Accurate Experimental and Theoretical Enthalpies of Association of $TiCl_4$ with Typical Lewis Bases Used in Heterogeneous Ziegler-Natta Catalysis

Supplementary Information

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Table S1. Formation constants and thermodynamic parameters (kJ mol^{-1}) previously reported for the complex formation between $TiCl_4$ with esters (L01-02), phthalates (L03-06) , succinates (L07-09) and ethers (L10-15) in TCE at 298.15 K. [27,29]

Ligand		$\log\beta_{j,2007}$	$\Delta G°_{j,2007}$	$\Delta H°_{j,2007}$	$T\Delta S°_{j,2007}$
L01	1:1	3.7	-21	-45	-24
	1:2	6.0	-34	-102	-68
L02	1:1	2.8	-16	-32	-16
	1:2	4.2	-24	-60	-37
L03	1:1	4.5	-26	-87	-61
L04	1:1	4.5	-27	-86	-60
L05	1:1	2.8	-16	-31	-15
	1:2	4.0	-23	-71	-48
L06	1:1	2.7	-15	-29	-13
	1:2	3.9	-22	-70	-48
L07	1:1	4.5	-26	-84	-58
L08	1:1	5.0	-29	-85	-56
L09	1:1	>5.5	-	-90	-
L10	1:1	4.8	-28	-60	-32
	1:2	7.9	-45	-120	-75
L11	1:1	>5.5	-	-103	-
L12	1:1	>5.5	-	-90	-
L13	1:1	4.4	-25	-88	-63
L14	1:1	>5.5	-	-96	-
L15	1:1	>5.5	-	-86	-

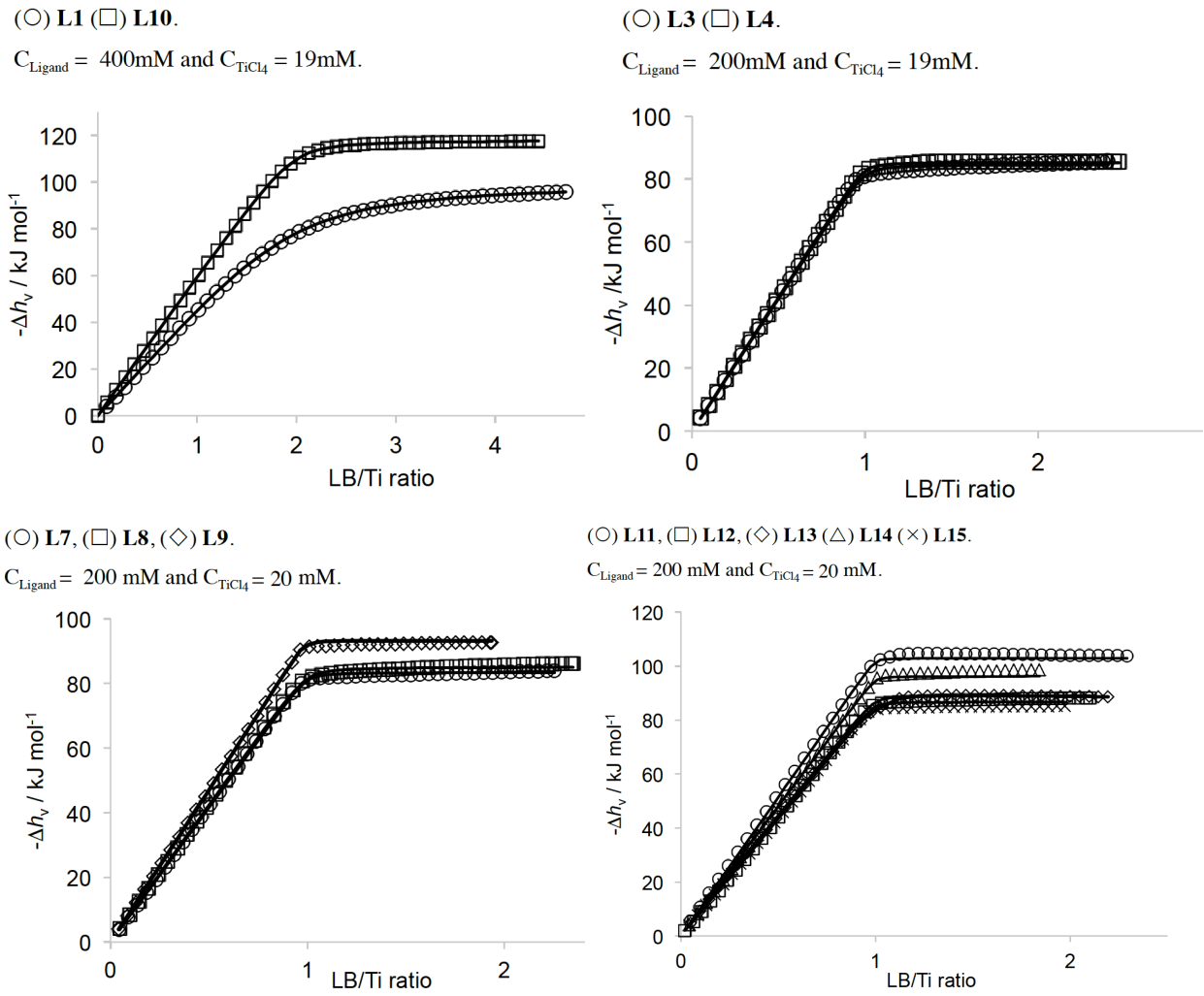

Figure S1. Experimental cumulative molar enthalpy changes per mole of Ti in the cell, Δh_v, as a function of the LB/Ti ratio in TCE at 298.15 K (old data, symbols). Solid lines are calculated with the new $\log\beta_j$ and $\Delta H°_j$ values obtained by the re-fit of the old data[27,29] and reported in Table 2.

Table S2. PBE energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1898.696745	-1898.676975	-1898.691112
L01	-307.443486	-307.314113	-307.329042
L02	-498.998893	-498.810755	-498.833459
L03	-923.053734	-922.660982	-922.706300
L04	-765.975698	-765.707763	-765.740853
L05	-765.985348	-765.718240	-765.749514
L06	-765.986084	-765.718593	-765.749762
L07	-613.696066	-613.455712	-613.482555
L08	-849.296785	-848.870622	-848.911644
L09	-849.301265	-848.874392	-848.915049
L10	-232.227453	-232.102830	-232.115651
L11	-308.577322	-308.422520	-308.436787
L12	-347.847604	-347.662049	-347.679414
L13	-387.117836	-386.900989	-386.921456
L14	-661.990730	-661.558961	-661.594584
L15	-808.313065	-807.974172	-808.010761
ML01	-2206.152824	-2206.000394	-2206.030050
$M(L01)_{2\ cis}$	-2513.608634	-2513.324391	-2513.367024
ML02	-2397.704988	-2397.494685	-2397.531209
ML03	-2821.761768	-2821.349934	-2821.409747
ML04	-2664.683407	-2664.397135	-2664.444273
ML05	-2664.691780	-2664.401469	-2664.446943
ML06	-2664.690909	-2664.401617	-2664.446108
ML07	-2512.405222	-2512.145636	-2512.188064
ML08	-2748.011175	-2747.565433	-2747.621847
ML09	-2748.016702	-2747.569619	-2747.627439
ML10	-2130.939737	-2130.793043	-2130.819894
$M(L10)_{2cis}$	-2363.182285	-2362.910072	-2362.947757
ML11	-2207.290647	-2207.119829	-2207.145584
ML12	-2246.557365	-2246.355512	-2246.384148
ML13	-2285.817899	-2285.584758	-2285.614562
ML14	-2560.700070	-2560.252441	-2560.298595
ML15	-2707.022598	-2706.665705	-2706.713759

