359611011 1.7582271213 0.1153884775
 C 0.3729719970 -1.7949246690 -0.0595482323
 N 0.5852619079 -2.9020796808 -0.3523931140
 C 0.8652317052 -4.2213125011 -0.8102099956
 H 0.0622055513 -4.5527934476 -1.4736581110
 H 0.9382207702 -4.9008552921 0.0427861598
 H 1.8102558758 -4.2194808303 -1.3597049086
 C -1.7950117092 -0.2168424728 -0.1165853693
 N -2.9019279798 -0.3627020536 -0.4484604476
 C -4.2229311587 -0.5214919874 -0.9569010455
 H -4.8613706582 0.2779475997 -0.5720299156
 H -4.6231105681 -1.4882101048 -0.6406570114
 H -4.1953683221 -0.4744029538 -2.0488018567
 C -0.2401304194 -0.2717573017 2.1704524302
 N -0.4130416301 -0.4606766075 3.3090266305
 C -0.6268301915 -0.6907403523 4.6980204643
 H 0.1149955289 -1.4024566766 5.0700435216
 H -1.6294956574 -1.0987182541 4.8514095755
 H -0.5313364304 0.2514263499 5.2443023663
 C 0.3222898581 0.3586899410 -1.5836820777
 N 0.4887173154 0.5468106634 -2.7237456989

Complex23: fe_2_water_water_water_water_water_chloride_s_1.xyz

Fe 0.0401968552 -0.0032431003 0.1924141246
O 0.5026292732 1.9566468333 0.4564047826
H 0.6115445998 2.2501560491 -0.4746093084
H -0.1385777802 2.5604634787 0.8684177872
O 2.0101131470 -0.3401117514 0.5062146702
H 2.4212778309 0.5130318683 0.7413499147
H 2.3722088166 -0.5295836637 -0.3832001653
O -0.2943426548 -1.9924868971 0.0005034846
H 0.2212020265 -2.3531190158 -0.7440943776
H -1.2274075505 -2.0989967122 -0.2639519614
O -1.9499478950 0.1457435146 -0.1889998990
H -2.5294117812 0.7364402258 0.3204970662
H -1.9940879323 0.4134149880 -1.1295058481
O -0.3509535581 -0.2792364345 2.1676129458
H 0.4158136206 -0.0888693124 2.7365040482
H -0.5195034636 -1.2308631191 2.3028996995
Cl 0.4104731351 0.3398910889 -2.0490502427

Complex24: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_1.xyz

Mn -0.0655267574 -0.0748997611 0.0105131196
C -0.5684430081 2.9854927650 -0.4378720067
N -0.3939249601 1.8478549179 -0.2803549909
C -0.7887549464 4.4055832121 -0.6350621689
H -1.2731600798 4.5800239269 -1.6035186006
H 0.1675675332 4.9412190681 -0.6038639616
H -1.4389225973 4.7904880594 0.1614165704
C 2.9932500761 0.3719746927 -0.4981002156
N 1.8601532171 0.1933377852 -0.3155463242
C 4.4085224592 0.5924837529 -0.7273119928
H 4.5864423395 1.6453231794 -0.9789114731
H 4.7607586785 -0.0417761273 -1.5494511686
H 4.9716615828 0.3465130752 0.1822651884
C 0.4885069306 -3.1288165097 0.4394263033
N 0.2858904278 -2.0013277006 0.2488109854
C 0.7411806131 -4.5377873702 0.6763127623
H 1.8170643355 -4.7398685022 0.6059964059
H 0.2083062485 -5.1461257338 -0.0641499552
H 0.3943964573 -4.8113366115 1.6810722402
C -3.1358127125 -0.4670794111 0.5058699736
N -2.0045089717 -0.3207720120 0.2884374554
C -4.5493188606 -0.6534173004 0.7756848501
H -4.6789731958 -1.4135433491 1.5567052285
H -5.0635332517 -0.9883483596 -0.1335145848
H -4.9930614726 0.2893059240 1.1172381731
C 0.4065899634 0.4562808091 3.0736554517
N 0.2414428795 0.2731267093 1.9388827818
C 0.6139048054 0.6879698889 4.4912527744
H -0.3479151516 0.6667392259 5.0176535281
H 1.0766666260 1.6719528056 4.6401381253

H 1.2732574258 -0.0832538768 4.9061011036
N -0.4455160579 -0.5222691246 -1.9456517267
H -0.7834963181 0.2955683109 -2.4615417500
H 0.3933018916 -0.8550492313 -2.4286982517
H -1.1568992681 -1.2504704446 -2.0483909436

Complex25: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_carbonyl_s_1.xyz
Mn -0.2225935195 -0.2258261828 0.2056398123
C 0.1034314183 2.5220755528 -1.2496977047
N -0.0127673398 1.5115742408 -0.6886500253
C 0.2468393239 3.7825282210 -1.9505730872
H -0.0881526971 3.6715338956 -2.9896855677
H 1.2952022390 4.1040311152 -1.9359026772
H -0.3685813547 4.5490420175 -1.4609188208
C 2.5662582682 -1.0306336971 -0.9438149787
N 1.5377396701 -0.7287192102 -0.4932821495
C 3.8481176490 -1.4099055019 -1.4997955622
H 4.3895382736 -0.5169687115 -1.8366301730
H 3.7032414560 -2.0938486146 -2.3454839340
H 4.4468244803 -1.9166577907 -0.7302281367
C -0.5146927355 -3.0232098074 1.5486402080
N -0.4040597019 -1.9852063638 1.0372330747
C -0.6568165776 -4.3157577033 2.1863036309
H 0.3167437262 -4.8214090384 2.2234312054
H -1.3690932821 -4.9344185291 1.6265489896
H -1.0239657258 -4.1828445274 3.2129305899
C -3.0950769646 0.6499669270 1.0310843643
N -2.0227407694 0.3269421892 0.7193414311
C -4.4304089910 1.0487105682 1.4238385227
H -4.6820884531 0.5919037317 2.3908846791
H -5.1565713602 0.7096059075 0.6737466930
H -4.4834999633 2.1400506377 1.5207650669
C 1.0790196967 0.9978847944 2.7649794847
N 0.6027087311 0.5508402902 1.8055880917
C 1.6741493797 1.5580939951 3.9636689892
H 0.9441631559 1.5388042559 4.7830830438
H 1.9738037364 2.5972256501 3.7808378973
H 2.5537674985 0.9719643889 4.2551408748
C -1.1226958180 -1.0793599520 -1.3981317546
O -1.6269898603 -1.5577972976 -2.2835215833

Complex26: mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_acetonitrile_s_1.xyz
Mn -0.1040141860 -0.0967713487 -0.0028331182
N -0.4072349237 1.9514012309 0.2919992233
H -1.3951483542 2.2251211236 0.3279609550
H 0.0098569333 2.3514587200 1.1405344677
H -0.0171420023 2.4994325401 -0.4850842520
N 1.9497855582 0.0493820950 0.3814777513
H 2.2575537168 0.9947653896 0.6406766124

H 2.3311998250 -0.5606829834 1.1141938896
H 2.4898402920 -0.1732528289 -0.4625346563
N 0.1984610500 -2.1493135076 -0.2707920713
H 1.0349481591 -2.5413153330 0.1762946853
H -0.5709014342 -2.7556297401 0.0427015265
H 0.3031622725 -2.3538717640 -1.2704664341
N -2.1377088948 -0.2482527793 -0.4636689511
H -2.4011287350 -1.1733327340 -0.8235166314
H -2.8020839257 -0.0662361995 0.2979105588
H -2.3965647162 0.3974699544 -1.2182002906
N -0.3988694475 -0.3023625552 2.0416788583
H -1.2305672415 0.1752535785 2.4087762857
H -0.5104242171 -1.2830143541 2.3290807946
H 0.3777252146 0.0446454792 2.6169581238
C 0.4086510002 0.3579909972 -3.0873465281
N 0.2100995245 0.1750074161 -1.9509209436
C 0.6535482413 0.5814412938 -4.4959684879
H 1.7331717856 0.5589364878 -4.6987437736
H 0.2435422114 1.5536769207 -4.8016548724
H 0.1666244891 -0.2099313001 -5.0852538003

Complex27: mn_3_ammonia_ammonia_ammonia_ammonia_water_s_1.xyz

Mn -0.0122267236 0.0111973794 -0.0202743544
N -0.4589112914 2.0054618753 0.4307928045
H -1.1724678061 2.1641318797 1.1525313871
H 0.3569770433 2.5428203868 0.7494419961
H -0.7908957396 2.5240845015 -0.3927268285
N 2.0591047157 0.2483961022 -0.2995661141
H 2.3113735628 1.2274098196 -0.4903643243
H 2.6481384045 -0.0133390044 0.5001387847
H 2.4621374170 -0.2733011953 -1.0884989105
N 0.2524222108 -2.0525915627 -0.2398782400
H 1.2154709504 -2.3864876477 -0.1145341031
H -0.3103814966 -2.6334119756 0.3968500327
H -0.0179921409 -2.3711277828 -1.1797848409
N -2.0776012493 -0.3458665929 0.1609238403
H -2.4277675386 -1.0548578289 -0.4961406640
H -2.3743675367 -0.6856404979 1.0853433974
H -2.6743401330 0.4747073774 0.0010575731
N 0.4225069634 -0.1083874957 2.0072066239
H -0.4109889278 -0.0633754553 2.6072308750
H 0.8897770941 -0.9834048794 2.2777226208
H 1.0335659381 0.6368399566 2.3645226754
O -0.2479536351 0.3369045435 -1.9498977438
H -1.0583219702 0.6762961430 -2.3880012428
H 0.3817856240 0.1258416344 -2.6735474031

Complex28: mn_3_ammonia_ammonia_ammonia_ammonia_phosphine_phosphine_s_1.xyz

Mn -0.0027443472 -0.0056131736 -0.0017740897

N -0.3655766020 2.0583612124 -0.1534927942
 H -1.1672541926 2.3866492443 0.3984398994
 H 0.4129353567 2.6567880616 0.1455889239
 H -0.5698443329 2.3668819440 -1.1124850955
 N 2.0809665955 0.2071888766 -0.1820820204
 H 2.4305392011 1.1485505716 0.0308389086
 H 2.6278232383 -0.4141703559 0.4264558350
 H 2.4337717246 0.0167289394 -1.1284901683
 N 0.3410307592 -2.0689293795 0.1634679952
 H 1.1682964815 -2.3963712282 -0.3495375892
 H 0.5001758906 -2.3753820922 1.1313831448
 H -0.4224322421 -2.6670001139 -0.1728037213
 N -2.0818933540 -0.2339907954 0.1853363026
 H -2.4393002249 -1.1495549894 -0.1101966664
 H -2.4210683974 -0.1298187486 1.1500939883
 H -2.6315435959 0.4432121231 -0.3571368357
 P 0.3713406365 0.4660424331 2.5108760127
 H 1.4727133922 1.2954583659 2.8043304250
 H -0.6809641151 1.1163818064 3.1868356485
 H 0.6134985909 -0.6519484031 3.3358549349
 P -0.3556431160 -0.4441252029 -2.5226534953
 H -0.0276106274 0.6296249242 -3.3770257433
 H 0.3854351630 -1.5048846588 -3.0813480550
 H -1.6726490244 -0.7500815478 -2.9205086529

Complex29: mn_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_1.xyz

Mn -0.1420056439 -0.1419735261 0.0111729566
 C -0.4180325011 1.7136530797 -0.7881183350
 O -0.5878980786 2.7158231370 -1.2659301010
 C 1.7135040234 -0.4180137365 -0.7883884296
 O 2.7156108812 -0.5878791785 -1.2663330551
 C 0.1612892985 -1.9633774723 0.8788778596
 O 0.3092287899 -2.9851673294 1.3212333192
 C -1.9633310578 0.1612857421 0.8790432082
 O -2.9850892468 0.3092078101 1.3214789092
 C 0.7790016508 0.7788568605 1.7185409187
 O 1.2565798962 1.2563112122 2.6159501276
 F -0.8388517408 -0.8387194895 -1.3602669152

Complex30: mn_3_cyanide_cyanide_ammonia_ammonia_ammonia_ammonia_s_1.xyz

Mn -0.0057617125 0.0643122056 0.0162137885
 C -0.8017002230 1.7766463054 0.3426127864
 N -1.3007634448 2.8269310512 0.4781282878
 C 1.8611337909 0.3413251054 0.3590235976
 N 3.0192659232 0.4426806878 0.5019754802
 N 0.3004631811 -2.0584380798 -0.0484922615
 H 1.3010365712 -2.1864410934 0.1218446340
 H -0.1867961299 -2.6075169727 0.6619614485
 H 0.1029962699 -2.5074151989 -0.9448363519

N -2.0843854182 -0.4264301279 -0.4430689374
H -2.2647820043 -1.1696733744 -1.1209646213
H -2.6074380839 -0.6753400683 0.3988496870
H -2.5436071212 0.4175193884 -0.7914978618
N -0.1280399163 -0.0773461090 2.1131055620
H -1.0687488240 -0.0595437131 2.5125982147
H 0.3699857343 -0.8652390164 2.5322731202
H 0.3405609287 0.7608989952 2.4626593290
N 0.3062157170 0.3621066332 -2.0176795040
H -0.4143912425 0.0737735997 -2.6815506999
H 0.3952442842 1.3779599476 -2.1153612752
H 1.1984075056 -0.0218278480 -2.3377861415

Complex31: mn_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_1.xyz

Mn -0.0006864340 -0.0017959853 0.0006977603
C 0.1869462119 1.9717429400 -0.3422787854
N 0.3186285026 3.1046524582 -0.5417444053
C 0.4856074083 4.5094782456 -0.7909531393
H 1.2332945852 4.6415239119 -1.5769945851
H 0.8221763255 4.9901470618 0.1318510778
H -0.4742967266 4.9287500732 -1.1032073026
C 1.9491658618 -0.4076188594 -0.2814282676
N 3.0760408555 -0.6165073403 -0.4461308642
C 4.4747374173 -0.8718387003 -0.6505588119
H 4.5891273219 -1.8564370905 -1.1116304277
H 4.9786728015 -0.8529971406 0.3197287856
H 4.8836756862 -0.0961382711 -1.3026484430
C -0.1858695196 -1.9755493403 0.3422063727
N -0.3133717014 -3.1095430573 0.5381273714
C -0.4724843688 -4.5163776080 0.7803208003
H -1.4365542813 -4.8358601005 0.3756457258
H -0.4450185560 -4.6908557077 1.8594869996
H 0.3428576742 -5.0541959511 0.2903178525
C -1.9499354368 0.4055651641 0.2840465151
N -3.0761480336 0.6165803921 0.4505447357
C -4.4736619446 0.8765706445 0.6577810839
H -4.6143640047 1.9496591073 0.8099294888
H -4.8091479080 0.3194403816 1.5361825509
H -5.0247301324 0.5472326556 -0.2275302168
C 0.4897414325 0.4621237439 3.0432326924
N 0.3012743351 0.2817679866 1.9102040013
C 0.7218056984 0.6869466692 4.4550553129
H -0.0198769525 0.1261877335 5.0405153126
H 0.6219198672 1.7541864361 4.6871513196
H 1.7250294256 0.3405270944 4.7317696138
C -0.4936826493 -0.4598449037 -3.0421113889
N -0.3031711193 -0.2845024220 -1.9086230892
C -0.7327837799 -0.6802158565 -4.4533758463
H -1.5126893418 -1.4441964595 -4.5767869864
H 0.1854851790 -1.0346756229 -4.9379916480
H -1.0665957926 0.2493853264 -4.9296736320

Complex32: mn_3_misc_misc_misc_misc_misc_misc_s_1.xyz

Mn 0.0001451946 -0.0001563211 0.0016069297
C 0.2189781618 1.9546805518 0.3784833803
N 0.3658209373 3.0864261044 0.5781941024
C 0.5481219364 4.4892963906 0.8225695873
H 1.5816777118 4.7535651159 0.5793981097
H 0.3529690927 4.6901004227 1.8797894052
H -0.1445754866 5.0518676489 0.1918004770
C 1.9364973011 -0.3923255548 0.3277843492
N 3.0632239384 -0.5989465409 0.5013627899
C 4.4596859266 -0.8548916997 0.7154233597
H 4.7441624226 -1.7519703674 0.1598528160
H 4.6316364056 -0.9951200250 1.7860573145
H 5.0298444405 0.0072893644 0.3563294398
C -0.2219959288 -1.9549192015 -0.3754037605
N -0.3718209387 -3.0856949807 -0.5783847821
C -0.5590008962 -4.4867168818 -0.8301994703
H -1.2842588359 -4.6078076482 -1.6385294786
H -0.9244911794 -4.9608980450 0.0851662137
H 0.4038392734 -4.9213975947 -1.1146596834
C -1.9365661581 0.3911443644 -0.3246481462
N -3.0638077042 0.5954803008 -0.4974370441
C -4.4609273204 0.8477338402 -0.7111143756
H -4.7059724550 1.8368508264 -0.3155217662
H -5.0366125486 0.0805167889 -0.1843229601
H -4.6683920212 0.8002583897 -1.7833412462
C -0.2584907063 -0.2394655321 1.9730858532
N -0.4272108077 -0.3924394972 3.1090617991
C -0.6360883170 -0.5822964548 4.5167713081
H -0.1853183050 -1.5312350355 4.8175933989
H -1.7120322039 -0.5912432946 4.7130628919
H -0.1675920921 0.2478718000 5.0537264641
C 0.2598947683 0.2390613003 -1.9697266824
N 0.4299228269 0.3915469183 -3.1055625006
C 0.6413799449 0.5807637674 -4.5129187384
H 0.1258372317 -0.2189253326 -5.0531728020
H 1.7150702423 0.5335184403 -4.7155084219
H 0.2399391713 1.5544982341 -4.8043711369

Complex33: mn_3_phosphine_phosphine_phosphine_phosphine_ammonia_ammonia_s_1.xyz

Mn -0.0141447207 -0.0309738888 -0.0060442055
P -0.5987056518 2.3860588563 0.3129184423
H -1.5489960166 2.6788226620 1.3112341507
H 0.4754818511 3.2241585311 0.6761788286
H -1.1306835947 3.0582259420 -0.8053060502
P 2.4487827605 0.0177412107 0.4004873475
H 3.0101687403 1.2798159371 0.6848237715
H 2.9124525310 -0.7621392762 1.4781297780

H 3.2569965736 -0.4347219235 -0.6607198230
P 0.3448583423 -2.5189738360 -0.3792847460
H 1.6366086030 -3.0731997388 -0.2929791318
H -0.3918793734 -3.3449610743 0.4948852787
H -0.0909857743 -2.9748473974 -1.6406272568
P -2.5110875897 -0.3063564133 -0.4543190766
H -2.9790798680 -1.5837298355 -0.8221881390
H -3.3549537824 0.0087363929 0.6301353320
H -3.0446258574 0.5027123410 -1.4778769939
N -0.1476257944 -0.1088692520 2.0794505933
H -1.1164237115 -0.0092346413 2.4080380656
H 0.1683278515 -1.0128411772 2.4524964066
H 0.3794445704 0.5873242511 2.6212579545
N 0.5063294219 0.5543626413 -1.9448539472
H -0.3163780519 0.8478542331 -2.4857570434
H 1.1666936132 1.3354480102 -2.0420317239
H 0.9280513030 -0.2088192589 -2.4892218274

Complex34: mn_3_phosphine_phosphine_phosphine_phosphine_phosphine_chloride_s_1.xyz

Mn -0.0657180402 -0.0737853681 0.0326197126
P -0.5427925621 2.3020605111 -0.2997230319
H -0.7037210335 3.1800006740 0.7915570140
H 0.4307830164 2.9916403062 -1.0479658501
H -1.6996006226 2.5848769044 -1.0496840237
P 2.3382233277 0.1306159028 -0.3496004667
H 2.7879536248 1.3821019950 -0.8150289725
H 3.2530015739 -0.0988737807 0.6980277727
H 2.8417370824 -0.7212175863 -1.3500263466
P 0.4174018082 -2.4491433038 0.3477089576
H 1.2211592142 -3.0223657889 -0.6552515344
H 1.0607614767 -2.9087562604 1.5144266165
H -0.7001748243 -3.3056139260 0.3088972712
P -2.4693872666 -0.2978681552 0.4319938748
H -2.9760666301 -1.6119937719 0.4052117619
H -3.0595239362 0.1843669740 1.6177773349
H -3.2749084204 0.3139957523 -0.5462261204
P 0.2999179172 0.3721368151 2.4566326468
H 1.4246967779 1.1514039793 2.7951986908
H -0.7060096807 1.0662694002 3.1567374566
H 0.4980878318 -0.7311280781 3.3103153641
Cl -0.3928476552 -0.4152145214 -2.0764620107

Complex35: mn_3_water_water_water_water_fluoride_fluoride_s_1.xyz

Mn 0.0000043711 -0.0002620558 0.0000119181
O 0.3390432616 1.9677466462 0.3375207155
H 0.4232068607 2.4317062812 -0.5173982195
H -0.4369519151 2.3583841580 0.7808181093
O 1.9483681271 -0.5213496704 0.2600607520
H 2.5871628921 0.0517879931 -0.2006645269

H 2.1833295521 -0.5068940715 1.2071451171
O -0.3388196438 -1.9683347071 -0.3376161642
H 0.4382841121 -2.3591270466 -0.7788333662
H -0.4245070666 -2.4317619366 0.5174616751
O -1.9482424025 0.5213107116 -0.2600377803
H -2.5877980764 -0.0524098668 0.1988621118
H -2.1827590907 0.5099016815 -1.2072500457
F -0.2742475016 -0.2945299900 1.6948418843
F 0.2739275338 0.2938321465 -1.6949212536

Complex36: fe_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_s_2.xyz

Fe 0.0554590421 0.0504992703 0.2483473545
C 0.5272404405 3.0824672497 0.5278487367
N 0.3381149329 1.9421036832 0.5110603455
C 0.7664027815 4.5154321569 0.5378970556
H 0.9815982690 4.8563125338 -0.4808873454
H 1.6193184884 4.7458985256 1.1855151306
H -0.1194025354 5.0375299511 0.9157155701
C 3.0928228277 -0.4198809342 0.4748332588
N 1.9485080745 -0.2557403217 0.4765688732
C 4.5309772215 -0.6255699134 0.4622990504
H 5.0334842093 0.2523722223 0.8830477855
H 4.8692384693 -0.7731362976 -0.5693312028
H 4.7887564700 -1.5056716932 1.0610493657
C -0.3512179774 -2.9229181061 -0.4523942697
N -0.2127011607 -1.8284974508 -0.1067720712
C -0.5243963533 -4.2954284807 -0.8961330943
H 0.2949740087 -4.9145043762 -0.5145891964
H -0.5212900582 -4.3279797754 -1.9913105889
H -1.4748334154 -4.6913452866 -0.5224601459
C -2.9077503183 0.5816565823 -0.4057222369
N -1.8207619963 0.3696040730 -0.0740746609
C -4.2700437053 0.8498191375 -0.8333192830
H -4.8971190583 -0.0294673629 -0.6497977637
H -4.2767732311 1.0825179454 -1.9039722650
H -4.6755468228 1.7000330070 -0.2741912151
C -0.4615779022 -0.4084568443 3.3931959571
N -0.2760036723 -0.2436998466 2.2639358529
C -0.6964829240 -0.6149754865 4.8157228493
H -1.7723817534 -0.6173612707 5.0188076601
H -0.2260497251 0.1887297336 5.3915307553
H -0.2718101932 -1.5744296578 5.1286459592
C 0.3615473889 0.3148155701 -1.5929149524
N 0.5480461129 0.4794732679 -2.7306096229

Complex37: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_chloride_s_2.xyz

Fe -0.0413207407 0.0321297574 0.0695983897
N -0.2376959763 2.0611479660 0.2949816702
H -1.2190794021 2.3530324572 0.2816391256