Table S3. PBE0 energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1898.792590	-1898.773139	-1898.786732
L01	-307.460411	-307.326783	-307.341385
L02	-499.029441	-498.836263	-498.858639
L03	-923.121303	-922.718558	-922.762877
L04	-766.010793	-765.735665	-765.768154
L05	-766.021193	-765.746848	-765.777557
L06	-766.021748	-765.747056	-765.777612
L07	-613.726953	-613.480248	-613.506566
L08	-849.376160	-848.939397	-848.979172
L09	-849.380328	-848.942804	-848.982130
L10	-232.254333	-232.125303	-232.137845
L11	-308.602994	-308.443891	-308.457678
L12	-347.880908	-347.690419	-347.707176
L13	-387.159230	-386.936742	-386.956515
L14	-662.089080	-661.646185	-661.680975
L15	-808.386875	-808.038678	-808.074635
ML01	-2206.268588	-2206.113241	-2206.142286
$M(L01)_{2\ cis}$	-2513.744887	-2513.454872	-2513.496023
ML02	-2397.834614	-2397.619665	-2397.655423
ML03	-2821.930940	-2821.510209	-2821.568456
ML04	-2664.820011	-2664.527537	-2664.573494
ML05	-2664.826659	-2664.529512	-2664.573952
ML06	-2664.825466	-2664.529337	-2664.572825
ML07	-2512.537704	-2512.272601	-2512.314077
ML08	-2748.192537	-2747.736965	-2747.791712
ML09	-2748.198145	-2747.741091	-2747.797349
ML10	-2131.065410	-2130.915495	-2130.941811
$M(L10)_{2cis}$	-2363.338623	-2363.060228	-2363.096624
ML11	-2207.417146	-2207.242574	-2207.267802
ML12	-2246.692731	-2246.486310	-2246.514095
ML13	-2285.961289	-2285.723090	-2285.751753
ML14	-2560.900679	-2560.442666	-2560.487271
ML15	-2707.198373	-2706.833105	-2706.879594

Table S4. B3LYP energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.501431	-1899.482380	-1899.495864
L01	-307.821983	-307.689365	-307.704008
L02	-499.619255	-499.427532	-499.449921
L03	-924.206896	-923.806877	-923.851572
L04	-766.898151	-766.625305	-766.657909
L05	-766.908756	-766.636658	-766.667474
L06	-766.909308	-766.636845	-766.667529
L07	-614.435990	-614.191259	-614.217734
L08	-850.379696	-849.945329	-849.986003
L09	-850.383246	-849.948193	-849.988476
L10	-232.532359	-232.404411	-232.416973
L11	-308.971691	-308.813805	-308.827729
L12	-348.299296	-348.110154	-348.127140
L13	-387.627481	-387.406486	-387.426525
L14	-662.900849	-662.460423	-662.495608
L15	-809.345112	-808.999414	-809.035449
ML01	-2207.334011	-2207.179380	-2207.208955
$M(L01)_{2\ cis}$	-2515.165967	-2514.877139	-2514.919425
ML02	-2399.128251	-2398.914545	-2398.950742
ML03	-2823.717537	-2823.298901	-2823.358356
ML04	-2666.408370	-2666.117611	-2666.164419
ML05	-2666.418057	-2666.122963	-2666.167944
ML06	-2666.416932	-2666.122816	-2666.166859
ML07	-2513.947388	-2513.683839	-2513.726116
ML08	-2749.895886	-2749.442272	-2749.498458
ML09	-2749.901612	-2749.446609	-2749.504225
ML10	-2132.047060	-2131.898165	-2131.924783
$M(L10)_{2cis}$	-2364.592052	-2364.315095	-2364.352406
ML11	-2208.485086	-2208.311180	-2208.337459
ML12	-2247.809915	-2247.604388	-2247.632934
ML13	-2287.133454	-2286.896541	-2286.926151
ML14	-2562.410277	-2561.954300	-2562.000065
ML15	-2708.854252	-2708.490814	-2708.538447

Table S5. TPSS energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.509575	-1899.490152	-1899.503938
L01	-307.861448	-307.730800	-307.745470
L02	-499.694012	-499.504207	-499.526619
L03	-924.340300	-923.944007	-923.988831
L04	-767.010666	-766.740519	-766.773128
L05	-767.020979	-766.751623	-766.782477
L06	-767.021691	-766.751923	-766.782695
L07	-614.517495	-614.274909	-614.301384
L08	-850.495307	-850.065077	-850.105610
L09	-850.499501	-850.068382	-850.108742
L10	-232.565642	-232.439711	-232.452333
L11	-309.009960	-308.853508	-308.867505
L12	-348.343116	-348.155614	-348.172709
L13	-387.676540	-387.457407	-387.477585
L14	-662.989537	-662.553349	-662.588529
L15	-809.474510	-809.132450	-809.168610
ML01	-2207.384885	-2207.231465	-2207.260972
$M(L01)_{2\ cis}$	-2515.259689	-2514.973401	-2515.015541
ML02	-2399.214738	-2399.003215	-2399.039463
ML03	-2823.866435	-2823.451933	-2823.511010
ML04	-2666.536296	-2666.248515	-2666.295041
ML05	-2666.541932	-2666.249823	-2666.294898
ML06	-2666.540981	-2666.249868	-2666.293975
ML07	-2514.043695	-2513.782555	-2513.824485
ML08	-2750.026889	-2749.577641	-2749.633495
ML09	-2750.032145	-2749.581672	-2749.638864
ML10	-2132.092639	-2131.945010	-2131.971644
$M(L10)_{2cis}$	-2364.675491	-2364.401165	-2364.438435
ML11	-2208.540866	-2208.369180	-2208.394509
ML12	-2247.871323	-2247.668096	-2247.696278
ML13	-2287.201317	-2286.967171	-2286.996171
ML14	-2562.517654	-2562.066371	-2562.111790
ML15	-2709.002321	-2708.642944	-2708.690374