H 0.1778780425 2.5023849768 1.1208940506
 H 0.1707297374 2.5141345595 -0.5285984135
 N 1.9676388391 0.3463015420 -0.2229286830
 H 2.3348938882 1.2268168349 0.1485095925
 H 2.5999408730 -0.3838829518 0.1186989125
 H 2.0997203238 0.3941594854 -1.2389285882
 N 0.1306029921 -1.9766283258 -0.3270874511
 H 1.0918426307 -2.2596510848 -0.5373348667
 H -0.2123755072 -2.6486735743 0.3657533909
 H -0.3874346725 -2.1541989787 -1.1943306894
 N -2.0502248642 -0.3001599060 0.3535366376
 H -2.2963761379 -1.2112888220 0.7499073606
 H -2.5579854188 0.3919166143 0.9125896283
 H -2.4718258955 -0.2697923068 -0.5807616220
 N 0.2828507870 -0.2057652126 2.1053374735
 H -0.4936891587 0.1443696784 2.6743494138
 H 0.3977152751 -1.1852596181 2.3798033887
 H 1.1172547132 0.2739161310 2.4553059525
 Cl -0.4027470467 0.3569901641 -2.1126136377

Complex38: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_misc_s_2.xyz

Fe -0.0782371075 -0.0851888143 0.0094767905
 N -0.2852197121 1.9515274623 0.2346347694
 H -1.2665559488 2.2513113709 0.2701493127
 H 0.1346585422 2.3272514931 1.0931241932
 H 0.1259583529 2.4911675163 -0.5353376915
 N 1.9435876371 0.0965103595 0.3426222021
 H 2.2487412920 1.0712441176 0.4409514093
 H 2.3090702220 -0.3902939646 1.1695901479
 H 2.4917341262 -0.2649236357 -0.4472609934
 N 0.1568558354 -2.1239612530 -0.1823282151
 H 0.9777497156 -2.5004073801 0.3063961097
 H -0.6333600635 -2.6822505214 0.1624961646
 H 0.2766869725 -2.4072323224 -1.1617759064
 N -2.0741929809 -0.3189540600 -0.4360518022
 H -2.2519350391 -1.1417371657 -1.0233248643
 H -2.6807360265 -0.4387009440 0.3837728366
 H -2.4760824771 0.4616855996 -0.9679290966
 N -0.4051496393 -0.3173216382 2.0371774596
 H -1.2344591749 0.1775110780 2.3890789915
 H -0.5448628501 -1.2931643859 2.3216615004
 H 0.3607703282 0.0216807267 2.6310051984
 C 0.1958605505 0.2113406311 -1.9537270852
 N 0.3537735032 0.3816903492 -3.0881237012
 C 0.5524153492 0.5927804417 -4.5031852522
 H -0.0227441287 -0.1596552040 -5.0505927541
 H 1.6200286513 0.4931805299 -4.7212782931
 H 0.2047175494 1.5991583081 -4.7554742529

Complex39: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_acetonitrile_s_2.xyz

Fe 0.0021789944 0.0013004236 -0.0448655451
C 0.0470004020 2.0023769907 -0.0077872134
O 0.0659341340 3.1237404774 -0.0147220266
C 2.0032653649 0.0456112050 -0.0064479560
O 3.1246384870 0.0641305551 -0.0126162757
C -0.0420572599 -1.9999399585 -0.0049815692
O -0.0606182474 -3.1213173569 -0.0096876818
C -1.9990805917 -0.0431255363 -0.0063318098
O -3.1204515728 -0.0619275629 -0.0118069291
C 0.0013719053 0.0014969735 1.9906133286
O 0.0009954364 0.0015604879 3.1118814348
C -0.0018371601 -0.0075034645 -3.0919579357
N 0.0009980125 -0.0009472373 -1.9151737717
C -0.0068855608 -0.0160936411 -4.5209233505
H 1.0309573523 -0.0203165971 -4.9050559146
H -0.4828435726 0.9151424590 -4.8949560890
H -0.5667812526 -0.8840758723 -4.9041990873

Complex40: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_fluoride_s_2.xyz

Fe 0.0000687684 0.0000142616 -0.0106297210
C 0.2832313486 1.9276973501 0.3323664973
O 0.4453733731 3.0241882751 0.5270702724
C 1.9146544236 -0.3244237860 0.2556432218
O 3.0136498879 -0.5135692248 0.4114180271
C -0.2837882517 -1.9281360030 -0.3513263870
O -0.4469254364 -3.0249601423 -0.5432679486
C -1.9142214481 0.3248710696 -0.2809183483
O -3.0123930488 0.5138891788 -0.4426174820
F -0.2745473688 -0.2721710125 1.6971968294
F 0.2748975578 0.2726014704 -1.7185652652

Complex41: fe_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_2.xyz

Fe 0.0001060531 0.0011622005 -0.0040619863
C 0.0497163823 1.9777425598 -0.0048723140
N 0.0673242015 3.1335743465 -0.0057998651
C 0.0878490863 4.5714849852 -0.0068632911
H 0.9313724028 4.9095529604 -0.6139769870
H 0.2012884955 4.9191541116 1.0232345451
H -0.8530430919 4.9355416529 -0.4269806546
C 1.9768065719 0.0477741619 -0.0035148301
N 3.1326896840 0.0615505749 -0.0025166826
C 4.5706846313 0.0754258959 -0.0006896621
H 4.9294727016 -0.7602038913 -0.6068639817
H 4.9187534115 -0.0300742995 1.0301144745
H 4.9136870386 1.0243981784 -0.4202922300
C -0.0497623791 -1.9754518857 -0.0041875585
N -0.0693823096 -3.1312595781 -0.0045176898
C -0.0928099147 -4.5691220451 -0.0048235235

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H -0.9368703008 -4.9057759715 -0.6119863237
H -0.2072734584 -4.9160040425 1.0254284080
H 0.8475337474 -4.9353586760 -0.4242783222
C -1.9765193905 -0.0470678336 -0.0032496036
N -3.1323369283 -0.0658135402 -0.0008350323
C -4.5701362692 -0.0878495044 0.0031797401
H -4.9355279673 0.9000696144 0.2942605569
H -4.9068120840 -0.8434619611 0.7174863462
H -4.9181984103 -0.3384358816 -1.0022728082
C 0.0011375066 0.0045131582 3.0883335517
N 0.0006827161 0.0016068330 1.9292680777
C 0.0018081943 0.0074510026 4.5395280208
H 0.6098164469 0.8399836029 4.9123939172
H 0.4182049793 -0.9372799884 4.9108138503
H -1.0247919825 0.1132431120 4.9111070822
C 0.0025009430 0.0039311892 -3.0963143234
N 0.0000819120 0.0022808416 -1.9372442445
C 0.0047642776 0.0050337135 -4.5475310513
H 0.7465037867 0.7206571778 -4.9209540447
H -0.9883000120 0.2866392841 -4.9189165606
H 0.2509964882 -0.9977517488 -4.9179248513

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Complex42: fe_3_misc_misc_misc_misc_water_water_s_2.xyz

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Fe 0.0015211064 0.0011069663 0.0006046188
C 0.2691225008 1.9532699246 0.2881691733
N 0.4444217710 3.0803327866 0.4773509075
C 0.6700704597 4.4823318029 0.7207651320
H 1.6112634470 4.7708568614 0.2448981638
H 0.7282961481 4.6390176187 1.8017666989
H -0.1633887798 5.0494932264 0.2978807657
C 1.9420254261 -0.3555989988 0.2719683076
N 3.0677042835 -0.5400141537 0.4591399189
C 4.4699453366 -0.7615410347 0.7034166239
H 4.8086309184 -1.5867743529 0.0712711836
H 4.5992532360 -1.0137767924 1.7598467558
H 5.0145622925 0.1551115473 0.4619012794
C -0.2662810587 -1.9507879217 -0.2885309797
N -0.4420683279 -3.0771696893 -0.4812485387
C -0.6693763694 -4.4776445670 -0.7317950248
H -1.4315200849 -4.5704850704 -1.5103605760
H -1.0149396107 -4.9440092146 0.1952051104
H 0.2702507814 -4.9310395663 -1.0584586227
C -1.9393269911 0.3564216250 -0.2694479288
N -3.0658769767 0.5381920436 -0.4538715611
C -4.4693520382 0.7554681471 -0.6936934064
H -4.7207890383 1.7787596026 -0.4026361804
H -5.0388943773 0.0367248110 -0.0980862145
H -4.6642133676 0.6033808888 -1.7592712692
O -0.2340618046 -0.1945258161 1.9339970407
H -0.1299113743 -1.0664141981 2.3644849124
H -0.9182751948 0.3048203106 2.4235162043

```

O 0.2363965922 0.1970261997 -1.9331801489
H 0.1317918182 1.0693854647 -2.3627305364
H 0.9227442424 -0.3001044413 -2.4219765627

Complex43: mn_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_water_water_s_2.xyz

Mn -0.0012445801 0.0022575844 -0.0002449560
C 0.4527141644 3.1071430500 -0.5230667933
N 0.2625457447 1.9886020928 -0.2902372485
C 0.6912248498 4.5129947374 -0.8211064987
H 0.4950122948 4.7040334584 -1.8815330619
H 1.7316851388 4.7721710925 -0.5999011507
H 0.0291866480 5.1430522901 -0.2181267714
C 3.1026431160 -0.4991252832 -0.4774931991
N 1.9754520305 -0.3406000503 -0.2625918025
C 4.5192819961 -0.7012173095 -0.7505260597
H 4.9670459565 0.2285835100 -1.1160977986
H 4.6447300998 -1.4799242799 -1.5101448746
H 5.0361006717 -1.0113362136 0.1637901917
C -0.4514982569 -3.1026411659 0.5253945234
N -0.2644426066 -1.9838220587 0.2913622320
C -0.6850218275 -4.5088353899 0.8256969748
H 0.2595381985 -5.0616056217 0.7954214982
H -1.3747860637 -4.9394994791 0.0923453541
H -1.1232022079 -4.6055491665 1.8247052739
C -3.1058240721 0.4986814795 0.4742544573
N -1.9779154024 0.3438473362 0.2605054754
C -4.5234650239 0.6931921418 0.7473644296
H -4.7895380631 0.2051214994 1.6909318958
H -5.1231381589 0.2580742695 -0.0590055087
H -4.7490553568 1.7619520813 0.8222990988
O 0.2414980064 0.2308328272 2.0183198254
H 1.0931542568 -0.0675919977 2.3816485870
H 0.0968266911 1.1303415412 2.3602626090
O -0.2444154675 -0.2232951951 -2.0190714122
H -1.1025066998 0.0615759720 -2.3781189354
H -0.0843691247 -1.1180674192 -2.3664044630

Complex44: mn_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_2.xyz

Mn -0.0001202127 -0.0001401207 -0.0002603854
N -0.2676794255 2.1046182812 -0.2010549337
H -1.2597072044 2.3349326806 -0.1621807618
H 0.1894091077 2.6174193924 0.5523476529
H 0.0637182084 2.4525305567 -1.1007422933
N 2.0950570590 0.2093146627 -0.3580462444
H 2.3139790358 1.1636925190 -0.6413883402
H 2.5988297719 0.0463464647 0.5130689919
H 2.4605521517 -0.4004449910 -1.0892558868
N 0.2673083898 -2.1048380590 0.2032341828
H 1.2604069502 -2.3330659886 0.1850800010

H -0.0817219896 -2.4550044906 1.0953348937
H -0.1739009921 -2.6170508157 -0.5599627152
N -2.0957355976 -0.2098502699 0.3561213061
H -2.3168789994 -1.1682264629 0.6237690101
H -2.4585406134 0.3890303599 1.0976211579
H -2.6006882755 -0.0318570178 -0.5113614216
C 0.3676999064 0.3202191470 1.9711132005
N 0.6111319902 0.5442729110 3.0974830551
C -0.3666747056 -0.3199555098 -1.9716874193
N -0.6064465427 -0.5419439056 -3.0992450268

Complex45: mn_2_carbonyl_carbonyl_carbonyl_carbonyl_phosphine_phosphine_s_2.xyz

Mn -0.0009943853 -0.0021277966 0.0632113713
C -0.3431453022 1.8997015993 0.3963082376
O -0.5439702964 2.9958176712 0.5889096186
C 1.9192245411 0.2530988157 -0.2361259768
O 3.0263789626 0.3966303464 -0.4157156995
C 0.3434815425 -1.9028414565 -0.2690351165
O 0.5464287254 -2.9986444458 -0.4606248772
C -1.9218560423 -0.2633290056 0.3602699819
O -3.0285625442 -0.4129082219 0.5376250766
P 0.4070591816 -0.3508235925 2.4960956198
H 1.5626161821 0.2855024688 2.9865752718
H -0.5973751279 0.1067550045 3.3678878774
H 0.5934146724 -1.6866039207 2.8964573211
P -0.4241813529 0.3658587228 -2.3640512284
H 0.6425302360 0.9445303872 -3.0762108607
H -0.6930411642 -0.8024688823 -3.1008607131
H -1.5101615964 1.1993970892 -2.6867878384

Complex46: mn_2_chloride_chloride_chloride_chloride_carbonyl_carbonyl_s_2.xyz

Mn 0.0000873839 0.0000112599 0.0000285442
Cl -0.3627581389 2.3959155530 -0.3869590442
Cl 2.3914196676 0.4046584907 0.3709562284
Cl 0.3633602256 -2.3957715366 0.3882881212
Cl -2.3909537820 -0.4041253156 -0.3716606590
C -0.3160451125 0.2641301423 1.8207204219
O -0.5138844024 0.4318702247 2.9437238119
C 0.3158576996 -0.2643587074 -1.8210109596
O 0.5129146592 -0.4323281938 -2.9440877811

Complex47: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_carbonyl

Mn 0.0192401536 -0.0978429660 0.1034584657
S 0.4130821934 2.3178115339 -0.2445878727
H -0.7416788373 2.9322017863 0.0948980404
H 0.2882285363 2.5799750188 -1.5652769484
S 2.4416524739 -0.4705884045 0.5178051126

H 3.0797205715 -0.0380214794 -0.5927807326
H 2.8588835367 0.5672122275 1.2768755083
S -0.3956577695 -2.5079076246 0.5481704396
H 0.2946905855 -2.7759884710 1.6786763793
H 0.4510903345 -3.1840187308 -0.2594686779
S -2.4115904200 0.2497458711 -0.2667786172
H -3.0411718896 -0.7292978800 0.4211622189
H -2.6869264356 -0.2870872456 -1.4764572542
S -0.3323804233 0.2632382408 2.5635815945
H 0.4541128239 1.2896637005 2.9573267315
H -1.4831853359 0.9466121490 2.7541900299
C 0.3065945203 -0.4272432436 -1.7160659983
O 0.4811119651 -0.6163648736 -2.8259870303

Complex48: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_phosphi

Mn -0.1238790460 0.0523942373 0.0871634750
S 0.2170596214 2.4952342722 -0.3560658958
H 0.7024133630 3.0189745978 0.7895771333
H 1.3729370791 2.6625782810 -1.0350292104
S 2.3143812042 -0.2198135797 0.6206191572
H 2.5177780373 -1.4331457288 1.1768908470
H 3.0119936565 -0.4994456780 -0.5010269033
S -0.7205152213 -2.3596470690 0.4601894909
H -0.5981282688 -2.6329851378 1.7775247584
H 0.3242508983 -3.1272964503 0.0839305459
S -2.6010487907 0.5268126329 -0.2212784963
H -3.1614391045 -0.6380781259 -0.6125591625
H -2.7670790559 1.1417781142 -1.4123066521
S -0.5549487770 0.3855175331 2.5378858701
H 0.4811082376 1.0918943390 3.0419802641
H -1.4421637406 1.3986644733 2.6489615139
P 0.1958008392 -0.3633006806 -2.3043247400
H 1.4499322140 -0.7969670385 -2.7825156846
H -0.6293380690 -1.3453623170 -2.8907135138
H -0.0405235336 0.7015866540 -3.1990185624

Complex49: mn_2_water_water_water_water_acetonitrile_acetonitrile_s_2.xyz

Mn -0.0000084241 0.0004258296 -0.0048960960
O 0.2048081988 2.0064851332 -0.3604849692
H 0.8159623432 2.2587124286 -1.0751899355
H 0.4186333766 2.5767452428 0.3984209550
O 2.0137485739 -0.2119044069 -0.3643303207
H 2.3119291092 -0.8452787909 -1.0401832643
H 2.5717318670 -0.3645836012 0.4186322484
O -0.2053392152 -2.0055903005 0.3511070379
H -0.4164904509 -2.5760093090 -0.4084442648
H -0.8198432396 -2.2571772409 1.0631752562
O -2.0138673787 0.2123642452 0.3544196833
H -2.3118524913 0.8441303175 1.0318769007

```

H -2.5716435807 0.3673526661 -0.4282400253
C 0.5141144034 0.4527686610 3.0991100557
N 0.3189894583 0.3185591208 1.9624737499
C 0.7593755368 0.6171324389 4.5249353033
H -0.1870842322 0.7853751987 5.0503272157
H 1.4198044167 1.4743571106 4.6955384898
H 1.2343200380 -0.2848815660 4.9264370080
C -0.5135879439 -0.4531247776 -3.1087387367
N -0.3185389743 -0.3177276099 -1.9722254080
C -0.7590787732 -0.6184563381 -4.5344162607
H 0.1857377213 -0.8007491146 -5.0580846120
H -1.2216243892 0.2885153481 -4.9392001093
H -1.4305019241 -1.4674375680 -4.7033475750

```

Complex50: mn_2_water_water_water_water_water_water_s_2.xyz

```

Mn 0.0001057081 -0.0005277389 -0.0001968969
O 0.3106313339 2.0719524435 -0.1466553249
H 0.9854347569 2.5243595497 -0.6830272223
H -0.4937766956 2.6210940237 -0.1796820840
O 2.0044124352 -0.5093520535 -0.3009455496
H 2.3152802047 -0.5182716058 -1.2244060972
H 2.7662465411 -0.2711914094 0.2559957801
O -0.3120778120 -2.0722178152 0.1475468030
H 0.4920567195 -2.6219420750 0.1784507533
H -0.9839669683 -2.5223791770 0.6894743162
O -2.0038334739 0.5101087872 0.3000306608
H -2.3146624286 0.5171736947 1.2235663388
H -2.7641995865 0.2660068082 -0.2564101990
O 0.1519272764 0.3362207903 2.0541826607
H 0.5198153469 -0.2657436192 2.7247059833
H 0.4011676027 1.2419261537 2.3128142822
O -0.1530374462 -0.3363777493 -2.0544091825
H -0.5159255090 0.2692545534 -2.7243517974
H -0.4055981518 -1.2400900568 -2.3166899164

```

S4.2 Intermediate spin geometries

Complex1: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_cyanide_s_3.xyz

```

Co 0.0034527507 0.0001027714 0.0074288509
C 0.5339862137 3.1554105941 -0.4595278317
N 0.3516718407 2.0287023819 -0.2842328977
C 0.7626859341 4.5759304641 -0.6830070612
H 0.6615391094 4.8036751391 -1.7487578997
H 1.7712148614 4.8446127426 -0.3535627131
H 0.0343041577 5.1631674512 -0.1153289920
C 3.1612675002 -0.4505402866 0.4728960341
N 2.0303662471 -0.2840284121 0.3101613044
C 4.5876016063 -0.6609649087 0.6760835785
H 5.1051189706 0.3033159211 0.6885157652
H 4.9914286970 -1.2741423370 -0.1354829483

```

H 4.7549933800 -1.1669643048 1.6320192657
 C -0.5368392882 -3.1555294322 0.4591989941
 N -0.3457394796 -2.0283776184 0.2965970751
 C -0.7794575616 -4.5767017680 0.6626710943
 H 0.1426951950 -5.0656258544 0.9920499774
 H -1.1108718285 -5.0337928342 -0.2749791901
 H -1.5499676006 -4.7162559745 1.4271673524
 C -3.1537053510 0.4511223807 -0.4644667146
 N -2.0235082419 0.2850231311 -0.2964941525
 C -4.5791291754 0.6600132503 -0.6755777449
 H -5.1506003744 0.0335601379 0.0165155683
 H -4.8449795793 0.3983169132 -1.7043936524
 H -4.8299187877 1.7096381967 -0.4935749137
 C -0.2761412252 0.3419913958 1.8847676790
 N -0.4378011931 0.5340867891 3.0246058073
 C 0.2821754181 -0.3420437244 -1.8703089945
 N 0.4420163449 -0.5345015503 -3.0103671167

Complex2: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_fluoride_fluoride_s_3.xyz

Co -0.0003870758 0.0036041759 -0.0022676639
 C -0.4890479083 3.0974000003 0.4476441169
 N -0.3088547763 1.9707378292 0.2798572736
 C -0.7173042606 4.5201377983 0.6605326369
 H -1.0483075296 4.9868001783 -0.2722763815
 H 0.2092043603 4.9995377867 0.9910600653
 H -1.4850058308 4.6618411404 1.4273629079
 C 3.2644204428 0.4955789634 0.5342897296
 N 2.1335834067 0.3354716381 0.3603004956
 C 4.6917858315 0.6953460459 0.7528539977
 H 4.8982259727 1.7554737636 0.9285197914
 H 5.2528239239 0.3653880907 -0.1268421594
 H 5.0195224023 0.1202250011 1.6242167795
 C 0.4865292994 -3.0913673351 -0.4476269178
 N 0.3078414794 -1.9639100908 -0.2835761457
 C 0.7112432270 -4.5155157754 -0.6550447643
 H 1.7765522782 -4.7421113946 -0.5489776582
 H 0.3839827218 -4.8005968507 -1.6595707623
 H 0.1482583073 -5.0918278820 0.0854907553
 C -3.2626959130 -0.4959218309 -0.5476694842
 N -2.1340414496 -0.3291114198 -0.3659722911
 C -4.6867158126 -0.7064836778 -0.7775605971
 H -5.0234083382 -1.5986236641 -0.2407599100
 H -4.8762591682 -0.8383914625 -1.8471930566
 H -5.2539425789 0.1578420910 -0.4189258357
 F -0.2601081219 -0.2668758609 1.6777734524
 F 0.2593631928 0.2739810948 -1.6823741670

Complex3: cr_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_misc_misc_s_3.xyz

Cr 0.0015950987 0.0050616850 0.0005077007

C -0.0258951533 3.2312574916 0.0000612760
 N -0.0187340722 2.0738663592 0.0000555238
 C -0.0384243194 4.6877900477 0.0008674637
 H -0.3495814424 5.0618796238 -0.9797813527
 H 0.9637931007 5.0675275487 0.2248972992
 H -0.7347068867 5.0553508204 0.7616465120
 C 3.2278374282 -0.0319953864 0.0027596486
 N 2.0704909640 -0.0194103421 0.0018787112
 C 4.6842238587 -0.0527375383 0.0035645627
 H 5.0708711390 0.9716532774 0.0028995233
 H 5.0523274357 -0.5713928322 -0.8875861761
 H 5.0514111643 -0.5699256109 0.8959402874
 C 0.0183213396 -3.2220182555 0.0013836447
 N 0.0178610215 -2.0646139745 0.0011629226
 C 0.0229540297 -4.6785517168 0.0016102754
 H 1.0541267404 -5.0467141429 0.0090990051
 H -0.4819020017 -5.0555818713 -0.8937038423
 H -0.4948054253 -5.0552737763 0.8896536078
 C -3.2252277883 0.0289917017 -0.0055053725
 N -2.0678328548 0.0248665749 -0.0018949576
 C -4.6817982657 0.0382179935 -0.0097875922
 H -5.0625253724 -0.6971559247 0.7064152266
 H -5.0564974501 -0.2082804215 -1.0084524907
 H -5.0477378389 1.0306560769 0.2728916134
 C 0.0011727075 0.0047905458 2.0811707905
 N 0.0015466446 0.0031345371 3.2454574025
 C 0.0026305055 -0.0018152302 4.6741383369
 H 0.6078494089 -0.8372499492 5.0345722077
 H -1.0236426631 -0.1068496687 5.0346830264
 H 0.4227005626 0.9399960751 5.0359916459
 C 0.0035123828 0.0039009664 -2.0802117847
 N 0.0052536412 0.0016592406 -3.2445071675
 C 0.0084900403 -0.0016690986 -4.6731867364
 H -0.5975104545 -0.8381039281 -5.0303839783
 H 1.0345668555 -0.1139088673 -5.0320257493
 H -0.4108214826 0.9384075443 -5.0400583808

Complex4: cr_2_acetonitrile_acetonitrile_ammonia_ammonia_ammonia_ammonia_s_3.xyz

Cr 0.0778222085 -0.0971956312 0.0007643949
 C -0.4169961777 3.0780674297 0.4748857985
 N -0.2532442512 1.9400842565 0.3042429814
 C -0.6150487186 4.5062550607 0.6885563782
 H -1.2475328269 4.9175712408 -0.1055160311
 H 0.3483531810 5.0267448618 0.6814759554
 H -1.1065137761 4.6767971609 1.6523638128
 C 3.2496490672 0.3981865608 -0.4693600012
 N 2.1156027406 0.2101864901 -0.2974591279
 C 4.6707176660 0.6384955166 -0.6870235524
 H 4.9306881914 1.6623659421 -0.3986925250
 H 4.9138378955 0.4943087795 -1.7452862962
 H 5.2654711918 -0.0626899768 -0.0918700605

N 0.4160387136 -2.2309682183 -0.2709918824
H 1.3170209444 -2.5253677776 0.1129190439
H -0.2751267095 -2.8783938127 0.1158677498
H 0.4738207347 -2.4637748971 -1.2649459911
N -2.0607603771 -0.4348291818 0.2605554504
H -2.4866411944 -1.2170712953 -0.2428334544
H -2.2923423613 -0.5940169906 1.2436852873
H -2.6032380965 0.3917643943 -0.0001264424
N 0.3993057312 -0.3011567195 2.1365706751
H -0.0521263218 0.4449442274 2.6699180794
H 0.1148715363 -1.1807562736 2.5735446267
H 1.3993447303 -0.2084027739 2.3272396176
N -0.2407741719 0.1853037341 -2.1277412848
H -0.4166202076 1.1782830428 -2.2957813120
H 0.5945032946 -0.0360735618 -2.6737465445
H -1.0146429212 -0.3164822316 -2.5688359991

Complex5: cr_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_3.xyz

Cr -0.0002802334 0.0002546718 0.0001718796
N -0.2478988409 2.1293179783 0.3668994734
H -1.2308051748 2.3022899716 0.5728795223
H 0.2846401253 2.4909535075 1.1582738155
H -0.0334379433 2.6742231328 -0.4681165217
N 2.1498256227 0.2764190526 -0.2820627040
H 2.3708260933 1.2686087191 -0.3560893919
H 2.6745029020 -0.0913114575 0.5110199130
H 2.4873615363 -0.1480806878 -1.1450582985
N 0.2472330320 -2.1287607229 -0.3673177670
H 1.2309278487 -2.3018609935 -0.5693729802
H 0.0291543315 -2.6752561828 0.4657285332
H -0.2821453492 -2.4886205542 -1.1616302061
N -2.1503036344 -0.2761520202 0.2825630907
H -2.3724659867 -1.2690344490 0.3427981670
H -2.4834136356 0.1360977194 1.1531867265
H -2.6779577448 0.1033203422 -0.5029419857
C 0.3474788365 -0.3448291075 2.0306350028
N 0.5941031351 -0.5543559659 3.1598663953
C -0.3469267917 0.3444742586 -2.0306200457
N -0.5904168407 0.5523251259 -3.1608279226

Complex6: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_ammonia_s_3.xyz

Cr 0.0375662380 0.0241379457 -0.0534215723
C -0.2942384977 2.0633628396 -0.2888323445
O -0.4782197463 3.1674018501 -0.4278259498
C 2.0779751941 0.3225695681 -0.3495422620
O 3.1816445030 0.4828327336 -0.5175036108
C 0.3855405219 -2.0082807548 0.2534629382
O 0.5774925249 -3.1071592839 0.4195479976
C -1.9878934114 -0.2768027906 0.3189080514

O -3.0852830623 -0.4444309216 0.5181194264
C 0.3525773029 0.3594873161 2.0885791719
O 0.5163556538 0.5378046515 3.1863067313
N -0.2747179446 -0.2375014690 -2.1303527751
H -1.1381023214 0.1977724877 -2.4769138635
H 0.4756780526 0.1479958688 -2.7159064779
H -0.3459205611 -1.2259923628 -2.3980894235

Complex7: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_s_3.xyz

Cr -0.0012682288 -0.0012625937 0.0581188480
C -0.0011987526 2.0276724028 -0.0280430372
O -0.0010295175 3.1548281620 -0.1349307916
C 2.0276683932 -0.0011946909 -0.0280275266
O 3.1548246940 -0.0010260273 -0.1349082524
C -0.0011976900 -2.0296776461 -0.0355288838
O -0.0010440833 -3.1564042665 -0.1468396699
C -2.0296811030 -0.0012057336 -0.0355451391
O -3.1564072293 -0.0010588255 -0.1468615119
C -0.0016832835 -0.0016548355 2.2442364608
O -0.0015118412 -0.0014713632 3.3718555202
C 0.0043968426 0.0043696628 -1.8926923964
N 0.0081317120 0.0080854107 -3.0671563630

Complex8: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_3.xyz

Cr 0.0415996402 0.0416548140 0.0047804531
C 0.0195394348 2.0702890271 0.2960794365
O 0.0185067436 3.1984936422 0.3852988032
C 2.0702014576 0.0202905905 0.2962547739
O 3.1983944720 0.0196756929 0.3856304278
C 0.0752930519 -1.9785197962 -0.3376723390
O 0.1060485625 -3.0811327911 -0.5911332916
C -1.9785761292 0.0746265660 -0.3377858377
O -3.0811764364 0.1049366610 -0.5913609113
C -0.3028396592 -0.3030642298 2.1563326377
O -0.4821013428 -0.4826199632 3.2554798413
F 0.3151094760 0.3153970924 -1.7073227353

Complex9: cr_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_s_3

Cr -0.2106931180 0.1410041016 0.0967645956
S 0.0952593755 2.5923672144 -0.2961098789
H 0.8342199946 3.1504043845 0.6866389662
H 1.0109250104 2.8021573701 -1.2651874976
S 2.2868787528 -0.2531531668 0.5895563570
H 2.5783089235 -1.3794902049 -0.0943407907
H 2.9427745616 0.5530800167 -0.2722397839
S -0.7419788923 -2.3009125414 0.5108225234
H -0.3132537739 -2.7064309233 1.7257351993

H 0.1096472499 -3.0782037538 -0.1889366770
S -2.7459440730 0.5650924374 -0.1980559049
H -3.1934883769 -0.5823161754 -0.7520063351
H -2.8056162016 1.2733741443 -1.3455808200
S -0.6658083206 0.4951602579 2.6223973251
H 0.5315146874 0.6927777085 3.2152672840
H -1.1047498206 1.7558382372 2.8310203134
C 0.0274857006 -0.2328533536 -1.8979695985
N 0.1470258737 -0.4473838349 -3.0366003758
C 0.2799772667 -0.7113316097 -4.4401518786
H -0.2962714474 -1.6056716349 -4.6904847003
H 1.3357803383 -0.8743420914 -4.6715827238
H -0.0955263438 0.1464222929 -5.0037314669

Complex10: cr_2_misc_misc_misc_misc_misc_misc_s_3.xyz

Cr -0.0000164004 -0.0006988013 -0.0016619387
C 0.3166113760 2.0198949883 -0.3340462654
N 0.4904136654 3.1543243399 -0.5252765601
C 0.7041032762 4.5478850332 -0.7604444755
H 1.6970801260 4.6883726585 -1.1948624828
H 0.6387210399 5.0861942765 0.1883285824
H -0.0569009490 4.9195299062 -1.4509961320
C 2.0081219677 -0.3259328273 0.3760402356
N 3.1361074631 -0.5122031531 0.5931072469
C 4.5205147083 -0.7439147200 0.8621993029
H 5.0114789847 -1.0871542957 -0.0518504839
H 4.6160258426 -1.5037539248 1.6416973910
H 4.9803764072 0.1890704271 1.1976345727
C -0.3162516570 -2.0216106507 0.3302947163
N -0.4895535330 -3.1560736825 0.5217342866
C -0.7024252791 -4.5497079423 0.7573288641
H -1.0527241371 -5.0222172145 -0.1636258445
H -1.4543400114 -4.6682598744 1.5415237110
H 0.2367498695 -5.0087872383 1.0757683525
C -2.0089033003 0.3241054717 -0.3766602703
N -3.1379992541 0.5086416418 -0.5892308338
C -4.5251782128 0.7343036013 -0.8486026734
H -4.7696587682 1.7724734115 -0.6099471472
H -5.1231418308 0.0624562259 -0.2279599950
H -4.7299710039 0.5429481214 -1.9049431922
C -0.2746665119 0.3026241513 2.0268121266
N -0.4250906506 0.4673560701 3.1689144446
C -0.6070204167 0.6688736972 4.5721260533
H 0.2036182716 0.1782895106 5.1165202016
H -1.5660710424 0.2399473023 4.8734020280
H -0.6012155981 1.7406767771 4.7854740175
C 0.2744741224 -0.3031236869 -2.0301996245
N 0.4247913811 -0.4661979170 -3.1725583530
C 0.6077985698 -0.6638292507 -4.5762611770
H 0.0198410486 -1.5283999110 -4.8944968503
H 1.6662574344 -0.8447797183 -4.7791478131

H 0.2742379154 0.2271618465 -5.1138589498

Complex11: cr_2_phosphine_phosphine_phosphine_phosphine_hydrogensulfide_hydrogensulfide_s_3.xyz

Cr -0.0190849792 -0.0825278616 -0.0301434985

P 0.3399953704 2.4165741515 0.3978460616

H 0.2287052578 2.8783531014 1.7254607125

H 1.5819914496 2.9960161467 0.0609957552

H -0.5153090747 3.3406651447 -0.2389179147

P 2.4493725852 -0.5074409430 0.3340628293

H 3.1890378911 0.3303824930 1.1968576386

H 2.8071496135 -1.7567933505 0.8837961948

H 3.3224532852 -0.5008639387 -0.7751680638

P -0.3743552013 -2.5964514333 -0.4718269480

H 0.4392392022 -3.5185695415 0.2184173750

H -1.6376814052 -3.1626548839 -0.2021626397

H -0.1831740545 -3.0353745171 -1.7970105981

P -2.5066338278 0.2699593532 -0.3657141120

H -3.3597916021 -0.4407762558 0.5056616576

H -3.0614753415 1.5587272649 -0.2130883514

H -3.1063611528 -0.0848396009 -1.5935606973

S -0.4767723443 -0.5477805153 2.4504427706

H 0.6127240381 -0.2132838914 3.1747732429

H -1.2313645850 0.4635534928 2.9300280794

S 0.3514029763 0.1771811023 -2.5110803916

H -0.3832866093 1.2162343394 -2.9656720839

H 1.5332145124 0.7997076270 -2.7139738809

Complex12: cr_2_phosphine_phosphine_phosphine_phosphine_phosphine_ammonia_s_3.xyz

Cr -0.0123643117 -0.0267299441 -0.0518400267

P -0.4126079306 2.4561383350 -0.3345399304

H -1.4362258479 3.0988163672 0.3945770542

H 0.6282157748 3.3834628090 -0.1119530690

H -0.7876866949 2.8693864716 -1.6323903962

P 2.4709608125 0.3149655471 -0.4106191445

H 3.0703548315 1.5679014899 -0.1570798968

H 3.3923964050 -0.5078804588 0.2721887280

H 2.9493718907 0.1151960947 -1.7250594760

P 0.3900044290 -2.4988956046 0.3154372160

H 1.6377056142 -2.9602402935 0.7877692082

H -0.4533174892 -3.2190235647 1.1886304163

H 0.2760884820 -3.3325622568 -0.8198725855

P -2.4813908156 -0.3714110418 0.3908548492

H -2.9528537125 -1.5454304590 1.0170622817

H -3.1909186653 0.5809672355 1.1537514193

H -3.3180839510 -0.3909402456 -0.7475645986

P 0.3513474265 0.3802523882 2.4966709011

H 1.5677025717 0.9583220513 2.9147258009

H -0.5523025685 1.2344814881 3.1617534440

H 0.3092147414 -0.7264559377 3.3696860617

N -0.3180538622 -0.2802618808 -2.1638621278
H -1.2030028128 0.1128618203 -2.4945549802
H 0.4077428293 0.1454654600 -2.7461276062
H -0.3426759079 -1.2675148787 -2.4311104452

Complex13: cr_2_water_water_water_water_ammonia_ammonia_s_3.xyz

Cr 0.0000698699 0.0002982124 -0.0001240199
O -0.3649862262 2.0905128301 0.1644520807
H 0.3023973571 2.7749781596 0.3466631206
H -1.1791839913 2.3756964306 0.6152458133
O 2.0924501822 0.1645122357 -0.4818867159
H 2.4688734888 0.8348785124 -1.0792902986
H 2.8111113186 -0.0545278645 0.1377758163
O 0.3641065909 -2.0901423980 -0.1646634117
H 1.1841182239 -2.3733009007 -0.6060976454
H -0.3002671035 -2.7746807939 -0.3572582297
O -2.0915567827 -0.1659374853 0.4830895078
H -2.4657212631 -0.8419837758 1.0755192993
H -2.8115608485 0.0558013305 -0.1340774990
N 0.4232668349 -0.2344906296 2.1076750780
H -0.3629517841 0.0100733555 2.7157230782
H 0.6205970738 -1.2214700348 2.2962532870
H 1.2191157805 0.2857978405 2.4870160338
N -0.4249952806 0.2356168498 -2.1076898195
H -0.6179477613 1.2235354221 -2.2958025179
H 0.3580673619 -0.0134357182 -2.7179651254
H -1.2247724758 -0.2804029222 -2.4845526323

Complex14: cr_2_water_water_water_water_carbonyl_carbonyl_s_3.xyz

Cr 0.0002731992 0.0000387896 -0.0002153462
O 0.8091066987 1.8319241974 -0.4465009081
H 1.7320854537 1.9513337625 -0.7367975147
H 0.4563691267 2.7051111099 -0.1942083170
O 1.7528850335 -0.9095883511 -0.6761776966
H 1.9326661986 -1.2058929137 -1.5868402682
H 2.5053761471 -1.2058880548 -0.1327131237
O -0.8098191087 -1.8315286119 0.4461070919
H -0.4535671250 -2.7053484253 0.2011434851
H -1.7335946671 -1.9512188555 0.7336319103
O -1.7526278427 0.9094344797 0.6754294651
H -1.9335133295 1.2040934907 1.5864002227
H -2.5039184566 1.2077117897 0.1313828967
C 0.8138196633 0.1074711444 1.9311049541
O 1.2588668489 0.1726383132 2.9678867684
C -0.8141705157 -0.1076423243 -1.9316495508
O -1.2602442109 -0.1726522909 -2.9679837784

Complex15: fe_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_3.xyz

Fe -0.0742566376 -0.0630841453 -0.0388403345
C 0.4143595552 3.1891479579 -0.5145378782
N 0.2399196569 2.0525508506 -0.3780101032
C 0.6350882344 4.6198272036 -0.6842071818
H 0.2937200313 4.9382880410 -1.6743207164
H 1.7016409440 4.8460274732 -0.5850521443
H 0.0814022788 5.1753633892 0.0795428965
C 3.1664080614 -0.5987806762 -0.5257282390
N 2.0321559762 -0.4121803654 -0.3851854453
C 4.5939798771 -0.8329638014 -0.7025331810
H 5.1091165201 0.1178218980 -0.8735949494
H 4.7630058631 -1.4889114207 -1.5625328263
H 5.0081861520 -1.3056789816 0.1937966658
C -0.5603170384 -3.3117472786 0.4410654961
N -0.3956510126 -2.1827306703 0.2419345589
C -0.7662513220 -4.7323154127 0.6930885828
H 0.1908636434 -5.2615195300 0.6439387269
H -1.4440610549 -5.1522591350 -0.0570145342
H -1.2016285644 -4.8752494255 1.6872746880
C -3.3192766631 0.4564027518 0.4505719681
N -2.1925669715 0.2796710452 0.2491561203
C -4.7367637115 0.6787784522 0.7059433686
H -5.0592994391 0.0784629477 1.5627628790
H -5.3261813131 0.3931046661 -0.1711982526
H -4.9144828270 1.7364623869 0.9256881948
C 0.4336701408 0.3503415221 3.0315163734
N 0.2469580204 0.1932702331 1.9011758259
C 0.6701787992 0.5486417559 4.4559346769
H -0.2587135388 0.3948753188 5.0143601381
H 1.0298495975 1.5666562368 4.6367247165
H 1.4217688282 -0.1629669580 4.8124755941
N -0.3996423922 -0.2771053566 -2.0148043397
H -1.2603464351 0.1861300933 -2.3104920947
H 0.3612410620 0.1172553595 -2.5696711545
H -0.4834967497 -1.2614031272 -2.2723364627

Complex16: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_chloride_chloride_s_3.xyz

Fe -0.0018633840 -0.0002434827 0.0000786766
C 0.3541553285 2.3230703361 0.3933147848
O 0.5385904672 3.4273230680 0.5692820599
C 1.8520529920 -0.3210698536 0.2707709471
O 2.9594180092 -0.5171197123 0.4363234311
C -0.3535399962 -2.3228082492 -0.4027115876
O -0.5275301790 -3.4258417999 -0.5961222781
C -1.8555878248 0.3200166174 -0.2699689042
O -2.9630751814 0.5158166179 -0.4351290758
Cl -0.3671495666 -0.3466971336 2.2339019639
Cl 0.3645343841 0.3475533977 -2.2339683036

Complex17: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_cyanide_s_3.xyz

Fe 0.0000021948 -0.0000022850 0.0010950023
C 0.0000027149 2.1570534585 0.0013647873
O 0.0000030088 3.2896556837 0.0016050303
C 2.1570736780 -0.0000017033 0.0012632010
O 3.2896758731 -0.0000021511 0.0014031814
C 0.0000028431 -2.1570644942 0.0011936799
O 0.0000030563 -3.2896667058 0.0012483987
C -2.1570727372 -0.0000017905 0.0012784489
O -3.2896748016 -0.0000019865 0.0014179363
C 0.0000085791 0.0000453021 1.9561610054
N 0.0000070552 0.0000861625 3.1239281820
C -0.0000117683 -0.0000350738 -1.9539752780
N -0.0000193879 -0.0000645198 -3.1217417060

Complex18: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_hydrogensulfide_hydrogensulfide_s_3.xyz

Fe -0.0294872085 -0.1751043919 0.0736658551
C 0.3280029828 1.9085789020 -0.2365048007
O 0.5217168538 3.0057851073 -0.4030785593
C 1.8469898016 -0.4562705023 0.4038532421
O 2.9455477411 -0.6236380234 0.6002984515
C -0.3894370118 -2.2808312109 0.3875862567
O -0.5814859022 -3.3767302529 0.5540003185
C -1.9067433295 0.0985246838 -0.2554928796
O -3.0063022960 0.2593889818 -0.4518620558
S -0.4396301357 0.1759809989 2.6674765733
H 0.6129555906 0.9046390508 3.1042086346
H -1.3245512327 1.1952664830 2.7539802805
S 0.3531341984 -0.7099063391 -2.4947053693
H -0.4377642923 0.1584855902 -3.1653353456
H 1.5070479118 -0.0841338994 -2.8207302196

Complex19: fe_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_misc_s_3.xyz

Fe 0.1439321613 0.5164003032 -0.1521546339
S 0.5014725730 3.0567711350 -0.5579522693
H 1.2079248491 3.4710179155 0.5152850943
H 1.5644968489 3.1039384918 -1.3888756185
S 2.7242832464 0.2551575461 0.2274482618
H 2.9023785328 -0.3255518612 1.4328293457
H 3.1192508743 -0.8313489629 -0.4688575223
S -0.4151238155 -2.0145581650 0.2233700328
H 0.2241065077 -2.3908771845 1.3508655315
H 0.3918039438 -2.7257080230 -0.5919197589
S -2.3838371706 0.9746322876 -0.5668934850
H -3.0039858842 0.2838248349 0.4133649140
H -2.7322062264 0.0956522843 -1.5305165590
C -0.1364846030 0.8561934943 1.7452976280
N -0.3168826415 1.0722655118 2.8727148137

C -0.5497808972 1.3503748098 4.2611811288
H -0.1001338666 0.5573420518 4.8636409843
H -1.6273249642 1.3892157100 4.4389819178
H -0.0956964065 2.3123969844 4.5112097446
C 0.4030039473 0.2036129250 -2.0573101604
N 0.5463371623 0.0375426608 -3.1984242885
C 0.7154147045 -0.1525187346 -4.6108214362
H 0.2410717195 -1.0927633097 -4.9025165863
H 1.7834232943 -0.1857245840 -4.8397551299
H 0.2462049465 0.6818138130 -5.1382474600

Complex20: fe_2_misc_misc_misc_misc_misc_acetonitrile_s_3.xyz

Fe -0.0099345300 -0.0145813243 0.0591481929
C 0.2717556920 1.8844792937 0.3594983922
N 0.4392650828 3.0208471714 0.5340741737
C 0.6452119669 4.4196434321 0.7460278887
H 1.5927521361 4.7167333016 0.2901103268
H 0.6731804443 4.6203035228 1.8198273329
H -0.1753899122 4.9770854544 0.2879754067
C 1.9992967481 -0.3310603665 0.2867191448
N 3.1364100764 -0.5118231790 0.4331791010
C 4.5373883223 -0.7353768758 0.6144278137
H 4.8726169400 -1.4969272978 -0.0936730346
H 4.7124212127 -1.0786328784 1.6370415605
H 5.0756418008 0.1991762202 0.4399154746
C -0.2833659337 -1.9062113232 -0.2922923607
N -0.4457459412 -3.0369815784 -0.5040300577
C -0.6466071478 -4.4276679255 -0.7680445266
H -1.3786103081 -4.5384957748 -1.5716585791
H -1.0154071850 -4.9158030393 0.1373599616
H 0.3027818038 -4.8770192610 -1.0691206330
C -1.9991476132 0.3183049255 -0.2913330948
N -3.1300002058 0.5023373754 -0.4769376226
C -4.5234138684 0.7270306477 -0.7073820286
H -4.7943268691 1.7183855811 -0.3366532503
H -5.1004360088 -0.0376800474 -0.1818565426
H -4.7203166231 0.6658357404 -1.7805524662
C -0.3768065151 -0.3450567031 2.2721979052
N -0.5632390096 -0.5119817275 3.4087738892
C -0.7916821742 -0.7158450583 4.8057570097
H -0.3277827468 -1.6563634653 5.1125538072
H -1.8678482527 -0.7585993195 4.9905090101
H -0.3539228692 0.1131240716 5.3669806712
C 0.5515614892 0.5194176363 -3.3618719838
N 0.3643338745 0.3399266282 -2.2325513039
C 0.7875178890 0.7452832087 -4.7834074829
H 1.8290998903 0.5164442546 -5.0302070996
H 0.5846276235 1.7908485308 -5.0356136872
H 0.1324871556 0.1018248399 -5.3791659667

Complex21: fe_2_misc_misc_misc_misc_misc_carbonyl_s_3.xyz

Fe 0.0902211775 0.0764704120 0.0350353156
C 0.4186101698 2.2901141568 0.3867063431
N 0.5891608221 3.4296258323 0.5406948545
C 0.8009427682 4.8341580843 0.7187743970
H 1.7202345209 5.1238101322 0.2041097260
H 0.8864193706 5.0519112731 1.7859385027
H -0.0465491910 5.3783878009 0.2950270784
C 2.1228502829 -0.2669142817 0.3344601174
N 3.2578699007 -0.4530795662 0.4853748068
C 4.6605336174 -0.6804173612 0.6601693213
H 5.0212581817 -1.3132862385 -0.1542649943
H 4.8260159747 -1.1739669431 1.6206207890
H 5.1793338840 0.2811588005 0.6401337077
C -0.2318614125 -2.1300030337 -0.3585338506
N -0.3929755920 -3.2592191415 -0.5825225303
C -0.5906329690 -4.6477226181 -0.8689158616
H -1.3284509646 -4.7447699361 -1.6689878989
H -0.9487478707 -5.1524051661 0.0314321620
H 0.3590278291 -5.0843812999 -1.1873805550
C -1.9431757900 0.4199038474 -0.2599761540
N -3.0735461472 0.6106610440 -0.4376413533
C -4.4667047600 0.8474501351 -0.6675656287
H -4.7509544757 1.7855397940 -0.1846466635
H -5.0421932896 0.0215113461 -0.2426754325
H -4.6438536933 0.9126128687 -1.7437325817
C -0.2300525308 -0.2026654688 1.9308309086
N -0.4203401330 -0.3692397156 3.0630661569
C -0.6553256971 -0.5739839761 4.4600353755
H 0.1144533477 -1.2395143037 4.8578625344
H -1.6413579850 -1.0251997548 4.5939555175
H -0.6149577047 0.3895305281 4.9736923248
C 0.4026893829 0.3507511744 -1.8039335848
O 0.5938175027 0.5196470381 -2.9095594006

Complex22: fe_2_misc_misc_misc_misc_misc_cyanide_s_3.xyz

Fe 0.0270136918 0.0239119893 0.4206838467
C -0.2721552460 1.9190027920 0.5755456703
N -0.4438024981 3.0710264068 0.6044482289
C -0.6419700232 4.4795558158 0.5514168096
H 0.1782362260 4.9392733741 -0.0063094173
H -0.6702804232 4.8873159103 1.5651474333
H -1.5872451068 4.6934161509 0.0455927239
C 2.3390709814 0.3655627769 0.7747963182
N 3.4703025361 0.5819562236 0.5883277335
C 4.8397725891 0.8527437855 0.3014595384
H 5.1504413023 0.2616783088 -0.5638924514
H 5.4545936760 0.5895170219 1.1658842644
H 4.9599084067 1.9156230796 0.0770888546
C 0.3534852787 -1.8335448910 0.0420501092