Table S6. PBE-D3 energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1898.704948	-1898.685178	-1898.699315
L01	-307.452531	-307.323157	-307.338087
L02	-499.019312	-498.831175	-498.853879
L03	-923.098757	-922.706005	-922.751323
L04	-766.007072	-765.739137	-765.772228
L05	-766.015360	-765.748253	-765.779527
L06	-766.016050	-765.748559	-765.779727
L07	-613.716871	-613.476518	-613.503360
L08	-849.345070	-848.918906	-848.959928
L09	-849.351019	-848.924146	-848.964803
L10	-232.236668	-232.112045	-232.124866
L11	-308.587175	-308.432372	-308.446640
L12	-347.860313	-347.674758	-347.692123
L13	-387.133425	-386.916578	-386.937045
L14	-662.035795	-661.604026	-661.639649
L15	-808.360017	-808.021124	-808.057713
ML01	-2206.176609	-2206.024178	-2206.053835
$M(L01)_{2\ cis}$	-2513.649751	-2513.365507	-2513.408141
ML02	-2397.741692	-2397.531389	-2397.567913
ML03	-2821.825980	-2821.414146	-2821.473960
ML04	-2664.733861	-2664.447588	-2664.494726
ML05	-2664.738221	-2664.447910	-2664.493384
ML06	-2664.737167	-2664.447875	-2664.492366
ML07	-2512.445756	-2512.186171	-2512.228599
ML08	-2748.080828	-2747.635085	-2747.691500
ML09	-2748.086760	-2747.639678	-2747.697497
ML10	-2130.965461	-2130.818768	-2130.845619
$M(L10)_{2cis}$	-2363.227696	-2362.955482	-2362.993168
ML11	-2207.322303	-2207.151485	-2207.177241
ML12	-2246.593521	-2246.391668	-2246.420304
ML13	-2285.859553	-2285.626412	-2285.656216
ML14	-2560.770889	-2560.323260	-2560.369415
ML15	-2707.096054	-2706.739160	-2706.787214

Table S7. PBE0-D3 energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.518162	-1899.499111	-1899.512595
L01	-307.837007	-307.704389	-307.719032
L02	-499.653969	-499.462246	-499.484635
L03	-924.281693	-923.881674	-923.926369
L04	-766.950834	-766.677988	-766.710592
L05	-766.959380	-766.687281	-766.718098
L06	-766.959868	-766.687405	-766.718090
L07	-614.470498	-614.225767	-614.252243
L08	-850.458181	-850.023814	-850.064488
L09	-850.463807	-850.028754	-850.069037
L10	-232.547744	-232.419797	-232.432359
L11	-308.987838	-308.829952	-308.843876
L12	-348.320114	-348.130971	-348.147958
L13	-387.653005	-387.432010	-387.452049
L14	-662.973757	-662.533331	-662.568516
L15	-809.423846	-809.078147	-809.114182
ML01	-2207.376933	-2207.222302	-2207.251876
$M(L01)_{2\ cis}$	-2515.237838	-2514.949010	-2514.991296
ML02	-2399.193430	-2398.979724	-2399.015921
ML03	-2823.827952	-2823.409315	-2823.468771
ML04	-2666.496500	-2666.205741	-2666.252549
ML05	-2666.499318	-2666.204224	-2666.249205
ML06	-2666.497935	-2666.203818	-2666.247862
ML07	-2514.018432	-2513.754882	-2513.797159
ML08	-2750.013194	-2749.559580	-2749.615766
ML09	-2750.019644	-2749.564640	-2749.622256
ML10	-2132.093636	-2131.944741	-2131.971359
$M(L10)_{2cis}$	-2364.671715	-2364.394758	-2364.432070
ML11	-2208.541857	-2208.367950	-2208.394230
ML12	-2247.874429	-2247.668901	-2247.697448
ML13	-2287.206827	-2286.969914	-2286.999525
ML14	-2562.530445	-2562.074468	-2562.120234
ML15	-2708.981344	-2708.617906	-2708.665539

Table S8. TPSS-D3 energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.520887	-1899.501464	-1899.515251
L01	-307.872568	-307.741920	-307.756590
L02	-499.719586	-499.529781	-499.552193
L03	-924.396500	-924.000207	-924.045031
L04	-767.050005	-766.779858	-766.812467
L05	-767.058563	-766.789207	-766.820061
L06	-767.059216	-766.789447	-766.820220
L07	-614.543220	-614.300634	-614.327110
L08	-850.555459	-850.125229	-850.165761
L09	-850.561366	-850.130247	-850.170608
L10	-232.576972	-232.451040	-232.463662
L11	-309.022004	-308.865552	-308.879549
L12	-348.358672	-348.171169	-348.188264
L13	-387.695643	-387.476510	-387.496689
L14	-663.045457	-662.609269	-662.644449
L15	-809.533800	-809.191740	-809.227901
ML01	-2207.416228	-2207.262808	-2207.292314
$M(L01)_{2\ cis}$	-2515.313351	-2515.027063	-2515.069203
ML02	-2399.262707	-2399.051184	-2399.087432
ML03	-2823.949272	-2823.534771	-2823.593848
ML04	-2666.602094	-2666.314312	-2666.360838
ML05	-2666.602077	-2666.309968	-2666.355043
ML06	-2666.600910	-2666.309797	-2666.353904
ML07	-2514.096581	-2513.835440	-2513.877370
ML08	-2750.116428	-2749.667180	-2749.723034
ML09	-2750.122367	-2749.671894	-2749.729086
ML10	-2132.126576	-2131.978947	-2132.005581
$M(L10)_{2cis}$	-2364.734673	-2364.460347	-2364.497617
ML11	-2208.582752	-2208.411066	-2208.436395
ML12	-2247.918924	-2247.715698	-2247.743880
ML13	-2287.256057	-2287.021910	-2287.050911
ML14	-2562.608757	-2562.157475	-2562.202894
ML15	-2709.097824	-2708.738447	-2708.785877

Table S9. M06L energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.462411	-1899.442339	-1899.456242
L01	-307.769452	-307.635351	-307.649652
L02	-499.539502	-499.345987	-499.367857
L03	-924.067354	-923.665116	-923.706359
L04	-766.784282	-766.508652	-766.540292
L05	-766.792533	-766.517926	-766.548022
L06	-766.793244	-766.518453	-766.548415
L07	-614.337921	-614.090530	-614.116334
L08	-850.254970	-849.816881	-849.855368
L09	-850.260767	-849.822920	-849.860046
L10	-232.488237	-232.358788	-232.371148
L11	-308.909685	-308.750240	-308.763763
L12	-348.230276	-348.039214	-348.055688
L13	-387.550907	-387.327722	-387.347170
L14	-662.790817	-662.346196	-662.380301
L15	-809.218086	-808.869071	-808.904306
ML01	-2207.254291	-2207.098082	-2207.126512
$M(L01)_{2\ cis}$	-2515.048797	-2514.757301	-2514.797994
ML02	-2399.022607	-2398.807017	-2398.842066
ML03	-2823.557520	-2823.136081	-2823.193407
ML04	-2666.275902	-2665.982644	-2666.027722
ML05	-2666.275792	-2665.978497	-2666.022052
ML06	-2666.274923	-2665.978113	-2666.020670
ML07	-2513.835261	-2513.569387	-2513.608340
ML08	-2749.755958	-2749.298889	-2749.351872
ML09	-2749.760198	-2749.301493	-2749.355861
ML10	-2131.977863	-2131.826899	-2131.853007
$M(L10)_{2cis}$	-2364.496454	-2364.217527	-2364.253284
ML11	-2208.408984	-2208.234111	-2208.258187
ML12	-2247.728947	-2247.521573	-2247.548472
ML13	-2287.043559	-2286.804443	-2286.832683
ML14	-2562.289844	-2561.829950	-2561.872967
ML15	-2708.717397	-2708.351351	-2708.396894

Table S10. M06 energy in vacuum (for comparison with the CCSD(T) values) and enthalpy values in TCE using the PCM and SMD solvation models (for comparison with the experimental values). All values in atomic units.

System	E In vacuum	H in TCE (PCM)	H in TCE (SMD)
M	-1899.338297	-1899.318199	-1899.331839
L01	-307.619327	-307.486061	-307.500484
L02	-499.265448	-499.072940	-499.095028
L03	-923.569915	-923.168707	-923.212021
L04	-766.390825	-766.116699	-766.148460
L05	-766.399390	-766.126156	-766.156515
L06	-766.399825	-766.126162	-766.156351
L07	-614.043871	-613.798890	-613.825304
L08	-849.803856	-849.368945	-849.407504
L09	-849.810791	-849.375722	-849.413198
L10	-232.362637	-232.234147	-232.246556
L11	-308.761568	-308.602898	-308.616469
L12	-348.055707	-347.865834	-347.882297
L13	-387.350259	-387.128615	-387.148047
L14	-662.408718	-661.967352	-662.001666
L15	-808.749619	-808.402603	-808.437979
ML01	-2206.976520	-2206.821230	-2206.850017
$M(L01)_{2\ cis}$	-2514.616710	-2514.326705	-2514.367674
ML02	-2398.620427	-2398.405775	-2398.441001
ML03	-2822.928112	-2822.508692	-2822.566998
ML04	-2665.749353	-2665.458073	-2665.503729
ML05	-2665.754594	-2665.458435	-2665.502427
ML06	-2665.753443	-2665.457798	-2665.500865
ML07	-2513.409154	-2513.143704	-2513.184153
ML08	-2749.172960	-2748.718731	-2748.772102
ML09	-2749.179334	-2748.723091	-2748.778282
ML10	-2131.725215	-2131.575121	-2131.601542
$M(L10)_{2cis}$	-2364.114013	-2363.836553	-2363.872458
ML11	-2208.129884	-2207.955463	-2207.980324
ML12	-2247.423071	-2247.216987	-2247.244146
ML13	-2286.710633	-2286.472933	-2286.501195
ML14	-2561.775556	-2561.318500	-2561.362650
ML15	-2708.117366	-2707.752877	-2707.798690

Table S11. DLPNO-CCSD(T) energy in calculated with the TZ and QZ basis sets, and extrapolated to CBS limit. All values in atomic units.

System	TZ	QZ	CBS
M	-2698.119284	-2698.237087	-2698.314769
L01	-307.375482	-307.470062	-307.528492
L02	-498.821972	-498.969141	-499.060726
L03	-922.765605	-923.039931	-923.210818
L04	-765.744563	-765.972395	-766.113917
L05	-765.752566	-765.981431	-766.123799
L06	-765.752896	-765.980758	-766.122403
L07	-613.556857	-613.744095	-613.860069
L08	-849.081279	-849.336774	-849.496107
L09	-849.087303	-849.342538	-849.501764
L10	-232.163484	-232.234533	-232.278669
L11	-308.520611	-308.617338	-308.677093
L12	-347.775091	-347.883481	-347.950552
L13	-387.030104	-387.150269	-387.224744
L14	-661.811769	-662.011840	-662.137026
L15	-807.993769	-808.229161	-808.376250
ML01	-3005.512405	-3005.725244	-3005.862156
$M(L01)_{2\ cis}$	-3312.908053	-3313.215458	-3313.411242
ML02	-3196.955806	-3197.221519	-3197.391708
ML03	-3620.906657	-3621.299177	-3621.548616
ML04	-3463.885042	-3464.231151	-3464.451292
ML05	-3463.887885	-3464.234232	-3464.454407
ML06	-3463.885685	-3464.231982	-3464.452129
ML07	-3311.699268	-3312.004551	-3312.198966
ML08	-3547.229747	-3547.603882	-3547.841876
ML09	-3547.235527	-3547.609621	-3547.847551
ML10	-2930.305420	-2930.494780	-2930.617378
$M(L10)_{2cis}$	-3162.494370	-3162.754421	-3162.921364
ML11	-3006.669040	-3006.883574	-3007.021661
ML12	-3045.921651	-3046.148030	-3046.293588
ML13	-3085.169715	-3085.407556	-3085.560486
ML14	-3359.958366	-3360.277415	-3360.481380
ML15	-3506.141779	-3506.495584	-3506.721258

Cartesian coordinates of all systems

PBE.M

Ti	0.000008	0.000049	-0.000097
Cl	1.732219	-1.129798	0.778749
Cl	-1.303273	-1.356648	-1.159606
Cl	0.713031	1.632883	-1.307445
Cl	-1.141995	0.853521	1.688420

PBE.L01

O	1.238388	1.368738	0.000001
C	1.075401	0.136076	-0.000001
O	-0.178091	-0.461177	-0.000002
C	2.166901	-0.898802	0.000000
C	-1.345831	0.467606	0.000001
C	-2.596372	-0.394352	-0.000001
H	-1.274061	1.109295	0.890739
H	-1.274062	1.109300	-0.890733
H	-3.489917	0.249745	0.000001
H	-2.633980	-1.036478	-0.892058
H	-2.633980	-1.036482	0.892053
H	3.139986	-0.395668	-0.000018
H	2.083153	-1.545002	0.886440
H	2.083131	-1.545029	-0.886417

PBE.L02

O	-1.465477	0.160122	1.077681
C	-0.323123	0.127704	1.580629
O	-0.113247	0.161935	2.951884
C	0.942986	0.049984	0.808833
C	-1.339078	0.240126	3.793522
C	0.858551	0.009335	-0.598279
H	-0.127869	0.036468	-1.062871
C	2.207094	0.016145	1.433519
C	3.370367	-0.057496	0.656403
C	3.280549	-0.097756	-0.744958
C	2.023021	-0.064235	-1.371125
H	1.952145	-0.095486	-2.460354
H	4.189232	-0.155177	-1.348289
H	4.347780	-0.083547	1.142980
H	2.266665	0.047770	2.520734
C	-0.880721	0.267458	5.241563
H	-1.894860	1.145882	3.509093
H	-1.969075	-0.632582	3.566173
H	-1.758176	0.325395	5.904966
H	-0.316549	-0.641744	5.495840
H	-0.242121	1.140935	5.438599