```

N 0.5568103830 -2.9430337232 -0.2496928706
C 0.8165124526 -4.2721612096 -0.6877098314
H 0.1616644279 -4.5093592243 -1.5303674616
H 0.6302759740 -4.9733817547 0.1298095969
H 1.8591122026 -4.3516171952 -1.0067640837
C -2.2847877230 -0.3090998890 0.0020562413
N -3.2936891485 -0.3964264136 -0.5776559913
C -4.4912838888 -0.4914341837 -1.3440235936
H -5.1748726670 0.3108162517 -1.0547517973
H -4.9672973100 -1.4583199265 -1.1619954007
H -4.2451561210 -0.3975259773 -2.4050774891
C -0.2668362848 -0.3016496745 2.4025366218
N -0.4376486387 -0.4864267480 3.5385568762
C -0.6479367696 -0.7117191276 4.9297489398
H 0.1323390147 -1.3751910179 5.3111606458
H -1.6263640771 -1.1766876621 5.0750843040
H -0.6125184943 0.2418175515 5.4625701258
C 0.2973444730 0.3370121514 -1.4934514493
N 0.4569554904 0.5210826715 -2.6364267483

```

Complex23: fe_2_water_water_water_water_water_chloride_s_3.xyz

```

Fe 0.0047671865 0.0072230556 0.1943307360
O -0.2914956214 1.9849236506 0.5549447687
H 0.6188626703 2.3234776925 0.6788916376
H -0.5877373160 2.3906138167 -0.2829839264
O 2.1687209925 0.8071931838 0.4348134071
H 2.4227376847 0.8853335730 -0.5051412717
H 2.9466124506 0.4614044371 0.9033929897
O 0.3076179732 -1.9800190220 -0.0564097393
H 0.7111713647 -2.0783579378 -0.9414835340
H -0.5955513847 -2.3438429418 -0.1546376950
O -2.1215907934 -0.7308396153 -0.2167054321
H -2.8836764130 -0.5294190855 0.3514400951
H -2.3751778001 -0.4831971796 -1.1235410538
O -0.3556461308 -0.3438570195 2.1700251522
H -0.3047302346 0.3909805217 2.8040082874
H -0.0006378059 -1.1402182311 2.5997416417
Cl 0.3338495876 0.3763316436 -2.0401961809

```

Complex24: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_3.xyz