PBE.L03

O	-0.904070	1.104818	0.389984
C	-0.036184	0.320559	0.818086
O	-0.283475	-0.590123	1.833650
C	1.383007	0.284260	0.368997
C	-1.660238	-0.569310	2.398900
C	1.735578	0.671416	-0.947350
C	0.735510	0.945185	-2.022419
O	0.773832	1.933046	-2.778598
O	-0.185608	-0.074590	-2.138830
C	-1.293525	0.157785	-3.105015
C	2.402154	-0.014596	1.295108

C	3.750911	0.092496	0.933690
C	4.097672	0.508899	-0.360526
C	3.092550	0.798914	-1.292093
H	3.345410	1.119474	-2.303755
H	5.147112	0.605680	-0.645355
H	4.528794	-0.137121	1.664503
H	2.122670	-0.311166	2.305639
C	-2.188459	-1.081415	-3.101276
H	-1.835568	1.057726	-2.777856
H	-0.857952	0.347045	-4.099197
C	-3.433348	-0.803853	-3.971227
C	-1.434487	-2.334751	-3.585307
H	-2.519779	-1.245824	-2.059912
C	-1.734088	-1.619670	3.507623
H	-1.865473	0.444502	2.779296
H	-2.367231	-0.784413	1.583538
C	-3.193948	-1.726870	3.998881
H	-1.441563	-2.589583	3.066076
C	-0.776577	-1.297312	4.670744
H	-2.084762	-3.222873	-3.541559
H	-1.103654	-2.209276	-4.631029
H	-0.545999	-2.526089	-2.966103
H	-4.111515	-1.671291	-3.959239
H	-3.995802	0.071432	-3.608431
H	-3.149059	-0.616626	-5.020797
H	-0.828688	-2.077734	5.446175
H	0.264178	-1.229438	4.321880
H	-1.044734	-0.335234	5.140711
H	-3.281119	-2.500990	4.776827
H	-3.535720	-0.773469	4.436450
H	-3.880931	-1.992052	3.179154

PBE.L04

O	-1.158944	1.007004	0.474503
C	-0.288789	0.235451	0.921383
O	-0.512792	-0.597369	2.007255
C	1.109739	0.136508	0.421409
C	-1.865272	-0.500974	2.626572
C	1.420521	0.455080	-0.923491
C	0.386946	0.716644	-1.969758
O	0.415137	1.681566	-2.755569
O	-0.554667	-0.289690	-2.025396
C	-1.687217	-0.063444	-2.968405
C	2.155635	-0.156537	1.319412
C	3.491180	-0.109410	0.901064
C	3.798056	0.240223	-0.422661
C	2.765688	0.523196	-1.326176
H	2.987996	0.792067	-2.359852
H	4.837622	0.290464	-0.752250
H	4.290467	-0.333555	1.610134
H	1.907095	-0.401700	2.351517
C	-2.603587	-1.269065	-2.854945
H	-2.181813	0.873733	-2.673579
H	-1.273874	0.062613	-3.979859
H	-3.457677	-1.149646	-3.540275
H	-2.074176	-2.195737	-3.121115
H	-2.993385	-1.371033	-1.831820
C	-1.887387	-1.471226	3.794844
H	-2.027154	0.541938	2.937156
H	-2.611224	-0.749140	1.857217