```

Mn -0.0724629471 -0.0636113244 -0.0011302967
C 0.3766164899 3.0061064381 -0.4648952621
N 0.2070216266 1.8680905764 -0.3168468014
C 0.5890978940 4.4300552530 -0.6517981906
H 0.2373363566 4.7309660593 -1.6464542811
H 1.6567772803 4.6632669761 -0.5631756380
H 0.0318412216 4.9917012262 0.1077179618
C 2.9920316693 -0.5723919686 -0.4594992047

```

N 1.8570491682 -0.3815350843 -0.3141870598
 C 4.4123012435 -0.8122775242 -0.6442027637
 H 4.9324619621 0.1360459614 -0.8235207324
 H 4.5710907812 -1.4796726386 -1.4997539793
 H 4.8264890621 -1.2827824671 0.2561195094
 C -0.5226813806 -3.1326896142 0.4769073130
 N -0.3603769366 -2.0021555730 0.2716704048
 C -0.7267875258 -4.5476444245 0.7286470130
 H 0.2299124950 -5.0801373478 0.6715285953
 H -1.4155267739 -4.9628907230 -0.0175243706
 H -1.1588915152 -4.6869274902 1.7272147895
 C -3.1401356519 0.4300588223 0.4730381584
 N -2.0115474517 0.2507314224 0.2734852422
 C -4.5538013281 0.6529774412 0.7197117942
 H -4.8801054586 0.0459040906 1.5730629480
 H -5.1366740731 0.3650258652 -0.1636874057
 H -4.7337812044 1.7113752300 0.9415268636
 C 0.4419009135 0.3654978110 3.0696762820
 N 0.2509333600 0.2051124541 1.9364218621
 C 0.6819408567 0.5681729614 4.4863623525
 H -0.2501705680 0.4267719714 5.0465777510
 H 1.0531802458 1.5859503933 4.6579246977
 H 1.4292638866 -0.1507406766 4.8435844296
 N -0.4064195992 -0.2818818795 -1.9869887949
 H -1.2567995375 0.2019310207 -2.2907126400
 H 0.3693604671 0.0779186776 -2.5507327937
 H -0.5191366695 -1.2721206830 -2.2220716843

Complex25: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_carbonyl_s_3.xyz
 Mn 0.0838880082 0.0747598662 0.0770815305
 C 0.5360856434 3.1342960364 0.5131776904
 N 0.3683272690 1.9961370596 0.3574023615
 C 0.7431405744 4.5560686368 0.7050323060
 H 0.7247818827 5.0683672601 -0.2652215835
 H 1.7148786194 4.7285179460 1.1846641140
 H -0.0498926013 4.9641629284 1.3441797184
 C 3.1426291729 -0.4205101155 0.4656830673
 N 2.0047429706 -0.2373180194 0.3264076130
 C 4.5631617422 -0.6517912450 0.6373997747
 H 5.0494834744 0.2677299212 0.9868847334
 H 5.0090038351 -0.9521691552 -0.3193149626
 H 4.7241971187 -1.4464313990 1.3766134356
 C -0.3529268537 -2.9667742152 -0.4789066008
 N -0.1905421137 -1.8369848744 -0.2669378397
 C -0.5532416457 -4.3773889784 -0.7455704342
 H 0.4085980850 -4.9034906459 -0.6976814913
 H -0.9835280713 -4.5085177594 -1.7465430671
 H -1.2347909239 -4.8049739020 0.0002770553
 C -2.9547386106 0.5824834835 -0.4325086586
 N -1.8257586996 0.3950535155 -0.2371959837
 C -4.3635287644 0.8180062950 -0.6786670484

H -4.9598243108 0.0180625785 -0.2221461166
H -4.5535306697 0.8385956615 -1.7593137979
H -4.6608047977 1.7804217675 -0.2431933619
C -0.4150591223 -0.3667566259 3.1286096250
N -0.2317798169 -0.2029877153 1.9953188046
C -0.6447925025 -0.5715488158 4.5472029405
H -1.7000541932 -0.8167881214 4.7198541239
H -0.3985642433 0.3438707466 5.0990817749
H -0.0193049916 -1.3939541350 4.9136195994
C 0.4175978124 0.3647218148 -1.9202541237
O 0.6027529906 0.5274044663 -3.0178933494

Complex26: mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_acetonitrile_s_3.xyz

Mn 0.0873966779 -0.0954494341 0.0127880582
N -0.1235526883 1.9537667815 0.3053117742
H -1.1097631482 2.2253548717 0.3882460676
H 0.3349512109 2.3591340389 1.1303530022
H 0.2225426752 2.4901321435 -0.4990385099
N 2.1421716323 0.1553723322 -0.2625507445
H 2.5044225886 1.0710298476 0.0300437148
H 2.7470137260 -0.5281580428 0.2090423353
H 2.3724938621 0.0931580294 -1.2609993846
N 0.2788689216 -2.1328569003 -0.3725431752
H 1.2508449405 -2.4015537647 -0.5640285905
H -0.0364644490 -2.7887650278 0.3527261011
H -0.2335605718 -2.3942896958 -1.2233676531
N -1.9702170742 -0.3400242074 0.2705417248
H -2.2569154705 -1.3233549737 0.3411038370
H -2.3813923968 0.1075115278 1.0985036856
H -2.4909480444 0.0291892128 -0.5336690968
N 0.3956703140 -0.3497750292 2.0541393239
H -0.3328961060 0.0487504003 2.6581412377
H 0.4603821281 -1.3339633479 2.3388792498
H 1.2710234407 0.0666612902 2.3944610027
C -0.3798781599 0.3737820003 -3.0969082070
N -0.2077928081 0.1997636119 -1.9570748131
C -0.5944545462 0.5893539975 -4.5147882370
H 0.3645133522 0.5538396202 -5.0486554756
H -1.0646707514 1.5679776483 -4.6789440628
H -1.2531100888 -0.1944039378 -4.9137804490

Complex27: mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_water_s_3.xyz

Mn -0.0129410988 0.0166303849 0.0190461410
N -0.2197235843 2.0536604048 0.3884701282
H -1.0932826366 2.3128815656 0.8645757049
H 0.5221583742 2.4851220183 0.9551081692
H -0.2336467167 2.5821315120 -0.4934918314
N 2.0503896862 0.2481213068 -0.3078906961
H 2.3244011369 1.2262830294 -0.4647882940

H 2.6615298738 -0.0695139502 0.4549115885
 H 2.4047389429 -0.2475805407 -1.1366720498
 N 0.2152039979 -2.0319357316 -0.2618595062
 H 1.1491921763 -2.3905092834 -0.0254206741
 H -0.4412144927 -2.6313694382 0.2553297578
 H 0.0805131027 -2.2774727899 -1.2517855265
 N -2.0802899273 -0.3015844184 0.2221730199
 H -2.4432956262 -1.0578346692 -0.3731512971
 H -2.3877094075 -0.5537179524 1.1695160482
 H -2.6603883031 0.5107288580 -0.0251857367
 N 0.2792539505 -0.2144292305 2.0558528301
 H -0.4659421823 0.1814680577 2.6426923127
 H 0.3397373205 -1.1998869758 2.3406276972
 H 1.1429483733 0.2102191697 2.4164565509
 O -0.3155949940 0.3127163099 -1.9604063824
 H -1.1812401361 0.3839989756 -2.4108916991
 H 0.3643692543 0.4543298226 -2.6495386148

Complex28: mn_3_ammonia_ammonia_ammonia_ammonia_phosphine_phosphine_s_3.xyz

Mn 0.0006652349 0.0030637842 0.0496014245
 N -0.1995962347 2.0435605864 0.4713206242
 H -1.1653768790 2.2880240588 0.7195574143
 H 0.3633339179 2.4018679062 1.2521143201
 H 0.0263418328 2.6566632543 -0.3208175611
 N 2.0691124618 0.2762645845 -0.1527047083
 H 2.4230190225 1.1381577544 0.2796596358
 H 2.6337364578 -0.4704507088 0.2696518375
 H 2.3846495605 0.3310465707 -1.1279911478
 N 0.1984211088 -2.0370623940 -0.3780911644
 H 1.1579502637 -2.2806347758 -0.6507415898
 H -0.0061687410 -2.6511573930 0.4190361092
 H -0.3832129160 -2.3957543776 -1.1448302147
 N -2.0700761721 -0.2625461628 0.2563023181
 H -2.4167350520 -1.1501667760 -0.1269011635
 H -2.3911096736 -0.2642280852 1.2314817632
 H -2.6368278410 0.4552893078 -0.2110158025
 P 0.3746765564 -0.4176928058 2.5736405817
 H 1.5514699928 0.1458983381 3.1080791951
 H -0.6140355688 0.0858436735 3.4434851308
 H 0.4796432155 -1.7619922723 2.9855284232
 P -0.3770733036 0.4194967308 -2.4752743265
 H 0.6537165469 -0.0013901057 -3.3401088059
 H -1.5035350355 -0.2265598786 -3.0248039200
 H -0.5801968307 1.7554568763 -2.8774450551

Complex29: mn_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_3.xyz

Mn 0.0492243717 0.0493342779 -0.0311657039
 C 0.0153648077 2.0737233780 0.3040607078
 O 0.0061140491 3.1902616398 0.4229744151

C 2.0734597096 0.0205736384 0.3050320720
O 3.1899083951 0.0143922471 0.4250245369
C 0.0750471503 -1.9810891826 -0.3310544572
O 0.0995632996 -3.0806605446 -0.5576738807
C -1.9811050574 0.0696339045 -0.3322297622
O -3.0805078721 0.0909252277 -0.5599919912
C -0.2899861880 -0.2900649148 2.1033102128
O -0.4651228231 -0.4654936300 3.1979872205
F 0.3080487826 0.3084737716 -1.6690180858

Complex30: mn_3_cyanide_cyanide_ammonia_ammonia_ammonia_ammonia_s_3.xyz

Mn -0.0577126621 -0.0037447816 0.0100350528
C -0.3917673882 1.8886165010 0.2980398834
N -0.7151568077 2.9969169983 0.4782287679
C 1.8483924665 0.2564523132 -0.2648642503
N 3.0008897102 0.2878828573 -0.4548654742
N 0.2685510815 -2.1035862642 -0.2908907725
H 1.2868687525 -2.1926973591 -0.3325656591
H -0.0561338677 -2.7440056481 0.4362310096
H -0.0863900336 -2.4734337304 -1.1748674813
N -2.1662050189 -0.3270185514 0.2662705152
H -2.6628411125 -0.8546035456 -0.4542320322
H -2.4323685374 -0.7449827992 1.1598541159
H -2.5583501288 0.6177507959 0.2687189010
N 0.3091501948 -0.1221735271 2.0565630868
H -0.3956826417 0.3425512002 2.6325569398
H 0.4822403964 -1.0470996909 2.4554809579
H 1.1735960703 0.4095358386 2.1888770067
N -0.2503550305 0.3203458994 -2.0458531387
H -1.1408134486 0.1029235493 -2.4978259975
H -0.1237955613 1.3311571548 -2.1417378347
H 0.4968135863 -0.1117210927 -2.5931485940

Complex31: mn_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_3.xyz

Mn -0.0006723344 -0.0008674898 -0.0120613893
C 0.3309639759 1.9911318594 -0.2970518137
N 0.5189993550 3.1204101107 -0.4591404361
C 0.7536719467 4.5232391508 -0.6598347865
H 1.7445013151 4.6514798382 -1.1040062843
H 0.7038846986 5.0279654190 0.3086640362
H -0.0158894696 4.9135975405 -1.3312968113
C 1.9711276905 -0.2865299701 0.3225554855
N 3.1008080828 -0.4506709666 0.5134255269
C 4.5030816631 -0.6555655827 0.7495870336
H 4.8200892156 -1.5568520194 0.2184112138
H 4.6673651605 -0.7690175398 1.8239440241
H 5.0506121880 0.2128348773 0.3731543017
C -0.3314214360 -1.9930002989 0.2727429377
N -0.5177146901 -3.1227296020 0.4336911728

C -0.7489581331 -4.5264659114 0.6321507965
 H -1.4149746805 -4.8856782425 -0.1570158383
 H -1.2104581982 -4.6696482471 1.6128205254
 H 0.2107162580 -5.0483071037 0.5849049912
 C -1.9731888655 0.2822828798 -0.3442069496
 N -3.1041488223 0.4430259521 -0.5302076062
 C -4.5080378412 0.6425550829 -0.7608333331
 H -4.7343456312 1.7052156856 -0.6374046328
 H -5.0701726051 0.0534322045 -0.0314627802
 H -4.7487161596 0.3206109609 -1.7769806492
 C -0.4588617601 0.5018836506 3.0474259639
 N -0.2891634629 0.3138903757 1.9158164293
 C -0.6725527958 0.7372427154 4.4644408012
 H 0.2574383018 1.0810206118 4.9319121449
 H -0.9932585848 -0.1932937418 4.9487295427
 H -1.4510948907 1.4965626967 4.6033710495
 C 0.4606261735 -0.4931071336 -3.0723263519
 N 0.2881297080 -0.3135070534 -1.9397735302
 C 0.6775725216 -0.7179437712 -4.4905945968
 H 1.7401899570 -0.5970410872 -4.7307305381
 H 0.0894509519 -0.0011247100 -5.0758407183
 H 0.3635703107 -1.7349499520 -4.7556530548

Complex32: mn_3_misc_misc_misc_misc_misc_misc_s_3.xyz

Mn 0.0003799328 0.0025931082 -0.0002700117
 C -0.0215462105 2.0257486837 -0.0004868580
 N -0.0346112606 3.1827799061 -0.0007483177
 C -0.0494875052 4.6193986581 -0.0004128928
 H 0.7849603975 4.9770069730 -0.6097846647
 H 0.0536674294 4.9712363859 1.0293210645
 H -0.9982435989 4.9591930079 -0.4246930957
 C 2.0234931535 -0.0209820983 0.0007364372
 N 3.1804813848 -0.0374319978 0.0028760259
 C 4.6170124161 -0.0584672112 0.0067790929
 H 4.9558788256 -0.9005930824 -0.6026727142
 H 4.9635704580 -0.1711276841 1.0373159582
 H 4.9807672498 0.8823422158 -0.4154097334
 C 0.0192392394 -2.0209041561 -0.0004218856
 N 0.0305362072 -3.1779496955 -0.0003476432
 C 0.0432247875 -4.6146011868 0.0006571594
 H -0.7915412034 -4.9712686187 -0.6088164289
 H -0.0608521468 -4.9657415692 1.0305433982
 H 0.9916558322 -4.9560227232 -0.4230389829
 C -2.0229728063 0.0221692363 -0.0001245888
 N -3.1800194616 0.0334830512 0.0006237275
 C -4.6165947135 0.0458928105 0.0012671694
 H -4.9571607657 1.0428372232 0.2941210761
 H -4.9721182537 -0.6993809857 0.7178929264
 H -4.9700962347 -0.1947520635 -1.0047394445
 C 0.0007287119 0.0017156230 2.0145493056
 N 0.0007040607 -0.0003330789 3.1721961647

C 0.0004063218 -0.0044312206 4.6091643242
 H 0.6080102884 -0.8421456184 4.9601056054
 H -1.0302300773 -0.1087400881 4.9584582280
 H 0.4207539697 0.9417759002 4.9608295428
 C 0.0005583530 0.0029206170 -2.0149884224
 N 0.0012986622 0.0025685160 -3.1726253261
 C 0.0029567184 0.0016942806 -4.6095893555
 H -0.6044975038 -0.8384302282 -4.9575118204
 H 1.0324789225 -0.1102054959 -4.9592810846
 H -0.4201883832 0.9449979072 -4.9637470039

Complex33: mn_3_phosphine_phosphine_phosphine_phosphine_ammonia_ammonia_s_3.xyz

Mn -0.0005716730 0.0045519883 0.0021748650
 P -0.4000214677 2.5034853348 0.3719198955
 H -0.9016657595 2.8373382340 1.6453589148
 H 0.7072582354 3.3669280723 0.2508350957
 H -1.3393391365 3.0997093241 -0.4927875945
 P 2.4764377213 0.4186937543 -0.4571282948
 H 3.1708963655 1.1511332270 0.5262508783
 H 3.2937964245 -0.7184376382 -0.6122471940
 H 2.7524701847 1.1509905495 -1.6289804598
 P 0.3987893298 -2.4943497582 -0.3677636326
 H 0.9005040618 -2.8280090225 -1.6412321423
 H 1.3381123316 -3.0906840713 0.4968754488
 H -0.7084492707 -3.3578734198 -0.2468367229
 P -2.4775000184 -0.4096155895 0.4614283404
 H -3.1718711719 -1.1421616051 -0.5219207900
 H -2.7535275854 -1.1417617564 1.6333643228
 H -3.2948357809 0.7275466172 0.6163380023
 N 0.4397771089 -0.1580711141 2.0583182634
 H -0.3560895110 0.0453988738 2.6715173790
 H 0.7482029483 -1.0950302789 2.3400390825
 H 1.1860009570 0.4656662492 2.3856307357
 N -0.4408717239 0.1672280298 -2.0540020110
 H -1.1870457720 -0.4565061712 -2.3814345878
 H -0.7492712713 1.1041941403 -2.3357206401
 H 0.3550668611 -0.0361859502 -2.6671305638

Complex34: mn_3_phosphine_phosphine_phosphine_phosphine_phosphine_chloride_s_3.xyz

Mn -0.0346850587 -0.0381087281 0.1835051196
 P -0.4569196071 2.3552133030 -0.3061406332
 H -0.4021153517 3.3454737839 0.6958108235
 H 0.3854846790 2.8957406324 -1.2939676990
 H -1.7227917004 2.5854299372 -0.8731390627
 P 2.3583931150 0.2665129542 -0.3890377828
 H 3.3328468566 0.5314188683 0.5942499380
 H 2.9102232959 -0.8394981187 -1.0590223238
 H 2.5994187998 1.2929467926 -1.3198332135
 P 0.3637334520 -2.4774982889 0.3555744124

H 1.3832660534 -2.9348073955 -0.4976091398
H 0.7019451578 -3.0955983906 1.5765160873
H -0.7212825715 -3.2629350350 -0.0733859458
P -2.4741693041 -0.3995554865 0.4541793389
H -2.9251387644 -1.6323896151 -0.0500162929
H -3.1035240119 -0.3526236958 1.7147288140
H -3.2513137405 0.5028460697 -0.2930723231
P 0.2938286933 0.3514711632 2.5901385745
H 1.5900105055 0.6636010775 3.0460705377
H -0.4451580886 1.3828534350 3.2028991855
H -0.0190830221 -0.7227630552 3.4468839357
Cl -0.3799967959 -0.3942243796 -2.0281900483

Complex35: mn_3_water_water_water_water_fluoride_fluoride_s_3.xyz

Mn -0.0005843952 -0.0001862254 0.0008354290
O -0.4062835774 1.9675151910 -0.3375591821
H 0.2619137672 2.3810616640 -0.9148679760
H -0.3972717617 2.4633901443 0.5028295430
O 1.9659461488 0.4371631706 0.2925027369
H 2.5602726984 -0.2373390639 -0.0834081560
H 2.1419610076 0.4547669227 1.2528321170
O 0.4034190710 -1.9676507913 0.3410863057
H 0.3965715460 -2.4665041151 -0.4974821402
H -0.2648776266 -2.3798828590 0.9192165543
O -1.9668514442 -0.4345906711 -0.2907577073
H -2.5587765332 0.2528588282 0.0651859934
H -2.1355438262 -0.4699319819 -1.2520205988
F -0.2575443701 0.2873215347 1.6954734907
F 0.2576523856 -0.2879871870 -1.6938642003

Complex36: fe_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_s_4.xyz

Fe 0.0511685841 0.0464971263 0.2810414964
C 0.5582786921 3.2816461227 0.5724301761
N 0.3638725288 2.1398041341 0.5877849292
C 0.8026170497 4.7147943646 0.5487209685
H 1.0418753090 5.0287537817 -0.4732314412
H 1.6424651603 4.9612602218 1.2068488386
H -0.0894498696 5.2506744458 0.8897743837
C 3.2009109012 -0.4347798807 0.4806213167
N 2.0551803874 -0.2737508159 0.4980274202
C 4.6402445058 -0.6373139835 0.4570012153
H 5.1413411729 0.2045356360 0.9467279156
H 4.9839238060 -0.7059117433 -0.5808601925
H 4.8956261909 -1.5621081324 0.9850354059
C -0.3917056583 -3.1280524908 -0.4597491232
N -0.2550230738 -2.0395008695 -0.0880895186
C -0.5635084091 -4.4930534964 -0.9305604236
H 0.2852367187 -5.1069325867 -0.6111003481
H -0.6186151055 -4.4989241735 -2.0246749606

H -1.4866763696 -4.9161118794 -0.5207680597
C -3.0126187925 0.5979169451 -0.4268282548
N -1.9288587105 0.3856073981 -0.0812515218
C -4.3732615445 0.8648054163 -0.8634867686
H -5.0106665645 0.0017436404 -0.6436393719
H -4.3811783308 1.0542455745 -1.9423737050
H -4.7667345431 1.7425816285 -0.3398569499
C -0.4601155198 -0.4079628830 3.4091707736
N -0.2751807933 -0.2443664654 2.2790460151
C -0.6926857960 -0.6126781377 4.8302142884
H -1.7678911207 -0.6015098608 5.0370448440
H -0.2079640504 0.1853282471 5.4028641035
H -0.2764075115 -1.5775026355 5.1390441619
C 0.3549501910 0.3088616028 -1.5613576949
N 0.5414055831 0.4717709270 -2.7026121010

Complex37: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_chloride_s_4.xyz

Fe -0.0380050481 0.0259827667 0.1065566711
N -0.2885620116 2.1995582202 0.3691363376
H -1.2850242017 2.4250212359 0.4309202926
H 0.1589834662 2.6804326897 1.1546625980
H 0.0309423683 2.6683118534 -0.4837912471
N 2.1287256031 0.3142424182 -0.2426389508
H 2.4520962735 1.2639546400 -0.0377849828
H 2.7949455979 -0.3127741183 0.2173920706
H 2.2670158583 0.2003367396 -1.2515266540
N 0.1863811457 -2.1253645406 -0.3202437136
H 1.1671900015 -2.3538956931 -0.5032135309
H -0.1406799040 -2.8253440191 0.3521084939
H -0.2990462134 -2.3209969666 -1.2012381142
N -2.2184056417 -0.2582208257 0.3402993613
H -2.4789766905 -1.2468589862 0.3877285300
H -2.6960407990 0.1893335012 1.1276396587
H -2.6626942737 0.0981502492 -0.5115315132
N 0.2736385209 -0.2074443598 2.1285287810
H -0.4694913014 0.1948290832 2.7061969743
H 0.3464276861 -1.1919076037 2.3997729849
H 1.1458707306 0.2306509057 2.4388533577
Cl -0.3760088500 0.3526860755 -2.0781595702

Complex38: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_misc_s_4.xyz

Fe 0.0949203546 -0.0725431196 0.0322496070
N -0.1706245712 2.1074500057 0.2801896189
H -1.1630275419 2.3655136911 0.3160242082
H 0.2421935048 2.5162230771 1.1265120544
H 0.2136253703 2.6538151303 -0.4984879093
N 2.2587823368 0.1864792016 -0.3270756937
H 2.5101939531 1.1806922477 -0.3616475069
H 2.8896505180 -0.2274576990 0.3694996472

H 2.5711370862 -0.1931879292 -1.2278972964
N 0.3378076019 -2.2523531451 -0.2817394799
H 1.3234335614 -2.5340796383 -0.3325652488
H -0.0773137860 -2.8607930098 0.4337572110
H -0.0705797501 -2.5712391372 -1.1672650575
N -2.0833444205 -0.3537199456 0.3285395226
H -2.3100996446 -1.3502906123 0.4168362844
H -2.5067003707 0.0891600918 1.1527443708
H -2.6456026529 -0.0266900798 -0.4648431111
N 0.4391802430 -0.2656512063 2.0262804067
H -0.3736559941 0.0012459758 2.5946983536
H 0.6540946317 -1.2322391207 2.2979079319
H 1.2206231744 0.3057452895 2.3684887642
C -0.2275694747 0.1649588748 -1.9224719120
N -0.4115959213 0.3067098250 -3.0556615792
C -0.6413655677 0.4828895963 -4.4697462211
H -1.2831390595 -0.3303487260 -4.8213603301
H 0.3264241640 0.4606303311 -4.9809253161
H -1.1281780678 1.4518186118 -4.6208698341

Complex39: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_acetonitrile_s_4.xyz

Fe 0.0075550664 -0.0002435194 -0.0652791780
C 0.0114853926 2.0967593569 -0.0608660273
O 0.0132717558 3.2175848615 -0.0860091507
C 2.3835327803 0.0003944775 0.1285799333
O 3.5057422904 0.0006903133 0.1636441095
C 0.0122439217 -2.0972227109 -0.0611558105
O 0.0143981990 -3.2180431076 -0.0864029039
C -2.3697801089 -0.0010838169 0.1241636978
O -3.4920575660 -0.0015335220 0.1574212271
C 0.0014102423 -0.0004882716 2.0056217537
O -0.0020613383 -0.0006323843 3.1266982352
C -0.0122578670 0.0009742302 -3.1122817618
N 0.0006015480 0.0003535794 -1.9373098203
C -0.0280501549 0.0016853958 -4.5434905871
H 1.0132742498 -0.0341888938 -4.9222313715
H -0.5017194710 0.9236998262 -4.9201623633
H -0.5604504944 -0.8886043470 -4.9192148307

Complex40: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_fluoride_s_4.xyz

Fe -0.0000859829 -0.0000827863 -0.0127227285
C -0.0318140624 2.2142722623 0.3442627073
O -0.0487713684 3.3249639343 0.5338603819
C 2.2221293532 -0.0315357609 0.3457255874
O 3.3327915272 -0.0482787371 0.5358089092
C 0.0330365628 -2.2151438706 -0.3656659894
O 0.0498896588 -3.3263959947 -0.5519356258
C -2.2230578643 0.0327072058 -0.3669627838
O -3.3343003467 0.0493041215 -0.5536138690

F -0.2621648387 -0.2621897599 1.6368159894
F 0.2623484024 0.2623801685 -1.6618606769

Complex41: fe_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_4.xyz

Fe -0.0000669195 0.0006524004 -0.0035281364
C 0.0016452958 2.0689144326 -0.0058566371
N 0.0034665349 3.2250692942 -0.0070773526
C 0.0067814845 4.6608644078 -0.0072767040
H 0.8456715380 5.0074391051 -0.6171410060
H 0.1154908135 5.0094701225 1.0232873923
H -0.9386097232 5.0119699377 -0.4301867596
C 1.9809106696 -0.0031697557 -0.0025573675
N 3.1361759114 -0.0071267570 -0.0006682385
C 4.5726443707 -0.0134948019 0.0037682976
H 4.9182459129 -0.8509768746 -0.6086727500
H 4.9193295760 -0.1232434307 1.0343978864
H 4.9252284588 0.9313931835 -0.4195122402
C -0.0036749896 -2.0675195930 -0.0045722207
N -0.0080696740 -3.2236588811 -0.0047648695
C -0.0151536757 -4.6594488270 -0.0038348846
H -0.8543321517 -5.0042217609 -0.6143416643
H -0.1259656869 -5.0069050725 1.0268968614
H 0.9298294491 -5.0134477709 -0.4252224789
C -1.9810059267 0.0003500992 -0.0027116919
N -3.1362723964 -0.0023612895 -0.0010933669
C -4.5726763219 -0.0081717091 0.0007984503
H -4.9229695650 0.9855111179 0.2946289843
H -4.9167683673 -0.7558560844 0.7206660588
H -4.9235259725 -0.2529738489 -1.0049702442
C 0.0004341152 0.0071997102 3.3509088674
N 0.0002359501 0.0029611291 2.1898773564
C 0.0013712922 0.0125109330 4.8051586487
H 0.6113485955 0.8448523773 5.1744931805
H 0.4199935722 -0.9282860671 5.1808210355
H -1.0220197387 0.1238554860 5.1804633617
C 0.0031579518 0.0039597149 -3.3587431928
N 0.0009410351 0.0014521570 -2.1977131509
C 0.0061818964 0.0064691739 -4.8130315967
H 0.7502930442 0.7205840135 -5.1836964618
H -0.9828553118 0.2906295224 -5.1893151041
H 0.2566041337 -0.9933875177 -5.1859958519

Complex42: fe_3_misc_misc_misc_misc_water_water_s_4.xyz

Fe 0.0008765737 0.0024232895 -0.0026202214
C 0.0022224001 2.0383832768 -0.0018306176
N 0.0042616109 3.1940454596 -0.0003781967