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  H     -2.875374    -1.440940     4.280821
  H     -1.700317    -2.500868     3.457093
  H     -1.127379    -1.207262     4.544769
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PBE.L05
  O      1.202340     0.158586     1.001648
  C      0.764825     1.217260     1.494017
  O      0.808133     1.483477     2.854538
  C      0.147166     2.324575     0.717241
  C      1.414501     0.419802     3.703796
  C      0.044071     2.176494    -0.676612
  H      0.411955     1.268766    -1.155018
  C     -0.330079     3.500834     1.333138
  C     -0.904086     4.515822     0.556280
  C     -1.006848     4.368302    -0.833280
  C     -0.531663     3.194703    -1.455815
  C     -0.615960     2.986915    -2.925767
  H     -1.451821     5.153062    -1.443577
  H     -1.272617     5.425085     1.035487
  H     -0.246742     3.608558     2.413766
  C      1.359455     0.913661     5.139087
  H      0.842124    -0.507370     3.553018
  H      2.443287     0.247183     3.354793
  H      1.799318     0.155571     5.806211
  H      1.927008     1.848046     5.259033
  H      0.321970     1.091614     5.457731
  O     -1.201661     4.060234    -3.580502
  O     -0.212833     1.971401    -3.526484
  C     -1.322968     3.928806    -5.059807
  C     -1.983847     5.199701    -5.564838
  H     -0.314892     3.782277    -5.474911
  H     -1.916327     3.028305    -5.276645
  H     -2.094573     5.146925    -6.659456
  H     -2.983105     5.329167    -5.124049
  H     -1.377788     6.084981    -5.322871
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PBE.L06
  O      1.103004     0.207757     0.879696
  C      0.699082     1.241438     1.450872
  O      0.828053     1.440445     2.815411
  C      0.036351     2.382886     0.766535
  C      1.484133     0.338448     3.574445
  C     -0.153313     2.297624    -0.628154
  H      0.191113     1.403162    -1.148511
  C     -0.400233     3.529395     1.462996
  C     -1.017372     4.573734     0.770725
  C     -1.207036     4.488472    -0.623964
  C     -0.770452     3.341963    -1.320426
  H     -0.919054     3.280398    -2.397554
  C     -1.869767     5.629919    -1.308301
  H     -1.361798     5.468195     1.291081
  H     -0.251631     3.590960     2.540125
  C      1.514548     0.762242     5.032552
  H      0.903658    -0.581882     3.412960
  H      2.490294     0.186388     3.156597
  H      1.993719    -0.025837     5.634675
  H      2.087750     1.691582     5.163663
  H      0.497907     0.921211     5.420623
  O     -1.998737     5.430913    -2.672841
  O     -2.273689     6.663601    -0.737125
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  C     -2.654817     6.532910    -3.431875
  C     -2.685232     6.109116    -4.889982
  H     -3.660979     6.684970    -3.014027
  H     -2.074342     7.453239    -3.270390
  H     -3.164403     6.897195    -5.492105
  H     -1.668592     5.950147    -5.278053
  H     -3.258435     5.179775    -5.021092
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PBE.L07
  C     -5.383793     0.612699     0.430519
  C     -4.319893    -0.319605    -0.121995
  O     -3.000782     0.337126     0.117253
  C     -1.885628    -0.356275    -0.319212
  O     -1.949716    -1.479462    -0.852779
  O      1.949558     1.477719    -0.856152
  C      1.885570     0.355618    -0.320293
  C      0.625936    -0.442535    -0.087464
  C     -0.625950     0.442345    -0.088233
  H     -0.541829     1.193291    -0.893502
  O      3.000805    -0.336894     0.117375
  C      4.319871     0.319351    -0.123448
  C      5.383870    -0.611806     0.430806
  H      0.541657    -1.195098    -0.891207
  H      0.724585    -1.012696     0.847967
  H     -0.724419     1.014385     0.846070
  H     -4.426289    -0.489507    -1.203600
  H     -4.311024    -1.298152     0.380200
  H      4.426082     0.487025    -1.205418
  H      4.311081     1.298930     0.376732
  H     -6.380041     0.168926     0.276031
  H     -5.243337     0.778470     1.508559
  H     -5.357783     1.587663    -0.077468
  H      6.380090    -0.168347     0.275233
  H      5.243599    -0.775354     1.509209
  H      5.357780    -1.587816    -0.075165
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PBE.L08
  C      0.735861     0.844572    -2.746338
  C     -0.540602     1.633202    -2.510156
  O     -0.135459     2.966211    -1.971848
  C     -1.171446     3.837416    -1.678721
  O     -2.365012     3.536003    -1.871127
  C     -0.723109     5.176970    -1.106000
  C     -1.093411     5.293592     0.426631
  C     -2.591511     5.079450     0.620881
  O     -3.145172     4.186310     1.284035
  C      0.739102     5.583772    -1.449108
  C      0.910946     5.711030    -2.980918
  C      1.135990     6.923530    -0.790462
  C     -0.200225     4.508494     1.432562
  C     -0.300732     2.968119     1.379818
  C     -0.454370     5.017002     2.871116
  O     -3.304590     6.071893    -0.036885
  C     -4.786160     5.915003    -0.037840
  C     -5.353620     7.061090    -0.857628
  H      1.294374     0.704316    -1.809341
  H      1.390384     1.354853    -3.468099
  H      0.485982    -0.149243    -3.150211
  H     -1.205615     1.157265    -1.774376
  H     -1.115645     1.798490    -3.433115
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  H     -1.389769     5.906753    -1.599036
  H     -0.940348     6.364159     0.649522
  H      1.421624     4.794840    -1.091075
  H      1.950420     5.980070    -3.227392
  H      0.675170     4.771491    -3.499391
  H      0.254900     6.504236    -3.379314
  H      2.135150     7.229784    -1.138300
  H      0.427520     7.723750    -1.066536
  H      1.174740     6.865557     0.307690
  H      0.839896     4.779158     1.171894
  H      0.361820     2.534416     2.146775
  H     -1.327171     2.634091     1.582747
  H      0.018961     2.570979     0.407015
  H      0.271581     4.568322     3.567642
  H     -0.350906     6.113315     2.936216
  H     -1.464267     4.742629     3.211848
  H     -5.016028     4.930695    -0.471086
  H     -5.135563     5.927171     1.005195
  H     -5.085551     8.034022    -0.419698
  H     -4.979875     7.028021    -1.891343
  H     -6.452343     6.986453    -0.886078
---------------------------------------------
PBE.L09
  C     -1.448824     0.651088     0.789379
  H     -1.746735     1.322337     1.606555
  H     -0.407301     0.343718     0.957412
  H     -2.093909    -0.242019     0.822976
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  H     -1.345568     0.670693    -1.397038
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  O     -0.630506     2.460119    -0.716913
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  H      1.884407     5.427015     0.636819
  C      0.561681     4.844952     2.250025
  C      1.912919     3.304746     0.776666
  C      1.736811     5.887062    -1.941573
  H      1.173853     3.797087    -1.984334
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  C     -0.649583     4.200791     1.150231
  C     -0.545211     4.345528    -0.249538
  C     -0.387405     3.210139    -1.059087
  H     -0.306910     3.319865    -2.137595
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  H      0.282976    -0.456940    -5.678474
  H     -0.765452     0.905573    -5.210407
  H      1.011478     1.049314    -5.065951
  O     -0.494040     5.732207    -2.193551
  O     -0.747802     6.756848    -0.136427
  C     -0.547242     7.075610    -2.842273
  C     -0.402326     6.851755    -4.336897
  H     -1.505041     7.545185    -2.574477
  H      0.265098     7.687894    -2.424196
  H     -0.436376     7.821718    -4.857418
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  H     -1.217908     6.224867    -4.725734
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PBE.ML06
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  Ti     0.013232    -2.516118    -0.225861
  Cl     0.167502    -4.730351     0.162806
  Cl     2.122337    -2.369221    -1.086509
  Cl    -0.213895    -1.912970     1.936452
  H     -0.393569     0.753194     1.400438
  C     -0.435972     1.746063     0.952102
  C     -0.330902     1.884663    -0.449526