C 0.0081517139 4.6314115403 0.0033884230
H 0.8491306953 4.9771336413 -0.6050402268
H 0.1140435325 4.9749476071 1.0364724263

H -0.9368082890 4.9818279703 -0.4224745848
 C 1.9943142548 0.0003017583 0.0004716463
 N 3.1503760375 -0.0024867975 0.0018286231
 C 4.5895680727 -0.0067031537 0.0033998055
 H 4.9336316772 -0.8459926321 -0.6083044146
 H 4.9360480764 -0.1154422892 1.0348354133
 H 4.9386329632 0.9395095519 -0.4209815437
 C -0.0006960274 -2.0335392889 -0.0022479982
 N -0.0031019147 -3.1891943299 -0.0009426206
 C -0.0076021334 -4.6265588739 0.0026882449
 H -0.8458887437 -4.9718547134 -0.6096972275
 H -0.1184091375 -4.9700984078 1.0352589333
 H 0.9392415116 -4.9773739740 -0.4186181214
 C -1.9925612994 0.0017143949 -0.0044327447
 N -3.1486199710 -0.0010456936 -0.0029021541
 C -4.5877149413 -0.0058346834 0.0001529536
 H -4.9359899914 0.9887975831 0.2947620577
 H -4.9300003848 -0.7558026774 0.7192869428
 H -4.9371452332 -0.2504782889 -1.0067914306
 O -0.0068155102 0.0028606009 2.2193683866
 H 0.7662186904 0.0278449926 2.8138052602
 H -0.7849202136 -0.0203465315 2.8072464177
 O 0.0080295716 0.0032290886 -2.2241571758
 H -0.7650180156 0.0314724191 -2.8184414281
 H 0.7858615287 -0.0229881569 -2.8122820095

Complex43: mn_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_water_water_s_4.xyz

Mn 0.0014019174 -0.0017752126 -0.0008571339
 C 0.5700829810 3.3679945619 -0.5746341248
 N 0.3681160340 2.2593660262 -0.3036774442
 C 0.8244139357 4.7618062380 -0.9161449252
 H 0.7382298006 4.9017057507 -1.9985528099
 H 1.8329663147 5.0464142207 -0.5996071656
 H 0.0985276185 5.4091714669 -0.4137067190
 C 3.1280823143 -0.4675512055 0.5176699234
 N 1.9968883170 -0.2971133435 0.3323825248
 C 4.5494163993 -0.6786527149 0.7509885773
 H 5.0736400358 0.2828171471 0.7352569564
 H 4.9652684658 -1.3244777954 -0.0295340176
 H 4.7015084029 -1.1530065958 1.7262647296
 C -0.5713189865 -3.3704653727 0.5687880260
 N -0.3649099752 -2.2622362328 0.2995326482
 C -0.8318334138 -4.7637234365 0.9078739206
 H 0.0947023838 -5.2498032201 1.2298929985
 H -1.2271010267 -5.2939678908 0.0355063281
 H -1.5630442536 -4.8187045586 1.7207883803
 C -3.1259308043 0.4658218676 -0.5142610819
 N -1.9943132793 0.2940843835 -0.3329301350
 C -4.5475527292 0.6828035561 -0.7404210927
 H -5.1328000492 0.0660466174 -0.0501641956
 H -4.8088579801 0.4148841321 -1.7695431869

H -4.7925819868 1.7370995971 -0.5733421256
O -0.3186081836 0.2635510496 2.0168268154
H 0.4309449084 0.5154067647 2.5810839904
H -1.0953972855 0.7582603646 2.3260918133
O 0.3207052801 -0.2675310890 -2.0186690580
H -0.4260715167 -0.5265263386 -2.5832802959
H 1.1031726727 -0.7525439332 -2.3288031083

Complex44: mn_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_4.xyz

Mn -0.0001161999 0.0000463706 -0.0002638252
N -0.8721383105 1.9213198936 0.4216871916
H -1.8652852933 1.7710840073 0.5924803573
H -0.4912481087 2.3627233426 1.2575181873
H -0.8059647713 2.5638510145 -0.3666561970
N 2.1871197824 1.0596767225 -0.2567061303
H 2.0578576413 2.0699229586 -0.2915160335
H 2.7786953860 0.8627001878 0.5494219015
H 2.6952338899 0.8117981661 -1.1047075486
N 0.8718740847 -1.9211984030 -0.4225245555
H 1.8647986541 -1.7706734983 -0.5943570025
H 0.8066820938 -2.5637525891 0.3658829153
H 0.4903027832 -2.3627199260 -1.2579824364
N -2.1871906846 -1.0597903373 0.2580417564
H -2.0570602588 -2.0698401721 0.2952822809
H -2.6952423247 -0.8103375908 1.1056133750
H -2.7792054812 -0.8652164609 -0.5483448842
C 0.3866375399 -0.2718082040 1.9830753865
N 0.6274306374 -0.4277616222 3.1201578127
C -0.3865334578 0.2719434072 -1.9835838414
N -0.6266562377 0.4280380235 -3.1207877065

Complex45: mn_2_carbonyl_carbonyl_carbonyl_carbonyl_phosphine_phosphine_s_4.xyz

Mn -0.0021088671 -0.0124699054 0.0599351532
C 0.3460528068 1.9700807528 0.3591056060
O 0.5410519509 3.0693828143 0.5282114863
C 2.4934895027 -0.4172520172 -0.3529629869
O 3.5896790275 -0.6018778363 -0.5388544798
C -0.3466812321 -1.9980568376 -0.2402371593
O -0.5395770232 -3.0974228623 -0.4094054432
C -2.5046557375 0.3582271555 0.4726688061
O -3.6045434770 0.5128130762 0.6639946071
P 0.3531202304 -0.4155743036 2.5309830496
H 1.6085376748 -0.0132995792 3.0251135590
H -0.5318279716 0.2763232817 3.3796901106
H 0.2539377395 -1.7347943966 3.0102785682
P -0.3625496318 0.4361930493 -2.4024611231
H 0.7876728314 0.8535208436 -3.0988828812
H -0.8297506196 -0.6196093228 -3.2067974019
H -1.2762496010 1.4645220535 -2.7014242904

Complex46: mn_2_chloride_chloride_chloride_chloride_carbonyl_carbonyl_s_4.xyz

Mn -0.0004795845 -0.0004707332 -0.0000002307
Cl 0.0220567513 2.5695630429 0.0000905187
Cl 2.5692824300 0.0227551355 0.0003602999
Cl -0.0201685003 -2.5699370220 -0.0001037910
Cl -2.5696725549 -0.0208510496 -0.0003445230
C -0.0003008025 -0.0003241370 1.9378127603
O -0.0001449623 -0.0002315890 3.0841976103
C -0.0003259822 -0.0003102543 -1.9378134280
O -0.0002467688 -0.0001934391 -3.0841992282

Complex47: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_carbonyl_s_4.xyz

Mn -0.0646782452 0.0336108980 0.1795075686
S 0.3134271484 2.5089422544 -0.1420920493
H -0.8474152981 3.0771304432 0.2557194840
H 0.1062037741 2.7671421874 -1.4522705172
S 2.7123664945 -0.3520660111 0.5500980647
H 3.2745504749 -0.8730517303 -0.5619063524
H 3.3448665960 0.8364299603 0.4432000581
S -0.4922696554 -2.4287886952 0.6105013239
H 0.6034244169 -2.8774433447 1.2638950025
H -0.2014365762 -3.0858441140 -0.5339859988
S -2.8222602042 0.4370317838 -0.2531337931
H -3.4777336645 -0.4962825189 0.4702056636
H -3.1769722572 -0.0849534107 -1.4472724859
S -0.4551189292 0.4535396355 2.5931627646
H 0.1823056725 -0.5313484910 3.2641196493
H 0.4286294851 1.4104737020 2.9555524756
C 0.2059626948 -0.2980533856 -1.7652757763
O 0.3662206957 -0.4944439864 -2.8689043044

Complex48: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_phosphine_s_4.xyz

Mn -0.1050637611 0.0597019134 0.0680880683
S 0.2698765630 2.5070897506 -0.3015534827
H 1.0570065703 2.9059392229 0.7219807319
H 1.2532533048 2.6304537065 -1.2192048167
S 2.6883031752 -0.0748080636 0.8609260171
H 2.8276393417 -0.8711997507 1.9410737131
H 3.4342321484 -0.8585977940 0.0546763373
S -0.5875819643 -2.3703691954 0.4040855420
H -0.2825874117 -2.6794098454 1.6842214146
H 0.4858625367 -3.0110013842 -0.1056720354
S -2.8861919037 0.4337979973 -0.3645545643
H -3.3661799932 -0.4417948369 -1.2725609146
H -3.0970138493 1.5228458018 -1.1335401384
S -0.5154765188 0.4665341205 2.5112534524

H -0.9936326272 1.7243974137 2.6393080644
H -1.7159294260 -0.1081721315 2.7465314085
P 0.2925850104 -0.3705716003 -2.3542458297
H 1.6303765830 -0.4727726391 -2.7876115979
H -0.2506727936 -1.5358063062 -2.9320229234
H -0.1901717523 0.6031460514 -3.2512662580

Complex49: mn_2_water_water_water_water_acetonitrile_acetonitrile_s_4.xyz

Mn -0.0265944274 0.0137783729 0.0216070058
O -0.1098793031 2.2905512700 0.2812354379
H -0.7205402968 2.8172860156 -0.2616666656
H -0.0775477823 2.7403059056 1.1429525219
O 1.9934501330 0.1968155836 -0.3448125062
H 2.2579597195 0.8686787687 -0.9976111574
H 2.5880648671 0.3059122634 0.4178808726
O 0.2585604751 -2.1640429279 -0.5603415021
H 1.1440557106 -2.4143188282 -0.8753025953
H -0.1027117439 -2.9552079644 -0.1271383088
O -2.0238431487 -0.2596768142 0.3228728019
H -2.4345616051 -0.5205765811 1.1633815665
H -2.6489255517 -0.4424104278 -0.3978268236
C 0.4996068544 -0.4698899928 3.1417241858
N 0.3100914594 -0.2812488555 2.0125607317
C 0.7373711932 -0.7084072245 4.5571514621
H -0.1167448496 -0.3548486041 5.1450747885
H 1.6397523669 -0.1778177562 4.8801585072
H 0.8725043285 -1.7815015382 4.7331533890
C -0.5342736492 0.4591370399 -3.1140192331
N -0.3653447523 0.3471025640 -1.9722942434
C -0.7448578650 0.5962662682 -4.5472294426
H 0.1337798343 0.2294248961 -5.0889099857
H -0.9073898013 1.6495354789 -4.8009506218
H -1.6218556019 0.0151976912 -4.8524017114

Complex50: mn_2_water_water_water_water_water_water_s_4.xyz

Mn 0.0002711654 0.0006913128 -0.0000860777
O -0.2755593231 2.0116250680 -0.1166149696
H 0.1835154254 2.6503916640 -0.6900191312
H -1.1761927438 2.3508086271 0.0404205872
O 1.8554499197 0.0084901263 -0.9448612686
H 1.7791999236 -0.0716855988 -1.9136234445
H 2.6159351461 0.5877185239 -0.7592517008
O 0.2759786290 -2.0107033121 0.1172843709
H 1.1757488843 -2.3507512660 -0.0425258471
H -0.1838685274 -2.6506692583 0.6886578830
O -1.8556502149 -0.0082860154 0.9435620742
H -1.7785432713 0.0760291439 1.9119575054
H -2.6117095415 -0.5944276984 0.7616419385
O 0.7104220458 0.3429027223 2.1581023160

H 1.1861872110 -0.2623712915 2.7535755520
H 0.9311651915 1.2406603342 2.4633103454
O -0.7108586786 -0.3421476724 -2.1577995977
H -1.1913679533 0.2619687737 -2.7506468124
H -0.9301294968 -1.2402437175 -2.4630775799

S4.3 High spin geometries

Complex1: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_cyanide_s_5.xyz

Co 0.0034836232 0.0040572099 0.0050360138
C 0.0012900972 3.3218708021 -0.0002277020
N 0.0033476193 2.1664675682 0.0032858675
C -0.0022922280 4.7782321362 -0.0059051083
H -0.2801779451 5.1445028360 -0.9991241831
H 0.9940667546 5.1525753203 0.2484675208
H -0.7212931999 5.1503708255 0.7305085598
C 3.3213155971 -0.0033223592 -0.0018232540
N 2.1659237849 0.0021255025 0.0016872167
C 4.7776143019 -0.0125970692 -0.0061826101
H 5.1557494781 1.0143440675 -0.0071840769
H 5.1424278704 -0.5282970648 -0.8999683673
H 5.1477958518 -0.5285495061 0.8852466244
C -0.0030952698 -3.3140712695 -0.0011957675
N 0.0018684774 -2.1586727064 0.0017821647
C -0.0117062764 -4.7703768980 -0.0048752161
H 1.0154011631 -5.1480383312 -0.0001559276
H -0.5225112519 -5.1358849797 -0.9011858189
H -0.5322658836 -5.1403373942 0.8839595784
C -3.3146155255 0.0012959936 -0.0019688858
N -2.1592150250 0.0038706489 0.0028115976
C -4.7709667519 -0.0030868920 -0.0096322566
H -5.1435478809 -0.7433701801 0.7051464808
H -5.1356077079 -0.2527037117 -1.0109470721
H -5.1464838704 0.9852269776 0.2727812271
C 0.0043607601 0.0025461014 2.0099095363
N 0.0049430290 0.0006989438 3.1850278656
C 0.0020830905 0.0049489586 -2.0008139397
N 0.0001787598 0.0054320996 -3.1758696904

Complex2: co_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_fluoride_fluoride_s_5.xyz

Co 0.0022123266 0.0034832147 0.0007522085
C 0.4753018333 3.2566240666 0.5329440365
N 0.3130425772 2.1264384784 0.3588110392
C 0.6780121733 4.6832230587 0.7504654996
H 0.6429984004 5.2135359936 -0.2060832725
H 1.6522413035 4.8540949806 1.2184875798
H -0.1050134701 5.0744548709 1.4071559116
C 3.2552597759 -0.5313309181 0.4747511961
N 2.1279396112 -0.3459115262 0.3051915055

C 4.6773031027 -0.7669048721 0.6887452313
 H 5.1598074002 0.1533434956 1.0318587307
 H 5.1462286708 -1.0881326663 -0.2463476169
 H 4.8155972222 -1.5445753869 1.4460773957
 C -0.4761307973 -3.2487310082 -0.5363725937
 N -0.3098370937 -2.1196956387 -0.3585653654
 C -0.6860642403 -4.6733524399 -0.7598777819
 H 0.2723421070 -5.2003101387 -0.7261188740
 H -1.1455357456 -4.8327258422 -1.7401337053
 H -1.3430175521 -5.0787529787 0.0156983393
 C -3.2511517411 0.5287409044 -0.4814400925
 N -2.1236408224 0.3508834464 -0.3051509797
 C -4.6735841817 0.7516007012 -0.7061493329
 H -5.2558528404 -0.0311431150 -0.2104468115
 H -4.8874914454 0.7336244755 -1.7791839180
 H -4.9673953471 1.7240390764 -0.2993677871
 F -0.2727983122 -0.2611221152 1.7018974367
 F 0.2773422364 0.2678750298 -1.7005511606

Complex3: cr_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_misc_misc_s_5.xyz

Cr -0.0015589609 -0.0010704381 -0.0017715375
 C 0.4731447606 3.2040531972 0.5142573602
 N 0.3068362123 2.0731282072 0.3338887699
 C 0.6814144554 4.6271225572 0.7403920278
 H 0.6524720554 5.1638379241 -0.2133863597
 H 1.6550943089 4.7906913273 1.2133969350
 H -0.1035449094 5.0187684786 1.3954627377
 C 3.2026465972 -0.5230576763 0.4758211575
 N 2.0721752415 -0.3407717221 0.3084720210
 C 4.6249124467 -0.7525524471 0.6859915059
 H 5.1627207145 0.2008013235 0.6649390532
 H 5.0180473128 -1.4012473362 -0.1034865728
 H 4.7856803346 -1.2322549251 1.6568871990
 C -0.4789028791 -3.2056991358 -0.5164800209
 N -0.3099337717 -2.0751146177 -0.3364384221
 C -0.6916381645 -4.6281421290 -0.7423488573
 H 0.2660520049 -5.1574930365 -0.7081571920
 H -1.1513888234 -4.7849611468 -1.7234927932
 H -1.3515779517 -5.0336157656 0.0314190669
 C -3.2047645538 0.5227380725 -0.4837251132
 N -2.0751045335 0.3389899156 -0.3125368687
 C -4.6259137678 0.7541449491 -0.6992609243
 H -5.2127644165 0.1257695348 -0.0214717908
 H -4.8905088231 0.5099926611 -1.7331626401
 H -4.8648536279 1.8052876832 -0.5080289237
 C -0.4041491304 -0.3615150767 2.4650269410
 N -0.5832287573 -0.5246554565 3.6053684218
 C -0.8025065895 -0.7233832918 5.0035933950
 H -0.3064530424 -1.6440723553 5.3202884944
 H -1.8757284335 -0.8004933149 5.1941377849
 H -0.3917169702 0.1240538679 5.5578176252

C 0.4028891134 0.3601398833 -2.4676869549
N 0.5858135616 0.5240574781 -3.6073005583
C 0.8101256007 0.7241387233 -5.0044473525
H 0.1558533981 0.0599839744 -5.5744265147
H 1.8537794999 0.5009359067 -5.2391463520
H 0.5912062300 1.7635541329 -5.2609979298

Complex4: cr_2_acetonitrile_acetonitrile_ammonia_ammonia_ammonia_ammonia_s_5.xyz

Cr -0.0903852009 0.0232760411 -0.0842621862
C -0.5172582816 3.2562256006 0.4157758920
N -0.3675504883 2.1196270104 0.2370198429
C -0.7043118245 4.6819757773 0.6407781729
H -1.0446768519 5.1635476210 -0.2822827650
H 0.2421910269 5.1361298940 0.9532207278
H -1.4538477877 4.8410841531 1.4235173833
C 3.7566827693 0.0788056991 -0.0861953630
N 2.5993898703 -0.0294533271 -0.0916645408
C 5.2089181965 0.2124787637 -0.0798384222
H 5.4890244737 1.2622686655 -0.2140501484
H 5.6430925802 -0.3782934939 -0.8930236158
H 5.6137407898 -0.1446126962 0.8726889197
N 0.2477484982 -2.1180074487 -0.3838807014
H 1.2587050650 -2.2731381975 -0.3933104706
H -0.1278381010 -2.7272965017 0.3459137115
H -0.1057601693 -2.5026473166 -1.2625328174
N -2.5404195568 -0.3419775982 -0.1318381636
H -2.9298356541 -0.8496279446 0.6655616632
H -3.0114503377 0.5649259470 -0.1218965315
H -2.9111602861 -0.8228710916 -0.9543426838
N 0.1647410209 -0.2371572356 2.0647273511
H -0.1759573448 0.5665245676 2.5965099346
H -0.2579306128 -1.0575956849 2.5041807801
H 1.1685902712 -0.2949152397 2.2551284186
N 0.1543002898 0.3996672216 -2.2146409661
H 1.1570075677 0.4716511013 -2.4066380456
H -0.2125129709 -0.2944519883 -2.8691482519
H -0.2513459268 1.2926535364 -2.5031086923

Complex5: cr_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_5.xyz

Cr -0.0019199427 -0.0007547103 -0.0023769720
N -0.2552115282 2.1470667354 0.3736345491
H -1.2428385435 2.3304358695 0.5432953803
H 0.2567225686 2.4578867979 1.1978794456
H 0.0198459290 2.7084978137 -0.4306629577
N 2.5690191425 0.3179805567 -0.1862545746
H 2.8458896582 1.2603391118 -0.4579175425
H 2.7943998801 0.2076479312 0.8019570196
H 3.1654111409 -0.3167107464 -0.7156362934
N 0.2547212217 -2.1486415235 -0.3751111865

H 1.2467642069 -2.3342583043 -0.5135627396
H -0.0485081848 -2.7154273748 0.4151212285
H -0.2313021410 -2.4514557481 -1.2179107684
N -2.5696606324 -0.3175530917 0.1893222139
H -2.8454251239 -1.2584258812 0.4672167975
H -3.1620036913 0.3198794398 0.7199704967
H -2.8023550327 -0.2114209201 -0.7976562834
C 0.4308513509 -0.3001693891 2.0639536789
N 0.7920704109 -0.4252251481 3.1714985490
C -0.4304086320 0.3007441422 -2.0688833809
N -0.7859972131 0.4295834091 -3.1778224538

Complex6: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_ammonia_s_5.xyz

Cr 0.0190725134 0.0370044267 -0.1009910688
C -0.3694580763 2.2868253002 -0.4022238538
O -0.5661983915 3.3855404191 -0.5432572626
C 2.5794890844 0.4543854242 -0.3920927116
O 3.6836766577 0.6455258558 -0.5100088604
C 0.3860766524 -2.2027662629 0.2983656837
O 0.5593592166 -3.2952129006 0.5042995411
C -2.5240281335 -0.3329901603 0.3878608680
O -3.6158879574 -0.4815676664 0.6237614982
C 0.3062364758 0.4154385950 2.1006029725
O 0.4553051845 0.6067019722 3.1985059077
N -0.1938877289 -0.3279935506 -2.1749314962
H -1.1677595199 -0.5071251798 -2.4468481340
H 0.1113755749 0.4550402056 -2.7644936903
H 0.3366460983 -1.1386638461 -2.5148664207

Complex7: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_s_5.xyz

Cr -0.0004068730 -0.0004010599 0.1633471978
C -0.0006132738 2.3943259801 0.0150566756
O -0.0004038138 3.4959939441 -0.2311683998
C 2.3908541985 -0.0006137082 0.0146914322
O 3.4926387912 -0.0004172707 -0.2309320290
C -0.0007040608 -2.3942067235 0.0090911279
O -0.0007290205 -3.4953100633 -0.2396429048
C -2.3907651715 -0.0006877369 0.0087039747
O -3.4919882408 -0.0007156298 -0.2394208856
C -0.0021234368 -0.0020559808 2.4023482065
O -0.0038143958 -0.0037131203 3.5300558607
C 0.0028407176 0.0027534103 -1.8247361386
N 0.0052147348 0.0050502286 -2.9951668568

Complex8: cr_2_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_5.xyz

Cr 0.0374776793 0.0384311887 0.0995428843
C -0.3710042881 2.5251428714 0.4615322949

O -0.5250677203 3.6436783228 0.4327951639
C 2.3194351404 0.3888774544 0.4170892728
O 3.4304388777 0.5871828802 0.4202682632
C 0.4394746997 -2.4449638179 -0.2864909730
O 0.6305798167 -3.4886100431 -0.6737838689
C -2.2260861081 -0.2877156774 -0.3465603767
O -3.2903020749 -0.4300941007 -0.6940035102
C -0.2929025190 -0.3290012405 2.3016922185
O -0.4574637378 -0.5184884280 3.4020990329
F 0.3054150231 0.3155654671 -1.6114031754

Complex9: cr_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_s_5

Cr 0.3885260383 -0.0377247887 -0.0252199160
S 0.8176353901 2.8206752982 -0.5586093501
H 1.6401553276 3.4201333582 0.3280809422
H 1.7164003537 2.8587508964 -1.5641500728
S 2.9372511457 -0.4817520279 -0.4417304103
H 2.9975079516 -1.8185477740 -0.6299987412
H 3.4923017319 -0.5275996544 0.7891392633
S 0.0362453820 -2.9559026304 0.4338216020
H -1.2400142023 -3.3805523474 0.3263157157
H 0.1703209298 -3.3637242724 1.7133333180
S -2.1620433859 0.4221673805 0.3420408263
H -2.7718316868 -0.2944539885 -0.6259294952
H -2.3515412061 1.6095185429 -0.2750865545
S 0.8014263817 0.3229432131 2.5094312731
H 0.3356547335 1.5632358409 2.7741903070
H -0.2466909906 -0.3047036678 3.0857040140
C 0.1145319275 -0.3758159550 -2.1189089698
N -0.0082184408 -0.5584253687 -3.2575853318
C -0.1498563632 -0.7850551157 -4.6667729356
H -0.2039497923 -1.8619681473 -4.8457876616
H 0.7181332103 -0.3617971914 -5.1787274984
H -1.0652123154 -0.2982679560 -5.0126163384

Complex10: cr_2_misc_misc_misc_misc_misc_misc_s_5.xyz

Cr 0.0000330616 0.0036449970 -0.0019100188
C 0.0018135785 2.3593011455 -0.0017311797
N 0.0052226461 3.5233429615 -0.0012771219
C 0.0103316132 4.9531037016 -0.0003123529
H 0.8472920482 5.3098328330 -0.6054414508
H 0.1187534052 5.3110325473 1.0263492846
H -0.9305980836 5.3165720122 -0.4204078437
C 2.3519376893 0.0031789464 -0.0012086471
N 3.5159236110 0.0013265745 0.0006542699
C 4.9456935564 -0.0018404062 0.0036380051
H 5.3043815916 -0.8381131356 -0.6012835183
H 5.3022309630 -0.1101308151 1.0307957688
H 5.3084345477 0.9397505268 -0.4156057303

C -0.0017484478 -2.3521548347 -0.0018861669
 N -0.0052074954 -3.5161976319 -0.0014751955
 C -0.0104642406 -4.9459632974 -0.0004679997
 H -0.8473225087 -5.3026196489 -0.6057811335
 H -0.1191928660 -5.3038364593 1.0261819370
 H 0.9305289791 -5.3095444753 -0.4203199860
 C -2.3518203673 0.0024542146 -0.0013112932
 N -3.5158020427 -0.0004275236 0.0001186526
 C -4.9455027432 -0.0047156794 0.0021844175
 H -5.3077869102 0.9841282536 0.2934497787
 H -5.3015648548 -0.7532251738 0.7141542142
 H -5.3054522920 -0.2489077835 -1.0001959853
 C -0.0003339817 0.0026215743 2.1388962643
 N -0.0010766981 0.0002574382 3.2995240421
 C -0.0027441120 -0.0038780110 4.7292343751
 H 0.6030873094 -0.8411410922 5.0840347764
 H -1.0304712454 -0.1120993230 5.0841061390
 H 0.4177754083 0.9380856099 5.0894885027
 C 0.0003927039 0.0031031721 -2.1426171281
 N 0.0011489639 0.0012372145 -3.3032344011
 C 0.0028099830 -0.0022656361 -4.7329430826
 H -0.6033687968 -0.8391270437 -5.0880931196
 H 1.0304876631 -0.1108569509 -5.0878426332
 H -0.4172637279 0.9400736916 -5.0927402290

Complex11: cr_2_phosphine_phosphine_phosphine_phosphine_hydrogensulfide_hydrogensulfide_s_5.xyz

Cr 0.0513286527 0.0879911667 0.0048402972
 P 0.4512348596 2.6642646188 0.3340794947
 H 0.0642045925 3.2621485715 1.5504662186
 H 1.7805055393 3.1239662186 0.2431858261
 H -0.1676564754 3.5377713548 -0.5823817458
 P 2.3143369194 -0.3712240389 1.2644091871
 H 2.5475481614 0.3772669981 2.4356095742
 H 2.5508503675 -1.6698545969 1.7581393339
 H 3.5236569989 -0.1420060937 0.5774259978
 P -0.2459936929 -2.4792914384 -0.4475983536
 H 0.9153928551 -3.2021117427 -0.7865774764
 H -0.7514720389 -3.3008512862 0.5809480568
 H -1.0885352732 -2.8702400019 -1.5078414566
 P -2.2755266416 0.5875586300 -1.1078480240
 H -3.2390941241 -0.4412188201 -1.1003995374
 H -3.0389271879 1.6325284028 -0.5494028027
 H -2.3227098830 0.9542779749 -2.4686199519
 S -1.2079401291 -0.2775812139 2.6785009943
 H -2.3504963149 -0.9942846184 2.6414485006
 H -1.8035084907 0.8373186363 3.1502327385
 S 1.4054360515 0.5287407330 -2.6084262597
 H 0.7977784771 -0.0820586259 -3.6467113177
 H 2.5668014475 -0.1408301800 -2.7620189917

Complex12: cr_2_phosphine_phosphine_phosphine_phosphine_phosphine_ammonia_s_5.xyz

Cr -0.0366138947 -0.0261419108 -0.0590822495
P -0.4002125988 2.6264241941 -0.3582883065
H -1.6472597367 3.1976638181 -0.0281318376
H 0.4467301280 3.5028613406 0.3517139928
H -0.2404125029 3.1684086038 -1.6520120568
P 2.9231872974 0.3926393915 -0.5413860839
H 3.5279089227 1.6318282951 -0.2275430918
H 3.8483759985 -0.4350429355 0.1355298566
H 3.4768959614 0.2504195851 -1.8356438271
P 0.4223147944 -2.6555368266 0.3393431230
H 1.6716284570 -3.0496103626 0.8622913417
H -0.4269250887 -3.3494240971 1.2266006769
H 0.3570808091 -3.5368881207 -0.7618789563
P -2.9504247702 -0.4868435513 0.4716633226
H -3.5351905824 -1.7496446640 0.2210684504
H -3.4333949338 -0.3248993541 1.7906249458
H -3.9324889078 0.2993259016 -0.1745170835
P 0.3335731470 0.3773313441 2.5055888962
H 1.5801981020 0.8848567597 2.9243048168
H -0.5264131292 1.2898495664 3.1500118571
H 0.2141923041 -0.7179932255 3.3851327812
N -0.3747218984 -0.2769536344 -2.1659600274
H -1.2189726548 0.1885146693 -2.5102928811
H 0.3979423674 0.0753646749 -2.7376207207
H -0.4818218128 -1.2614212483 -2.4231533046

Complex13: cr_2_water_water_water_water_ammonia_ammonia_s_5.xyz

Cr -0.0001424301 0.0000310167 0.0008999513
O -0.3915694201 2.0763876522 0.1851878976
H 0.1860974867 2.8126078411 0.4504092103
H -1.3043163464 2.3026190725 0.4376714712
O 2.4430225131 -0.0331152569 -0.3917983379
H 2.8980685626 0.2094504615 -1.2170452134
H 3.1422712852 -0.0000033970 0.2841786694
O 0.3910686782 -2.0763819846 -0.1837274957
H 1.3058607298 -2.3008257871 -0.4304125111
H -0.1839702836 -2.8121666772 -0.4557412498
O -2.4435041814 0.0329766109 0.3909234457
H -2.9010380215 -0.2228537764 1.2107894086
H -3.1407370159 0.0112717564 -0.2875729506
N 0.3471927641 -0.2536938286 2.1220866810
H -0.4204250676 0.0577781826 2.7226205559
H 0.4745925664 -1.2491841605 2.3251138234
H 1.1786594285 0.2164891540 2.4899681508
N -0.3473684321 0.2536844989 -2.1205275292
H -0.4744523639 1.2492333632 -2.3234282558
H 0.4198333686 -0.0581846278 -2.7213532074
H -1.1791492408 -0.2161058726 -2.4882177674

Complex14: cr_2_water_water_water_water_carbonyl_carbonyl_s_5.xyz

Cr -0.0007424675 -0.0015114743 0.0011250175
O -0.2792420800 2.0133080985 0.3526606210
H 0.3636732811 2.7393056834 0.2622317017
H -1.1616900458 2.4089586051 0.4690297175
O 2.0579284620 0.2628435760 -0.3228029251
H 2.4799020788 0.4536781124 -1.1804260240
H 2.7364717174 0.3851650310 0.3661071510
O 0.2789075771 -2.0169036082 -0.3478235291
H 1.1593586095 -2.4143332331 -0.4727589542
H -0.3658470484 -2.7420940758 -0.2643545558
O -2.0604197041 -0.2609385426 0.3228088840
H -2.4808435232 -0.4595176211 1.1795066149
H -2.7379146141 -0.3875821149 -0.3664080972
C 0.4384982448 -0.3883540027 2.6390478175
O 0.6500665936 -0.5384331575 3.7371877950
C -0.4363865738 0.3936160262 -2.6386185331
O -0.6415063544 0.5530746965 -3.7366616750

Complex15: fe_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_5.xyz

Fe -0.0771820548 -0.0742474017 -0.0147254632
C 0.4195697121 3.2207972265 -0.5170408645
N 0.2438109584 2.0855562963 -0.3699059128
C 0.6408891249 4.6494978927 -0.7014273135
H 0.3020456505 4.9545712812 -1.6967714001
H 1.7065435489 4.8790551159 -0.6021710270
H 0.0819642474 5.2137799031 0.0519525565
C 3.2085882959 -0.6166767897 -0.5026475572
N 2.0745243901 -0.4300288785 -0.3592998287
C 4.6353958199 -0.8521449414 -0.6829316165
H 5.1520443450 0.0954169649 -0.8656047934
H 4.7992934999 -1.5183617441 -1.5361152296
H 5.0516991898 -1.3182269210 0.2159799198
C -0.5654899141 -3.3611820447 0.5118193080
N -0.4003378794 -2.2330740506 0.3074361961
C -0.7729004242 -4.7803431083 0.7698040615
H 0.1824884011 -5.3127213810 0.7257689962
H -1.4509400009 -5.2012712945 0.0203375013
H -1.2128504885 -4.9172275231 1.7628878884
C -3.3642057087 0.4543108616 0.4974164376
N -2.2375553411 0.2753880454 0.2969582397
C -4.7817618439 0.6788715146 0.7502145957
H -5.1064938733 0.0814755965 1.6081871316
H -5.3682737725 0.3871890443 -0.1270805209
H -4.9616379499 1.7374475676 0.9629368908
C 0.4638130267 0.4079266631 3.2638599390
N 0.2753428360 0.2362466299 2.1346697955
C 0.7013045321 0.6238335822 4.6844691131
H -0.2310405139 0.4916516706 5.2427465650

H 1.0757040586 1.6392805315 4.8494265163
H 1.4421881401 -0.0937314452 5.0515276817
N -0.4346235449 -0.3152197029 -2.1552558138
H -1.2787221050 0.1693994761 -2.4643977133
H 0.3381641139 0.0424713973 -2.7186600623
H -0.5507999112 -1.2995048790 -2.4013071995

Complex16: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_chloride_chloride_s_5.xyz

Fe 0.0003313882 0.0000785164 -0.0050851257
C 0.3650891008 2.3179477564 0.3682849911
O 0.4650612525 3.4361810449 0.5139488575
C 2.3192379947 -0.3782255790 0.3462919340
O 3.4082983793 -0.6383306020 0.5140920349
C -0.3654030877 -2.3178658008 -0.3750800847
O -0.4669373227 -3.4365384052 -0.5161885474
C -2.3186533482 0.3778321350 -0.3552856078
O -3.4077039843 0.6383513684 -0.5225077211
Cl -0.3739418769 -0.3555371035 2.2872317957
Cl 0.3746197757 0.3561045388 -2.2969248480

Complex17: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_cyanide_cyanide_s_5.xyz

Fe 0.0000152827 0.0000115833 0.0000071834
C -0.0001059269 2.5103117083 -0.0003351661
O 0.0001608665 3.6418786118 -0.0004637778
C 2.4925738502 -0.0006251748 -0.0000030940
O 3.6249273216 -0.0005565957 -0.0000167784
C 0.0000727245 -2.5102902776 0.0003633833
O -0.0002421604 -3.6418572509 0.0005050383
C -2.4925500293 0.0005846142 0.0000138409
O -3.6249038270 0.0004722219 0.0000198287
C 0.0000144456 0.0004415411 2.0293390994
N 0.0000123290 0.0007567067 3.1988440634
C 0.0000132307 -0.0004096259 -2.0293839402
N 0.0000123362 -0.0007181318 -3.1988894056

Complex18: fe_2_carbonyl_carbonyl_carbonyl_carbonyl_hydrogensulfide_hydrogensulfide_s_5.xyz

Fe -0.0744183172 -0.0932745765 0.0138270399
C -0.4196271443 2.1454079731 -0.3387710126
O -0.5897099471 3.2398741016 -0.5432185920
C 2.1674822717 0.2647749235 0.3251658687
O 3.2645289566 0.4421953335 0.5085032591
C 0.2519303144 -2.3523620903 0.3456648010
O 0.4173478684 -3.4575125893 0.4820411381
C -2.3296275783 -0.4797732961 -0.2787387523
O -3.4322725398 -0.6755940983 -0.3937779522
S -0.5723962443 0.2572294477 2.6147541852
H 0.2827805190 -0.5902564512 3.2310875466

H 0.1260275067 1.3701426369 2.9356254860
S 0.3339382560 -0.5432615058 -2.5876560067
H -0.6896514474 0.0995715287 -3.1947662983
H 1.2636844252 0.3728567664 -2.9422108519

Complex19: fe_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_misc_misc_s_5.xyz

Fe -0.0366376773 0.0371472148 -0.0092617289
S 0.2833183081 2.6762113610 -0.5177634402
H -0.5768439931 3.2774923792 0.3321118334
H 1.3824756633 3.0089020713 0.1923233956
S 2.6531101961 -0.1278260471 -0.3388659164
H 3.1114551386 -1.1224833111 0.4486257149
H 2.9065026927 -0.7753927299 -1.4947471223
S -0.5221507168 -2.6136289296 0.3489175709
H 0.2201587898 -2.9678010262 1.4194593296
H 0.2774952438 -3.2425994163 -0.5385484755
S -2.6618146561 0.5476629093 0.3971823257
H -3.0591309044 -0.3402166426 1.3325394093
H -3.3164597395 -0.0655610381 -0.6106151700
C 0.2973334182 0.3370399679 2.1147754926
N 0.4660734592 0.5136857859 3.2500801784
C 0.6735401323 0.7407514692 4.6508190998
H 0.9968814031 -0.1934068962 5.1167434910
H -0.2648645898 1.0773165254 5.0982332275
H 1.4443344618 1.5055307619 4.7742142498
C -0.3760767196 -0.2440558564 -2.1320308084
N -0.5610899324 -0.3273229785 -3.2750755607
C -0.7914988900 -0.4106520777 -4.6876373491
H -1.6259466432 -1.0918885210 -4.8713912602
H 0.1126642828 -0.7845070309 -5.1740335624
H -1.0327359628 0.5872281236 -5.0626722438

Complex20: fe_2_misc_misc_misc_misc_misc_acetonitrile_s_5.xyz

Fe -0.0069164298 -0.0092830371 0.0349541608
C 0.3146275419 2.2123564336 0.3834544219
N 0.4607992968 3.3533938694 0.5479385307
C 0.6399454695 4.7574505561 0.7501738973
H 1.5943926809 5.0629848481 0.3147636567
H 0.6377774442 4.9682058779 1.8222936248
H -0.1775287928 5.2962537587 0.2651034747
C 2.1983199799 -0.3596616157 0.3138031390
N 3.3348897367 -0.5552436115 0.4623096975
C 4.7324987945 -0.7942486504 0.6452979878
H 5.0938552156 -1.4406091782 -0.1581735188
H 4.8913978567 -1.2798071318 1.6110761610
H 5.2650968668 0.1594942164 0.6187662556
C -0.3250720334 -2.2216443687 -0.3630650969
N -0.4741849426 -3.3587061414 -0.5506127544
C -0.6584853292 -4.7576146165 -0.7821203453

H -1.4055164151 -4.8949185090 -1.5675320018
 H -1.0000856291 -5.2314510278 0.1412470541
 H 0.2920990906 -5.1968555115 -1.0940614476
 C -2.1995701705 0.3579916043 -0.3117910042
 N -3.3312656558 0.5628329346 -0.4833488737
 C -4.7231762585 0.8135876350 -0.6924116632
 H -4.9917383329 1.7600178940 -0.2168738032
 H -5.3045338380 0.0008611152 -0.2503473239
 H -4.9215123756 0.8695715373 -1.7653922625
 C -0.3568056007 -0.3318173257 2.2225582531
 N -0.5341661439 -0.5079899327 3.3584134744
 C -0.7515963094 -0.7243086933 4.7547377735
 H -0.3085935538 -1.6803171265 5.0440046071
 H -1.8259247305 -0.7383069304 4.9535168437
 H -0.2826214510 0.0853287938 5.3192469680
 C 0.5316291691 0.4902956937 -3.2766038084
 N 0.3458132821 0.3152734922 -2.1470988621
 C 0.7659810998 0.7115043311 -4.6979602917
 H 1.0981902840 -0.2179903299 -5.1711944699
 H 1.5388971318 1.4748321117 -4.8334999895
 H -0.1560190443 1.0487453811 -5.1820013768

Complex21: fe_2_misc_misc_misc_misc_misc_carbonyl_s_5.xyz

Fe 0.0747533284 0.0655376544 0.1778787164
 C 0.4087116363 2.2727422459 0.4507753224
 N 0.5577705276 3.4152032233 0.5986200801
 C 0.7421826934 4.8229745910 0.7773599405
 H 1.5439503251 5.1636356737 0.1177670444
 H 1.0079540159 5.0186134236 1.8189202313
 H -0.1882209556 5.3385156298 0.5274691522
 C 2.2870413053 -0.2789099285 0.3874788550
 N 3.4259902537 -0.4754674971 0.5027655929
 C 4.8298361964 -0.7158066113 0.6404577094
 H 5.1702360908 -1.3286483869 -0.1976906831
 H 5.0121516707 -1.2380538633 1.5826642889
 H 5.3564131770 0.2416253550 0.6377710122
 C -0.2275280853 -2.1130476497 -0.2813966130
 N -0.3623484791 -3.2458779142 -0.4999173327
 C -0.5271006756 -4.6413890729 -0.7697911196
 H -1.4994884075 -4.8004324853 -1.2421182433
 H -0.4752755732 -5.1949340890 0.1707801139
 H 0.2696023920 -4.9712193922 -1.4409176066
 C -2.1055942028 0.4402196337 -0.2282816741
 N -3.2307485189 0.6515300584 -0.4245814327
 C -4.6158262776 0.9126174974 -0.6716481088
 H -4.9545966745 1.7050747349 -0.0000477461
 H -5.1884304758 0.0001895173 -0.4887436057
 H -4.7390207386 1.2269513027 -1.7108854241
 C -0.2772694002 -0.2503794422 2.3408620691
 N -0.4621560959 -0.4156953084 3.4761397208
 C -0.6904635982 -0.6189357921 4.8734418455

H 0.0830763484 -1.2803315387 5.2707954267
H -1.6742656105 -1.0742134746 5.0111784841
H -0.6544992295 0.3454701774 5.3857904889
C 0.4625824632 0.4223389067 -2.1877552813
O 0.6526111680 0.5972564726 -3.2879035739

Complex22: fe_2_misc_misc_misc_misc_misc_cyanide_s_5.xyz

Fe -0.0366829896 0.0376049915 0.3979342646
C -0.3583087294 2.2436392229 0.7572411491
N -0.5641421477 3.3873416689 0.6691283705
C -0.8245844063 4.7767123725 0.4915853252
H -0.9251872958 4.9873727664 -0.5763915713
H 0.0030419396 5.3591794282 0.9042280955
H -1.7508689162 5.0429847892 1.0068638538
C 2.1657274860 0.4059231606 0.0607516745
N 3.2186804709 0.6271577165 -0.3871576489
C 4.4726007024 0.9037272861 -1.0043165797
H 4.3319484595 0.9614127594 -2.0868928561
H 5.1804493084 0.1053214610 -0.7677468939
H 4.8594577356 1.8562506783 -0.6335459492
C 0.2887795284 -2.1694838576 0.0321410795
N 0.4100629209 -3.2388430958 -0.4150881943
C 0.5441328004 -4.5188400371 -1.0260004924
H 0.2445659788 -4.4470448970 -2.0749092565
H -0.0957153638 -5.2390251179 -0.5098539371
H 1.5852784468 -4.8453959041 -0.9641187118
C -2.2432189478 -0.3309198198 0.7211477766
N -3.3949310545 -0.4754490341 0.6167716267
C -4.7962496747 -0.6396678247 0.4194353654
H -5.3396036264 0.0654727620 1.0534849850
H -5.0845325466 -1.6613797537 0.6792426033
H -5.0339098766 -0.4478407732 -0.6302738404
C 0.3441193228 -0.2940962834 2.6788424355
N 0.5317043501 -0.4599867417 3.8160125660
C 0.7617780293 -0.6634277327 5.2083281178
H 1.7451166281 -1.1187351911 5.3498380719
H -0.0099830090 -1.3248892204 5.6097288449
H 0.7253939631 0.2986561188 5.7253963559
C -0.3822388195 0.3261337957 -1.6336593436
N -0.5727038312 0.4901524131 -2.7763812419

Complex23: fe_2_water_water_water_water_water_chloride_s_5.xyz

Fe 0.0113755799 -0.0548701995 0.1183862813
O 0.6450194908 2.0481541160 -0.2381396809
H 0.7400034019 2.1018437971 -1.2088892712
H 0.1736689141 2.8505304832 0.0415295964
O 2.1384829452 -0.1441931826 0.7970135280
H 2.5869286579 0.5885389636 0.3396400053
H 2.6728018257 -0.9354202028 0.6128233772

O -0.4345089297 -2.1535522330 0.6079211536
H 0.0459575725 -2.7535180154 0.0105639089
H -1.3765130153 -2.2991678729 0.4068759500
O -2.1724066950 0.0120787192 -0.2780145797
H -2.7679282526 0.7248435350 0.0080185730
H -2.2317404368 -0.0219713108 -1.2525481435
O -0.2943201915 0.3607596013 2.1802371692
H 0.5909303419 0.4808703246 2.5725055312
H -0.6870714406 -0.3865156156 2.6652100273
Cl 0.3565777846 -0.4180828285 -2.1332820275

Complex24: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_ammonia_s_5.xyz
Mn -0.0687093646 -0.0570902800 0.0446432855
C 0.4061107354 3.1957676829 -0.4841364208
N 0.2354381572 2.0559940613 -0.3371543902
C 0.6195263327 4.6206179201 -0.6706921520
H 0.2488693005 4.9280067801 -1.6558067735
H 1.6896290280 4.8491853957 -0.6037581091
H 0.0833492858 5.1819480726 0.1035045577
C 3.0915888341 -0.5918281822 -0.4437106122
N 1.9544212724 -0.3990622518 -0.3051982696
C 4.5114046824 -0.8319496599 -0.6225133498
H 5.0253594554 0.1132903860 -0.8351083265
H 4.6696393658 -1.5231286676 -1.4594445039
H 4.9313398615 -1.2724988109 0.2898834545
C -0.5621697658 -3.3198600964 0.4957635428
N -0.3946322003 -2.1871811685 0.2972509027
C -0.7712852754 -4.7366443878 0.7386491151
H 0.1870143732 -5.2675427627 0.6976214339
H -1.4429070913 -5.1506189857 -0.0228797704
H -1.2204747597 -4.8823667039 1.7280921541
C -3.2402923922 0.4422645546 0.5105086145
N -2.1105058261 0.2653543843 0.3059006934
C -4.6524678677 0.6632698721 0.7605103627
H -4.9707964297 0.0812810564 1.6338820456
H -5.2387137509 0.3486870110 -0.1116656547
H -4.8351394613 1.7278646287 0.9503517951
C 0.4387856752 0.3605594380 3.1056629448
N 0.2488890964 0.2036684615 1.9709486247
C 0.6767104429 0.5558867968 4.5216025038
H -0.2458652759 0.3629726191 5.0832362625
H 1.0008903648 1.5880746703 4.7041952131
H 1.4580968221 -0.1337843078 4.8645764789
N -0.3869157966 -0.2669207771 -1.9345830042
H -1.2615962115 0.1873702182 -2.2169376231
H 0.3768813893 0.1498762148 -2.4763327614
H -0.4508078037 -1.2610876578 -2.1776939748

Complex25: mn_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_carbonyl_s_5.xyz

Mn -0.0060241362 -0.0059768416 0.3940823295
C 0.4721351536 3.0745978139 0.0648752521
N 0.2966026101 1.9323037026 0.1837048499
C 0.6885213566 4.4982092555 -0.0861883785
H 0.4792969769 4.7966359175 -1.1216480484
H 1.7300701831 4.7440099898 0.1568731020
H 0.0214531541 5.0479449397 0.5901716671
C 3.0740706894 -0.4924133562 0.0730986232
N 1.9321579455 -0.3116261089 0.1877274885
C 4.4970142255 -0.7175791059 -0.0710600300
H 5.0248609354 0.2443200044 -0.0931587421
H 4.6945545245 -1.2585995119 -1.0054577614
H 4.8650690910 -1.3112271000 0.7756073080
C -0.4939064759 -3.0896447025 0.1211032993
N -0.3124112602 -1.9462505150 0.2187901403
C -0.7200106523 -4.5143030411 -0.0023703122
H 0.2412668947 -5.0437368619 -0.0083656835
H -1.2538542730 -4.7256906608 -0.9378969462
H -1.3211371343 -4.8681534615 0.8450940438
C -3.0900889034 0.4742727678 0.1106656550
N -1.9463816437 0.2977591786 0.2136409487
C -4.5153513462 0.6918857839 -0.0209922418
H -5.0569927740 0.0156214652 0.6527827924
H -4.8256476622 0.4959915472 -1.0556086698
H -4.7587464607 1.7300711721 0.2384273660
C 0.0432921442 0.0383579736 3.6943318856
N 0.0244226777 0.0218839924 2.5318105983
C 0.0651213510 0.0570757545 5.1454709443
H -0.9467596170 -0.1070067121 5.5348801120
H 0.4329462229 1.0270767078 5.5005378440
H 0.7252812109 -0.7351593902 5.5182321254
C -0.0274772766 -0.0271633863 -2.2809876814
O -0.0327654050 -0.0332123629 -3.4092858555

Complex26: mn_3_ammonia_ammonia_ammonia_ammonia_ammonia_acetonitrile_s_5.xyz

Mn 0.0895799802 -0.1014849756 -0.0168164114
N -0.1285128733 1.9764523947 0.2615207412
H -1.1110960904 2.2724349578 0.2964661697
H 0.2985375977 2.3446581429 1.1204943274
H 0.2773912666 2.5045617897 -0.5209057588
N 2.1624155797 0.1566911155 -0.2848332448
H 2.5192477269 1.0581092872 0.0546034923
H 2.7494892610 -0.5513778455 0.1734668216
H 2.3959502444 0.1298877061 -1.2855281222
N 0.2721640527 -2.1583845494 -0.4413405155
H 1.2276125671 -2.4378556214 -0.6942471469
H -0.0009514141 -2.7946549502 0.3179220686
H -0.3011866778 -2.4100755359 -1.2563936074
N -1.9842746473 -0.3463587123 0.2683578719
H -2.2625782033 -1.3289666650 0.3749928792
H -2.3708307275 0.1294899933 1.0929451657

H -2.5107455009 0.0015602984 -0.5432475597
N 0.4690364268 -0.4005568455 2.2897819551
H -0.2977156278 -0.1018861922 2.9034547806
H 0.6236258722 -1.3793742319 2.5570154319
H 1.2898766884 0.0848944791 2.6701919582
C -0.4247835940 0.4137973137 -3.3538650011
N -0.2496178280 0.2369016352 -2.2140227169
C -0.6421580874 0.6335471233 -4.7712808181
H 0.3155914555 0.5964571104 -5.3063970177
H -1.1036064573 1.6166368688 -4.9311080143
H -1.3060900451 -0.1429467072 -5.1728642350

Complex27: mn_3_ammonia_ammonia_ammonia_ammonia_water_s_5.xyz

Mn -0.0098335939 -0.0030923506 0.1256357690
N -0.2989312312 2.0543385536 -0.0474926185
H -1.1131531091 2.4302834173 0.4564039825
H 0.4883192640 2.6354540360 0.2688301779
H -0.4423247216 2.2761304532 -1.0427833084
N 2.0527153902 0.2163398808 -0.3130978077
H 2.2976602536 1.1281471722 -0.7201135482
H 2.6356606176 0.1376169911 0.5309036758
H 2.4303476954 -0.4741415883 -0.9751429922
N 0.2075789900 -2.0701478739 -0.0099701051
H 1.1507475784 -2.4133107523 0.2124883240
H -0.4201552648 -2.6181135943 0.5933661001
H 0.0206351495 -2.3686379274 -0.9778633010
N -2.0976957503 -0.2897100160 0.3169740361
H -2.4484171085 -1.1326398042 -0.1566644829
H -2.3973084328 -0.3861737899 1.2964940100
H -2.6665755503 0.4771115400 -0.0647811641
N 0.4068686030 0.0896237117 2.4004962797
H -0.4390463626 0.1047777935 2.9829963506
H 0.9486257650 -0.6953086613 2.7834271569
H 0.9215660796 0.9231703254 2.7108034779
O -0.3533451277 -0.0020139410 -2.2331189729
H -1.1970967567 -0.0536829856 -2.7246208631
H 0.3221623529 0.0350219587 -2.9387542033

Complex28: mn_3_ammonia_ammonia_ammonia_ammonia_phosphine_phosphine_s_5.xyz

Mn 0.0052526361 0.0043897260 0.0323166399
N -0.1476169068 2.0811777536 0.4722253608
H -1.0001028098 2.3242131511 0.9908710780
H 0.6333453685 2.4568394473 1.0233555906
H -0.1776711038 2.6602561624 -0.3751224189
N 2.2889252790 0.2646274336 -0.4343051621
H 2.5331374003 1.2121053467 -0.7438721733
H 2.9202070335 0.0991427754 0.3577043975
H 2.6569651338 -0.3401832916 -1.1771105164
N 0.2361519379 -2.0996729233 -0.2078065533

H 1.1533060427 -2.4368391123 0.1074278717
H -0.4611660457 -2.6594492636 0.2970473396
H 0.1672332614 -2.4004368389 -1.1870140879
N -2.3125476686 -0.2660881447 0.2672657756
H -2.6960441893 -1.0982971891 -0.1950411815
H -2.6421750405 -0.3513156252 1.2354849575
H -2.8719068189 0.5043035040 -0.1163153853
P 0.4199894097 -0.3776854094 2.6728161398
H 1.6061156871 0.1965269333 3.1724701673
H -0.5852862518 0.1572771113 3.5030545891
H 0.5047210925 -1.7246642995 3.0782279967
P -0.4736553789 0.3934339937 -2.6235282278
H 0.6554056881 0.3856762425 -3.4670100695
H -1.3255422713 -0.5639106647 -3.2108774223
H -1.1057815683 1.6128651097 -2.9416815692

Complex29: mn_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_s_5.xyz

Mn -0.0546702050 -0.0547436128 -0.0176966813
C -0.0770306784 2.2520900567 -0.3366403165
O -0.1018363576 3.3501550608 -0.5724772016
C 2.2514738724 -0.0765877902 -0.3374918347
O 3.3494331414 -0.1010917955 -0.5738575557
C -0.0057594090 -2.3451115585 0.3892201413
O 0.0050161051 -3.4629913320 0.4989200173
C -2.3446084407 -0.0065711146 0.3883148046
O -3.4625118212 0.0038206560 0.4978242541
C 0.2891788377 0.2894823610 2.1405531911
O 0.4645334390 0.4651918838 3.2348677979
F -0.3131846710 -0.3136240275 -1.6442809718

Complex30: mn_3_cyanide_cyanide_ammonia_ammonia_ammonia_ammonia_s_5.xyz

Mn -0.0480175677 -0.0189224619 0.0116958261
C -0.2665343225 1.9095417032 0.3372407913
N -0.5309573870 3.0295993411 0.5370460773
C 1.8774722364 0.2970520647 -0.2391640852
N 3.0315231944 0.3308391218 -0.4182813698
N 0.2716070228 -2.1188147850 -0.3678325732
H 1.2784513084 -2.2223696284 -0.5154063665
H 0.0247917189 -2.7371013937 0.4068382803
H -0.1857581473 -2.4807098138 -1.2064727440
N -2.1770449141 -0.1686045357 0.2848274484
H -2.6230889283 -1.0532326034 0.0346729800
H -2.4080221035 0.0144021690 1.2631257053
H -2.6391638463 0.5669538451 -0.2534256594
N 0.3147138663 -0.3772775058 2.3332576962
H 0.1961620323 0.5564420343 2.7342324000
H -0.1566441244 -1.0277811516 2.9645081796
H 1.3163469613 -0.5671350268 2.4151246543
N -0.3880637651 0.3511476821 -2.3148677974

H -0.5921698683 1.3526659077 -2.3588564424
H 0.5382196644 0.2580533960 -2.7376148615
H -1.0469457480 -0.1078868664 -2.9462372878

Complex31: mn_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_5.xyz

Mn 0.0013760762 -0.0001114961 -0.0008451757
C 0.0035395174 2.0749576888 -0.0007703127
N 0.0072303887 3.2309581231 -0.0007789269
C 0.0133941923 4.6669169761 0.0002105401
H 0.8532880598 5.0120295441 -0.6089445596
H 0.1226980864 5.0141174666 1.0311394728
H -0.9312201470 5.0201143139 -0.4224031877
C 2.0764461849 -0.0017082735 -0.0000393775
N 3.2324503288 -0.0045976166 0.0011488581
C 4.6684129433 -0.0095489359 0.0037047366
H 5.0149359640 -0.8484290491 -0.6060453675