  C     -0.165546     0.676112    -1.274759
  O     -0.110329    -0.494347    -0.786692
  O     -0.076272     0.909495    -2.603424
  C      0.094805    -0.256632    -3.545498
  C     -0.592979     2.878755     1.751733
  C     -0.646808     4.159551     1.165692
  C     -0.541794     4.297847    -0.234540
  C     -0.384856     3.168134    -1.038771
  H     -0.303213     3.267876    -2.120169
  H     -0.584367     5.291119    -0.678689
  C     -0.815440     5.333482     2.068216
  H     -0.675982     2.792816     2.835416
  C      0.162469     0.325760    -4.942967
  H      1.015435    -0.780768    -3.255459
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  H     -0.760454     0.866423    -5.196797
  H      1.016750     1.009141    -5.051252
  O     -0.853031     6.529950     1.378140
  O     -0.912983     5.259511     3.308826
  C     -1.019922     7.758154     2.210547
  C     -1.032656     8.940731     1.258695
  H     -1.956935     7.659181     2.777893
  H     -0.186674     7.798505     2.927294
  H     -1.154380     9.872143     1.833648
  H     -0.091285     9.006712     0.694092
  H     -1.865557     8.867228     0.544424
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PBE.ML07
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  Ti     0.073314    -1.758230     0.010263
  Cl    -0.354765    -3.126231     1.764752
  Cl    -0.109417    -3.251338    -1.677758
  Cl     2.408733    -1.814233     0.185894
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  C      0.073970     2.054458    -0.659232
  C      0.459801     1.017850    -1.677817
  O      0.535183    -0.219361    -1.466068
  O      0.731650     1.532587    -2.901438
  C      1.081460     0.547931    -3.993151
  H      0.933979     3.100324     1.049725
  H      0.058913     3.033668    -1.152670
  C      1.312077     1.358479    -5.252677
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  H      0.409798     1.917730    -5.538486
  H      2.142231     2.068107    -5.126032
  C      1.269273     1.138718     5.263151
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  H      2.321002     1.455583     5.218649
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PBE.ML08
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  Cl     0.028266    -2.965161     2.206474
  Cl    -0.247357    -3.246013    -1.252216
  Cl     2.388730    -1.595358     0.127036
  O      0.423896     0.065859     1.620601
  C      0.316513     1.322372     1.571380
  O      1.049155     2.096050     2.411208
  C     -0.597692     2.074371     0.626626
  C      1.978873     1.380600     3.361533
  C      0.085269     2.339765    -0.760410
  C      0.176005     1.067791    -1.575762
  O      0.143384    -0.105329    -1.126602
  O      0.291175     1.293174    -2.909203
  C      0.400411     0.073843    -3.796437
  H     -1.429342     1.372484     0.437552
  C      1.457520     3.115836    -0.693315
  C      0.539915     0.580264    -5.218085
  H      1.269139    -0.505188    -3.454321
  H     -0.505201    -0.527608    -3.638089
  H      0.617604    -0.281636    -5.898943
  H     -0.333862     1.176387    -5.518023
  H      1.444452     1.193728    -5.338581
  C      2.751063     2.452582     4.104895
  H      1.355306     0.761584     4.021568
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  H      3.434985     1.971527     4.821329
  H      3.352647     3.062304     3.415358
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  H      2.523062     4.694130    -1.761372
  H      1.574576     3.623312    -2.824084
  H      0.750991     4.858179    -1.835031
  C     -2.134749     4.118860     0.313748
  C     -2.024783     2.942901     2.538925
  H     -0.396561     4.018487     1.603571
  H     -2.666611     4.912856     0.860270
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  H     -2.896009     3.452446    -0.126086
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PBE.ML09
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  Ti    -0.000273     1.914131    -0.000382
  Cl     1.713313     3.369328     0.295991
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  Cl    -0.393468     1.588555     2.292327
  O      1.363535     0.253300     0.199177
  C      1.595412    -0.982246     0.243426
  O      2.860314    -1.446020     0.068647
  C      0.590904    -2.081215     0.514102
  C      3.935423    -0.412652    -0.173390
  C     -0.590208    -2.081525    -0.513881
  C     -1.595056    -0.982801    -0.243479
  O     -1.363562     0.252826    -0.199527
  O     -2.859815    -1.446926    -0.068593
  C     -3.935247    -0.413835     0.173188
  H      1.130247    -3.029773     0.369773
  H     -1.129257    -3.030214    -0.369319
  C     -5.232661    -1.172889     0.368999
  H     -3.636450     0.171345     1.053670
  H     -3.951622     0.252350    -0.700587
  H     -6.047377    -0.452525     0.541392
  H     -5.484751    -1.770129    -0.519065
  H     -5.177254    -1.841770     1.239918
  C      5.233073    -1.171348    -0.369022
  H      3.636440     0.172220    -1.054013
  H      3.951594     0.253751     0.700222
  H      6.047563    -0.450772    -0.541595
  H      5.485354    -1.768293     0.519186
  H      5.177871    -1.840459    -1.239777
  C     -0.123112    -2.046766    -2.013005
  C      0.123802    -2.046225     2.013218
  C     -0.759941    -3.268883     2.335705
  C      1.332197    -1.991653     2.970479
  H     -0.461223    -1.122953     2.166890
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PBE.ML10
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  Cl     2.248653    -0.220717     0.710986
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  Cl    -0.171764    -1.549844     2.603484
  Cl    -0.636632     1.758204     2.461155
  O      0.211325     1.660772    -0.431237
  C     -0.786027     2.773294    -0.628862
  C     -0.320114     3.480137    -1.899151
  C      0.237712     2.322664    -2.757043
  C      0.941063     1.424520    -1.736804
  H     -1.776875     2.306659    -0.742388
  H     -0.754507     3.381266     0.279787
  H      0.470582     4.210282    -1.667096
  H     -1.147448     4.007561    -2.393709
  H      0.933657     2.670625    -3.532910
  H     -0.584631     1.778461    -3.246274
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  H      1.987117     1.701537    -1.552441
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PBE.ML10-cis
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  Cl     2.337024    -0.002083     0.628450
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  Cl     0.008651    -1.725253     2.395813
  Cl    -0.008649     1.725253     2.395813
  O     -0.027305     1.435455    -0.744446
  O      0.027305    -1.435455    -0.744446
  C     -0.978233     2.607063    -0.806816
  C     -0.344729     3.571476    -1.811230
  C      0.429555     2.635328    -2.766928
  C      1.014401     1.591895    -1.816183
  C      0.978232    -2.607064    -0.806815
  C      0.344728    -3.571477    -1.811230
  C     -0.429555    -2.635327    -2.766928
  C     -1.014401    -1.591894    -1.816183
  H     -1.946083     2.205927    -1.135567
  H     -1.065272     2.996691     0.213511
  H      0.349995     4.258377    -1.303592
  H     -1.106461     4.169232    -2.330771
  H      1.218174     3.159953    -3.324172
  H     -0.257165     2.168688    -3.491376
  H      1.172681     0.598357    -2.250080
  H      1.938627     1.927857    -1.327258
  H      1.946082    -2.205929    -1.135566
  H      1.065270    -2.996692     0.213512
  H      1.106459    -4.169233    -2.330771
  H     -0.349998    -4.258377    -1.303592
  H      0.257166    -2.168688    -3.491376
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  Cl    -1.874012    -3.025936    -1.701910
  Cl     1.099380    -2.041940    -0.380919
  O     -0.528906    -0.616208     1.771907
  C     -0.815548     0.800145     1.453172
  O     -1.085058     0.024713    -0.792427
  C     -0.400643     1.050771     0.017033
  H     -1.897069     0.925160     1.586453
  H     -0.263710     1.449798     2.147077
  H     -0.732933     2.046600    -0.318355
  H      0.687786     0.943701    -0.124999
  C     -0.817430     0.180898    -2.238232