H 5.0145515936 -0.1197370794 1.0348947973
H 5.0212820864 0.9359158875 -0.4172761194
C 0.0008001025 -2.0751661725 -0.0014227787
N -0.0006430397 -3.2311682598 -0.0013462901
C -0.0037305909 -4.6671376861 0.0000555418
H -0.8428607962 -5.0142619271 -0.6090078650
H -0.1121932656 -5.0142380448 1.0311076956
H 0.9417133982 -5.0184067401 -0.4223105659
C -2.0737319104 -0.0008878903 0.0002022019
N -3.2297339119 -0.0034575974 0.0023835811
C -4.6656118495 -0.0083202982 0.0052689904
H -5.0171459533 0.9847743218 0.2982362969
H -5.0100429184 -0.7588419303 0.7219636404
H -5.0154957807 -0.2536227093 -1.0011139870
C -0.0083073292 0.0016645946 3.4143377426
N -0.0017270222 0.0000887197 2.2524761641
C -0.0175969719 0.0037089033 4.8680660738
H -0.5347525816 -0.8884625429 5.2392813181
H -0.5359576513 0.8962511405 5.2367132105
H 1.0101798990 0.0048902718 5.2486970743
C 0.0015113050 0.0052176445 -3.4156029809
N 0.0016014615 0.0017095551 -2.2537229503
C 0.0015370475 0.0099164552 -4.8693645625
H -0.3825509710 -0.9449171639 -5.2460870473
H 1.0217308271 0.1566071825 -5.2420826550
H -0.6342686274 0.8220763740 -5.2400022378

Complex32: mn_3_misc_misc_misc_misc_misc_misc_s_5.xyz

Mn -0.0000309380 0.0036063437 -0.0021772031
C 0.0034796219 2.0793590730 -0.0019044189
N 0.0068320903 3.2356554688 -0.0016341803
C 0.0122541662 4.6714711675 -0.0000198140
H 0.8518410793 5.0174302624 -0.6092005077

H 0.1216394977 5.0183421131 1.0311116520
 H -0.9327384423 5.0244430027 -0.4220776302
 C 2.0755680121 0.0001283058 0.0004024548
 N 3.2318461489 -0.0029131096 0.0037568231
 C 4.6676579412 -0.0077913278 0.0097448537
 H 5.0158493022 -0.8463855579 -0.5995200342
 H 5.0113289965 -0.1184986786 1.0418094196
 H 5.0215785872 0.9379552302 -0.4098119259
 C -0.0037539985 -2.0723250741 -0.0026119028
 N -0.0075087051 -3.2286231011 -0.0024816287
 C -0.0135352434 -4.6644439327 -0.0008901575
 H -0.8527628609 -5.0100379544 -0.6107734432
 H -0.1239682634 -5.0112594143 1.0301500896
 H 0.9316806752 -5.0178341916 -0.4220880855
 C -2.0756086478 0.0054552715 -0.0017972070
 N -3.2318927213 0.0047483864 -0.0009557570
 C -4.6676421994 0.0019042339 0.0000461879
 H -5.0182904648 0.9957821542 0.2915164956
 H -5.0141778402 -0.7475693760 0.7169056668
 H -5.0166051205 -0.2439292345 -1.0066244662
 C -0.0010381434 0.0021472638 2.3410927983
 N -0.0027305277 -0.0004409153 3.5019191306
 C -0.0056614296 -0.0047530524 4.9371816562
 H 0.6002464066 -0.8435359958 5.2892195095
 H -1.0351896656 -0.1125562738 5.2878970068
 H 0.4156803319 0.9382526614 5.2946974116
 C 0.0009831723 0.0031847446 -2.3446959647
 N 0.0028751973 0.0011863072 -3.5055040351
 C 0.0060641852 -0.0024357417 -4.9407480855
 H -0.6020856432 -0.8393892884 -5.2932755497
 H 1.0353589044 -0.1130613596 -5.2912762738
 H -0.4125166045 0.9419594481 -5.2978474528

Complex33: mn_3_phosphine_phosphine_phosphine_phosphine_ammonia_ammonia_s_5.xyz

Mn -0.0121571045 -0.0064243353 -0.0018394148
 P -0.4173409097 2.6170211811 0.4582337751
 H -1.4648521215 2.9297563746 1.3472808383
 H 0.6740571876 3.3118440044 1.0158950853
 H -0.7329568073 3.3829342440 -0.6812887200
 P 2.6230139239 0.3567488115 -0.3882208909
 H 3.0628356978 1.6931605661 -0.4648211864
 H 3.4573367898 -0.1934632105 0.6048366701
 H 3.1274967574 -0.2050801478 -1.5776047737
 P 0.3330687379 -2.6369309961 -0.4068723879
 H 1.6618196101 -3.1025281565 -0.4563333797
 H -0.2505200033 -3.4644456519 0.5728729293
 H -0.2193388410 -3.1240995333 -1.6077397986
 P -2.6331071876 -0.4645809149 0.3233635702
 H -3.1445149967 -1.6210202809 -0.2976536636
 H -3.0416088897 -0.6146259413 1.6630355985
 H -3.4842143808 0.5485939871 -0.1605001798

N 0.3905581366 -0.2390492436 2.2695580987
H -0.4063256812 0.0201061706 2.8605073850
H 0.6101765274 -1.1985652318 2.5577794477
H 1.1691820669 0.3179755207 2.6374008179
N -0.2802481389 0.3887060872 -2.2726807176
H -1.2559667187 0.5588453225 -2.5388420013
H 0.2237076966 1.2025849118 -2.6412611016
H 0.0108644329 -0.3849747470 -2.8794303878

Complex34: mn_3_phosphine_phosphine_phosphine_phosphine_phosphine_chloride_s_5.xyz

Mn -0.0494517835 -0.0610293296 0.1091349709
P -0.5014526888 2.6861640198 -0.2946646902
H -0.4557665691 3.7092892171 0.6778452510
H 0.3302381864 3.2657604563 -1.2754183113
H -1.7548058335 2.9777459304 -0.8725229733
P 2.4709858905 0.2701933987 -0.4330327932
H 2.7076037469 1.3254891100 -1.3332703147
H 3.4415036899 0.5117918929 0.5604189568
H 3.0255538690 -0.8229322195 -1.1234104969
P 0.4170525412 -2.8133717408 0.4744649521
H 1.4459638663 -3.3401417975 -0.3342444396
H 0.7314786929 -3.4585643261 1.6907841516
H -0.6385373834 -3.6444602113 0.0438865477
P -2.5922256710 -0.4631371800 0.4405928268
H -3.0161425399 -1.6949056499 -0.0902566083
H -3.2134750208 -0.4579355018 1.7059988948
H -3.3862766735 0.4494671490 -0.2779736112
P 0.2930331036 0.4000028007 2.5932040964
H 1.4517124945 1.1190624208 2.9423157462
H -0.7080105812 1.1656152168 3.2203088903
H 0.3788030025 -0.7157906832 3.4469128023
Cl -0.3803837791 -0.4039806736 -2.0280128882

Complex35: mn_3_water_water_water_water_fluoride_fluoride_s_5.xyz

Mn -0.0003500474 0.0002556370 0.0011484394
O -0.2013169808 2.1034705284 0.3187391665
H -0.4794992830 2.6026615655 -0.4691173987
H -0.8038058905 2.3488326582 1.0423652974
O 2.0969193480 0.1757151767 0.3483116393
H 2.5558905825 0.7978909542 -0.2422412898
H 2.3233807114 0.4253367618 1.2616255263
O 0.2007338016 -2.1033190496 -0.3157738961
H 0.7909364270 -2.3487145860 -1.0494355572
H 0.4926576631 -2.6014913238 0.4677146180
O -2.0977601494 -0.1763245017 -0.3446951695
H -2.5526251908 -0.8074293249 0.2395951894
H -2.3245799248 -0.4172739232 -1.2602810984
F -0.2638868215 -0.2756938097 1.6909889990
F 0.2632995296 0.2760960126 -1.6889279300

Complex36: fe_3_acetonitrile_acetonitrile_acetonitrile_acetonitrile_acetonitrile_cyanide_s_6.xyz

Fe -0.0591307973 0.0627569456 0.2408768688
C 0.4394965173 3.2818417811 0.5593630610
N 0.2866797184 2.1335727913 0.5813882308
C 0.6285479509 4.7221922214 0.5232275592
H 0.3669243264 5.1004687635 -0.4712241391
H 1.6747928474 4.9659055742 0.7366528172
H -0.0113444874 5.2015451646 1.2717307354
C 3.1154283240 -0.3863365650 -0.4202870324
N 2.0228538177 -0.2503569062 -0.0595543735
C 4.4835556975 -0.5561356063 -0.8797249764
H 5.1047682113 0.2669387452 -0.5105673917
H 4.5042739814 -0.5587859312 -1.9751720249
H 4.8867560693 -1.5043139561 -0.5084522472
C -0.6065244559 -3.1013252246 -0.3803025070
N -0.3947913294 -2.0171675063 -0.0307229099
C -0.8731003588 -4.4581910614 -0.8267017784
H 0.0034250526 -5.0892011018 -0.6447582505
H -1.0970868615 -4.4530449896 -1.8992279824
H -1.7298002948 -4.8684848204 -0.2814499305
C -3.2719484902 0.5542755044 0.6083802003
N -2.1296631570 0.3603532849 0.6113351624
C -4.7043630462 0.7981568428 0.5967062962
H -5.2362659523 -0.0912996982 0.9510344151
H -5.0280968404 1.0286845042 -0.4243344006
H -4.9439248987 1.6435522584 1.2505276367
C 0.4245341125 -0.4720025314 3.5095430194
N 0.2553230039 -0.2863994836 2.3790009824
C 0.6373000916 -0.7056368556 4.9294763910
H -0.2978726743 -1.0317463848 5.3968167549
H 0.9759883632 0.2174606086 5.4116153532
H 1.3969546078 -1.4820701196 5.0685723468
C -0.3303769320 0.3921721464 -1.7047280360
N -0.4930454471 0.5828829035 -2.8522334795

Complex37: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_chloride_s_6.xyz

Fe -0.0610460262 0.0458021128 -0.0147840869
N -0.3019266169 2.2347223875 0.3702665833
H -1.2891199434 2.4778733824 0.4898996041
H 0.1894470882 2.6645624843 1.1586504114
H -0.0114093917 2.7422785988 -0.4710379391
N 2.1402699534 0.3123390275 -0.2846207014
H 2.4133705675 1.2947969245 -0.1908095449
H 2.7860951718 -0.2156493051 0.3090159223
H 2.3683506642 0.0707901187 -1.2540206112
N 0.1846057296 -2.1547779041 -0.3140757290
H 1.1690587514 -2.4243054735 -0.3940462824
H -0.2265901644 -2.8050217612 0.3614907285

H -0.2291387003 -2.3859180230 -1.2229834432
N -2.2472730165 -0.2572591152 0.3673839071
H -2.4825228880 -1.2362450724 0.5505193079
H -2.6996360536 0.2780124575 1.1136660424
H -2.7403782768 -0.0176883628 -0.4985273076
N 0.3135915513 -0.2113778249 2.1798439244
H -0.4822859950 0.0619454683 2.7625985817
H 0.5108844927 -1.1828535484 2.4346994684
H 1.1084220098 0.3271266218 2.5353234101
Cl -0.4126992301 0.3809238164 -2.2013209652

Complex38: fe_3_ammonia_ammonia_ammonia_ammonia_ammonia_misc_s_6.xyz

Fe -0.0874850029 -0.0964474690 0.0166568067
N -0.3751691187 2.0854712209 0.3443231562
H -1.3608925207 2.3455788059 0.4654046914
H 0.1038277021 2.4722596266 1.1663265593
H -0.0493375513 2.6431912082 -0.4537738583
N 2.1080446472 0.1583210390 0.2741207484
H 2.3846978439 1.1465299856 0.2925624874
H 2.5154844650 -0.2524896703 1.1226815639
H 2.6339594373 -0.2502616229 -0.5069862900
N 0.3092744120 -2.2709517996 -0.2156785120
H 1.0998254816 -2.6303545368 0.3320992649
H -0.4845681336 -2.8759889410 0.0248922878
H 0.5307645625 -2.4971066408 -1.1926697381
N -2.2239595049 -0.4894125718 -0.4504796624
H -2.3452162255 -1.1861700589 -1.1945861586
H -2.7906183016 -0.8240555070 0.3377851862
H -2.7061371977 0.3487047093 -0.7951884424
N -0.4483887484 -0.3547429969 2.1829735360
H -1.2809733214 0.1342653359 2.5336614069
H -0.5808366010 -1.3366197020 2.4523403293
H 0.3215475531 -0.0205207727 2.7749526699
C 0.1970431331 0.2715167157 -2.1489435369
N 0.3391479799 0.4667080842 -3.2829445990
C 0.5152693213 0.7091551787 -4.6912102024
H -0.0311062423 -0.0590131342 -5.2473780990
H 1.5839821469 0.6605515722 -4.9219996429
H 0.1191618064 1.7024704269 -4.9247312273

Complex39: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_carbonyl_acetonitrile_s_6.xyz

Fe 0.0034076490 -0.0003576076 -0.2041958037
C 0.0040306440 2.2954840178 0.0552563102
O 0.0042145126 3.4132912901 0.1543574303
C 2.2995520480 0.0030352521 0.0523513008
O 3.4174844841 0.0047152690 0.1500044860
C 0.0083175910 -2.2959556316 0.0550475163
O 0.0108268556 -3.4137581693 0.1541385013
C -2.2918867647 -0.0012092503 0.0579542658

O -3.4095644236 -0.0017514003 0.1584865504
C 0.0057131720 -0.0004774295 2.1669979822
O 0.0068950592 -0.0003532501 3.2897721914
C -0.0054385692 -0.0003190704 -3.3121928944
N -0.0004529033 -0.0000587353 -2.1277388755
C -0.0124041011 -0.0005432320 -4.7336243049
H 1.0250135532 -0.0329393790 -5.1213979215
H -0.5060655378 0.9159140580 -5.1131971747
H -0.5622736165 -0.8846260299 -5.1126498517

Complex40: fe_3_carbonyl_carbonyl_carbonyl_carbonyl_fluoride_fluoride_s_6.xyz

Fe 0.0003282293 0.0003205487 -0.0107761996
C -0.0469027523 2.3744279749 0.3763201609
O -0.0691275383 3.4845943319 0.5671920352
C 2.3744480305 -0.0456528373 0.3764256478
O 3.4846247612 -0.0671239047 0.5673261876
C 0.0454088691 -2.3730957949 -0.3974402881
O 0.0670214159 -3.4831594328 -0.5889628596
C -2.3730792238 0.0441898529 -0.3975465277
O -3.4831472260 0.0650589893 -0.5891289586
F -0.2727365127 -0.2725967255 1.6850203287
F 0.2731622491 0.2730361434 -1.7064852853

Complex41: fe_3_misc_misc_misc_misc_acetonitrile_acetonitrile_s_6.xyz

Fe 0.0004018015 0.0020831157 -0.0031416639
C 0.0024356882 2.2013963407 -0.0030784801
N 0.0049227954 3.3597223236 -0.0048031667
C 0.0086522988 4.7947452039 -0.0065793217
H 0.8480891844 5.1425447462 -0.6146078797
H 0.1161929988 5.1467896516 1.0227509596
H -0.9354467880 5.1477471115 -0.4302051888
C 2.1998175039 0.0005386665 -0.0027129940
N 3.3581483368 -0.0021054101 -0.0019241821
C 4.7931768529 -0.0059183511 -0.0004206040
H 5.1423622367 -0.8451239457 -0.6079696863
H 5.1428060663 -0.1139496330 1.0296788861
H 5.1472564890 0.9384119281 -0.4226209592
C -0.0008325200 -2.1974289158 -0.0027878187
N -0.0024521189 -3.3557638688 -0.0022753532
C -0.0050874328 -4.7907975441 -0.0013202747
H -0.8439144599 -5.1404340760 -0.6091357524
H -0.1130226356 -5.1409361919 1.0286124947
H 0.9396323320 -5.1439315833 -0.4234394045
C -2.1989719653 0.0012156164 -0.0021287109
N -3.3572951261 -0.0018222987 -0.0004882195
C -4.7922382762 -0.0067431902 0.0018846765
H -5.1462302067 0.9853467687 0.2948337744
H -5.1393778194 -0.7575045424 0.7168221279
H -5.1443232996 -0.2513131177 -1.0037654177

C -0.0033395678 0.0046219464 3.2452640495
N -0.0008043113 0.0029747946 2.0827340125
C -0.0067251390 0.0062780606 4.6948167064
H -0.7967498654 0.6715691055 5.0643181332
H 0.9627391803 0.3573025325 5.0690910780
H -0.1892117613 -1.0091552242 5.0674687535
C 0.0003374103 0.0017558421 -3.2511891559
N 0.0005048699 0.0019284397 -2.0886426133
C -0.0001021155 0.0010742508 -4.7007226228
H -0.7892668158 0.6658902132 -5.0729176888
H -0.1818720190 -1.0149867578 -5.0720524357
H 0.9701676999 0.3514553179 -5.0735363789

Complex42: fe_3_misc_misc_misc_misc_water_water_s_6.xyz

Fe 0.0011709404 -0.0002745567 0.0018988957
C 0.3515178359 2.1325770057 -0.3696442472
N 0.5271159017 3.2686187348 -0.5134474424
C 0.7442883613 4.6778256622 -0.6879750640
H 1.7160273506 4.8249277878 -1.1682536479
H 0.7297061370 5.1569171395 0.2953166909
H -0.0550415274 5.0790329972 -1.3178286427
C 2.1303433686 -0.2831041265 0.4352057732
N 3.2644842968 -0.4422897821 0.6095818421
C 4.6714484890 -0.6403838578 0.8207103715
H 5.0567804865 -1.2798254771 0.0212135565
H 4.8150744475 -1.1192536807 1.7936453471
H 5.1684166720 0.3339014827 0.7999805779
C -0.3296705749 -2.1538494230 0.2317585628
N -0.5114787323 -3.2840923413 0.4091539258
C -0.7372896779 -4.6848675378 0.6330633525
H -1.3912863210 -5.0642180080 -0.1574693038
H -1.2107143877 -4.8093792314 1.6112841371
H 0.2263577100 -5.2020325270 0.6092064105
C -2.1500403585 0.3060117266 -0.2919926088
N -3.2791148114 0.4570333473 -0.5028279726
C -4.6784916135 0.6425185649 -0.7686078162
H -4.9900659517 1.6036125252 -0.3492607295
H -5.2344177851 -0.1744165437 -0.2993519821
H -4.8314071496 0.6328449485 -1.8517223312
O -0.3056562745 0.3185883410 2.0248847216
H 0.3887327694 0.3941577988 2.7080166357
H -1.1722609378 0.4593409784 2.4534184438
O 0.3028144914 -0.3243455472 -2.0213580483
H 0.4543824229 0.3685370156 -2.6931850872
H 0.3374615108 -1.1935867949 -2.4661929330

Complex43: mn_2_acetonitrile_acetonitrile_acetonitrile_acetonitrile_water_water_s_6.xyz

Mn -0.0024164828 0.0004273184 -0.0012577117
C 0.4831960872 3.3206143904 -0.5585513967

N 0.3345947349 2.1955033544 -0.3264105713
 C 0.6701537782 4.7349630868 -0.8512440768
 H 0.3421810141 4.9497954483 -1.8735249433
 H 1.7279332058 4.9995727928 -0.7526167014
 H 0.0846021597 5.3414831078 -0.1527353048
 C 3.3234160812 -0.5600371797 -0.4960399230
 N 2.1919502602 -0.3596431259 -0.3445261166
 C 4.7450843136 -0.8114095457 -0.6862295298
 H 5.2635785968 0.1265661562 -0.9102534883
 H 4.8922964815 -1.5086336274 -1.5176511343
 H 5.1708352686 -1.2473398100 0.2235897114
 C -0.4824348619 -3.3194283195 0.5603753876
 N -0.3391507095 -2.1942086950 0.3253884224
 C -0.6612469564 -4.7339911712 0.8571157074
 H 0.3081943999 -5.2425043805 0.8439107018
 H -1.3156237291 -5.1933612417 0.1091830278
 H -1.1121761234 -4.8522168935 1.8477631273
 C -3.3288786077 0.5584268658 0.4931243116
 N -2.1973191394 0.3590496655 0.3409586931
 C -4.7506346661 0.8086785082 0.6840961070
 H -5.1105563022 0.2653574247 1.5639715364
 H -5.3089997147 0.4717786337 -0.1956092172
 H -4.9250080406 1.8799832935 0.8279877359
 O 0.3569595982 0.1994013993 2.1779831038
 H 1.1851251871 0.5347671397 2.5577637778
 H -0.3524106661 0.4397589834 2.7958107324
 O -0.3566620670 -0.1983244789 -2.1808781387
 H -1.1898041526 -0.5152669830 -2.5654610384
 H 0.3508423666 -0.4512067744 -2.7957508762

Complex44: mn_2_ammonia_ammonia_ammonia_ammonia_cyanide_cyanide_s_6.xyz

Mn -0.0001269570 0.0010578909 -0.0039811072
 N -0.3047195399 2.3293441378 0.3570445610
 H -1.2837435807 2.5151001291 0.5702146885
 H 0.2433165754 2.7164247970 1.1241267780
 H -0.0919272505 2.8397669894 -0.4993556533
 N 2.3312358523 0.3399339929 -0.3109962505
 H 2.5235913027 1.3400795477 -0.3410041255
 H 2.8624799420 -0.0457557266 0.4687668628
 H 2.6875055979 -0.0484779073 -1.1832330922
 N 0.3052035214 -2.3302701365 -0.3547819590
 H 1.2658414004 -2.5163517632 -0.6391314376
 H 0.1630089768 -2.8122544817 0.5322228730
 H -0.2975635447 -2.7456447519 -1.0635687125
 N -2.3313249956 -0.3375783165 0.3116708852
 H -2.5223851079 -1.3376434859 0.3511222409
 H -2.6849941254 0.0575367641 1.1819635224
 H -2.8660452685 0.0408285423 -0.4693035016
 C 0.3541495920 -0.3477995667 2.1433774754
 N 0.5639471902 -0.5833226076 3.2713843794
 C -0.3546493765 0.3480658666 -2.1492293570

N -0.5628106109 0.5769949772 -3.2788501370

Complex45: mn_2_carbonyl_carbonyl_carbonyl_carbonyl_phosphine_phosphine_s_6.xyz

Mn 0.0018223735 -0.0020855722 0.0383528791
C 0.0036452192 2.4513000075 0.0495634290
O 0.0051383130 3.5775671861 0.0558054540
C 2.4546711990 -0.0036857247 0.0493146107
O 3.5809376627 -0.0049745939 0.0545842912
C 0.0021115977 -2.4549254040 0.0433348162
O 0.0024606549 -3.5812026621 0.0451632793
C -2.4515326088 -0.0033306938 0.0441274975
O -3.5778121976 -0.0046542290 0.0475540447
P -0.0009487506 0.0005981213 2.8012569547
H 1.1422371959 0.5071116976 3.4520713112
H -1.0110330561 0.7417624643 3.4473871182
H -0.1376813068 -1.2407622652 3.4547477374
P -0.0022198155 0.0034316164 -2.7208287420
H 1.2013678204 0.3362786911 -3.3745911689
H -0.3231973016 -1.2034384504 -3.3744874362
H -0.8940631961 0.8863828187 -3.3627387864

Complex46: mn_2_chloride_chloride_chloride_chloride_carbonyl_carbonyl_s_6.xyz

Mn 0.0000142499 -0.0000902280 -0.0000271326
Cl 0.0000102993 2.5746445189 0.0026577261
Cl 2.5747500193 -0.0001411949 -0.0002217934
Cl 0.0000196504 -2.5748236722 -0.0024459905
Cl -2.5747195997 -0.0000302744 0.0001337507
C -0.0000306525 0.0003154624 2.4175183715
O -0.0000982012 0.0009455414 3.5576920759
C 0.0000199114 -0.0002247216 -2.4175667983
O 0.0000343103 -0.0005954319 -3.5577402673

Complex47: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_carbonyl

Mn -0.0112188277 -0.0763536386 0.1404229238
S 0.4117099734 2.5986087256 -0.3115691569
H -0.6955161170 3.2480308679 0.1084125049
H 0.2134679706 2.8753424525 -1.6190205858
S 2.6452851114 -0.5258915035 -0.3410078211
H 3.1191705657 -1.0418031348 0.8135096788
H 3.2775387348 0.6592390868 -0.1963602775
S -0.4332122601 -2.7531839015 0.5745378705
H 0.4161920408 -3.1007286537 1.5653317973
H 0.2422109729 -3.4149172417 -0.3903958724
S -2.6955253782 0.3220257758 0.5107642233
H -3.2764178340 -0.8956365024 0.4431256044
H -3.1997433818 0.7504703876 -0.6665557386
S 0.4027904368 0.2799171736 2.8052676236

H 1.1721598481 1.3852134891 2.9058503675
H -0.7065251784 0.8688614954 3.3025301363
C -0.3523539186 -0.4904696854 -2.2517434487
O -0.5298267207 -0.6880365393 -3.3470554544

Complex48: mn_2_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_hydrogensulfide_phosphi

Mn 0.0341013772 0.0387582577 0.0009930235
S -0.4108557557 2.7278957659 -0.4077127636
H 0.4788512310 3.3920900829 0.3612612552
H 0.2391167842 3.0043931110 -1.5585666634
S 2.7171428723 0.4455817871 -0.4267849511
H 3.2133265174 -0.7110202285 -0.9171796556
H 3.3287659161 0.3221120844 0.7713403364
S 0.5105269062 -2.6467105569 0.3865630303
H 1.2370250921 -2.7509997977 1.5201655689
H -0.5977608817 -3.2055869736 0.9193545081
S -2.6440839538 -0.3371111937 0.5256116364
H -3.2351978941 -0.8294947097 -0.5840978583
H -3.1962249709 0.8891598770 0.4013334114
S 0.4235257100 0.4320987756 2.7030031118
H -0.0202949462 1.6567950495 3.0596745697
H -0.6004433873 -0.2224658608 3.2916071962
P -0.2994627176 -0.4564891190 -2.7024440321
H 0.8228123179 -0.4371051126 -3.5571154414
H -0.8449028530 -1.7042087225 -3.0705422368
H -1.1573758759 0.3939633638 -3.4314597220

Complex49: mn_2_water_water_water_water_acetonitrile_acetonitrile_s_6.xyz

Mn 0.0134109161 0.0484383058 0.0060270424
O 0.2793541711 2.2019908951 0.3429760971
H 0.4256805286 2.8886470808 -0.3282767496
H 0.4776352515 2.5967405840 1.2080815058
O 2.1385426180 -0.5195290760 -0.3833287808
H 2.6475719661 -0.2260680388 -1.1580126722
H 2.7804128341 -0.6227402255 0.3400029627
O -0.3276012267 -2.0944906140 -0.2188394940
H 0.3536128001 -2.7046647178 -0.5454865164
H -1.1956541592 -2.4809864608 -0.4198111227
O -2.1989458756 0.1216548638 0.2727955630
H -2.6176406782 0.0746502879 1.1496922764
H -2.7561598133 0.7166884681 -0.2572659903
C 0.5061496202 -0.4953767070 3.3164274697
N 0.3600835436 -0.2328883006 2.1958314181
C 0.6894452789 -0.8254690147 4.7217459390
H -0.2721022566 -0.7750548687 5.2438808320
H 1.3850968012 -0.1172938130 5.1846022384
H 1.0937420899 -1.8391814142 4.8150146825
C -0.4759094049 0.6016043164 -3.3038872036
N -0.2892987053 0.4665116133 -2.1668550790

C -0.7096509506 0.7718092908 -4.7301383859
H 0.2408815793 0.7196276626 -5.2718931760
H -1.1756697157 1.7450496127 -4.9181573985
H -1.3730488425 -0.0196866807 -5.0951412849

Complex50: mn_2_water_water_water_water_water_water_s_6.xyz

Mn 0.0000438805 -0.0002126033 -0.0002607084
O -0.1985275770 2.1974217948 -0.0531243321
H 0.3853240494 2.7702597393 -0.5808887622
H -0.9809772158 2.7319050565 0.1698993870
O 1.9476439207 0.3028636154 -0.9613514903
H 2.2725704051 0.2061290961 -1.8731556067
H 2.7255457241 0.4068622124 -0.3866041620
O 0.1963286201 -2.1982208385 0.0518966806
H 0.9783753032 -2.7341610183 -0.1690932978
H -0.3905803209 -2.7704786803 0.5769088438
O -1.9469609838 -0.3022286336 0.9630131497
H -2.2695442852 -0.2060275452 1.8757107070
H -2.7264746323 -0.4053392167 0.3902550586
O 1.1887351661 0.3165865970 1.8494692115
H 1.1938660196 1.1794581535 2.3007905495
H 1.4505145588 -0.3412556396 2.5177862218
O -1.1874402588 -0.3162374089 -1.8502998738
H -1.4461562911 0.3418715642 -2.5195306971
H -1.1922907637 -1.1792057341 -2.3014312300