  H     -1.078256     1.208096    -2.532350
  H      0.240724    -0.038472    -2.445380
  H     -1.461424    -0.540764    -2.746597
  C      0.633598    -0.841520     2.656889
  H      1.560507    -0.526209     2.156838
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  H      0.659870    -1.917949     2.847463
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PBE.ML12
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  Cl    -2.423444    -0.002265     0.429650
  Cl    -1.608461    -2.731959     2.244857
  Cl    -2.637897    -3.074532    -1.035852
  Cl     0.636609    -3.466839    -0.196751
  O      0.534896    -0.689305     1.030010
  C      0.764077     0.736021     0.678188
  O     -0.386363    -0.947982    -1.655696
  C      1.091639     0.867186    -0.807865
  H     -0.145069     1.290779     0.951970
  H      1.608724     1.090707     1.286584
  H      1.346969     1.925644    -0.997680
  H      1.985535     0.268141    -1.046750
  C     -0.061066    -1.704697    -2.884128
  H      1.027762    -1.705457    -3.038945
  H     -0.418663    -2.725061    -2.731779
  H     -0.585756    -1.238989    -3.731136
  C      1.325879    -1.149454     2.191314
  C     -0.054423     0.499643    -1.747989
  H      0.220072     0.703049    -2.793124
  H     -0.977988     1.038999    -1.498943
  H      0.930810    -0.689004     3.108640
  H      1.220170    -2.235801     2.232298
  H      2.380221    -0.879830     2.032651
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PBE.ML13
  Ti    -0.664688    -2.213813     0.047272
  Cl    -2.600927    -1.060772     0.709111
  Cl    -0.474933    -3.435508     1.961582
  Cl    -1.787904    -3.791073    -1.154976
  Cl     1.461000    -2.787093    -0.768552
  O      0.385517    -0.535386     1.039315
  C      1.549285     0.237313     0.508235
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  C      1.187759     1.000884    -0.778042
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  H      1.850649     1.880376    -0.826019
  H      1.424797     0.376127    -1.650709
  C     -0.584321    -1.445397    -3.072297
  H      0.026661    -0.772428    -3.691350
  H     -0.087018    -2.411340    -2.964688
  H     -1.588053    -1.575295    -3.502043
  C      0.141357    -0.269632     2.477135
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  H     -0.376276     2.473831    -1.214356
  H     -0.728773     1.448109     0.181815
  H      0.093785     0.817861     2.633725
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  Cl    -3.341565    -2.172822    -0.354362
  Cl    -0.369879    -3.777056    -0.084547
  O      0.789121    -1.107166     0.909015
  C      1.437084     0.142228     0.419719
  O     -0.491303    -1.124072    -1.566182
  C      1.644722     0.121432    -1.110742
  H      0.781113     0.967046     0.725349
  H      2.400870     0.230649     0.939304
  C      2.375013     1.454880    -1.492999
  C      2.513332    -1.129932    -1.521502
  C     -1.228891    -1.624140    -2.749531
  H     -0.564178    -1.584838    -3.623726
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  H     -2.129588    -1.015614    -2.913478
  C      1.560224    -1.816425     1.954661
  C      0.279767     0.124529    -1.828545
  H      0.426290     0.192702    -2.915845
  H     -0.345130     0.961610    -1.490110
  H      1.485062    -1.260319     2.900214
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  C      1.569868     2.770445    -1.383034
  H      3.271498     1.541221    -0.852889
  C      2.451631     4.042952    -1.467920
  H      0.810673     2.826740    -2.184851
  H      1.014124     2.804828    -0.429949
  C      1.595834     5.301254    -1.215052
  H      3.210441     3.977385    -0.662808
  C      3.192520     4.154864    -2.817104
  H      2.217849     6.210585    -1.222654
  H      0.826107     5.415055    -1.997648
  H      1.082013     5.248634    -0.241692
  H      3.784691     5.082704    -2.861105
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  H      3.240095    -2.236040    -3.246641
  H      1.586424    -1.655715    -3.460722
  H      2.958343    -0.521486    -3.602890
  H      4.448615    -2.047758    -1.129407
  H      4.565827    -0.321738    -1.525267
  H      4.024726    -0.833192     0.089016
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PBE.ML15
  Ti    -0.950270    -2.140014     0.296094
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  C     -1.184721    -0.423846    -0.134122
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PBE1.L11
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  C      1.346897     1.314420    -5.180485
  H      2.011238     0.006354    -3.570608
  H      0.307865    -0.195155    -4.003659
  H      1.631325     0.629346    -5.982905
  H      0.441891     1.840861    -5.487576
  H      2.149111     2.043422    -5.054987
  C      1.376111     1.058573     5.168652
  H     -0.201166     0.165567     3.961657
  H      1.419671    -0.439899     3.587620
  H      1.292977     0.334576     5.982944
  H      2.426198     1.337135     5.067957
  H      0.803357     1.946204     5.442128
  H     -0.999649     1.824351    -0.371914
  H      1.986784     2.093139     0.292051
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PBE1.ML08
  Ti     0.051883    -1.619760     0.347471
  Cl    -2.208908    -1.051973     0.488331
  Cl     0.055223    -2.916922     2.169407
  Cl    -0.258825    -3.169792    -1.255504
  Cl     2.366200    -1.554014     0.095562
  O      0.411397     0.082287     1.582199
  C      0.310765     1.325701     1.549059
  O      1.041657     2.070718     2.377649
  C     -0.603873     2.077347     0.621675
  C      1.963435     1.369257     3.305201
  C      0.063686     2.342233    -0.756445
  C      0.163313     1.077335    -1.560516
  O      0.114609    -0.075511    -1.099370
  O      0.303546     1.277376    -2.870511
  C      0.425654     0.077107    -3.738684
  H     -1.435683     1.386435     0.442263
  C      1.422850     3.113093    -0.698731
  C      0.603125     0.572770    -5.149307
  H      1.274393    -0.506212    -3.379375
  H     -0.478766    -0.517727    -3.606018
  H      0.688705    -0.283768    -5.822443
  H     -0.250686     1.172656    -5.468593
  H      1.508620     1.173859    -5.248080
  C      2.731798     2.431805     4.045920
  H      1.355069     0.747202     3.963290
  H      2.601006     0.714627     2.709596
  H      3.418570     1.955138     4.749680
  H      3.320009     3.044586     3.360662
  H      2.063734     3.084170     4.610765
  H     -0.638191     2.970508    -1.309584
  C     -1.195254     3.342677     1.290305
  C      1.541532     4.112517    -1.851928
  H      1.395564     3.679122     0.238886
  C      2.645381     2.191189    -0.660377
  H      3.545595     2.775383    -0.454324
  H      2.576986     1.407230     0.096299
  H      2.794719     1.694578    -1.623928
  H      2.476764     4.673227    -1.772495
  H      1.536011     3.600236    -2.816936
  H      0.718429     4.833189    -1.845312
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  C     -2.103762     4.123668     0.335603
  C     -1.996110     2.934870     2.534014
  H     -0.374237     3.993731     1.607197
  H     -2.627791     4.908166     0.887060
  H     -1.555722     4.614977    -0.471795
  H     -2.863697     3.472479    -0.109190
  H     -2.400215     3.819668     3.031860
  H     -2.835835     2.289806     2.258190
  H     -1.386078     2.399172     3.264484
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PBE1.ML09
  Cl     0.455322     1.553782    -2.266508
  Ti    -0.000263     1.855258    -0.000376
  Cl     1.688715     3.296692     0.341085
  Cl    -1.689690     3.296080    -0.342197
  Cl    -0.455753     1.554205     2.265830
  O      1.325688     0.224664     0.232586
  C      1.574669    -0.994290     0.253452
  O      2.821753    -1.426139     0.064399
  C      0.581902    -2.091377     0.513421
  C      3.874280    -0.405048    -0.171679
  C     -0.581202    -2.091685    -0.513199
  C     -1.574309    -0.994843    -0.253502
  O     -1.325706     0.224193    -0.232932
  O     -2.821260    -1.427033    -0.064349
  C     -3.874105    -0.406213     0.171475
  H      1.123532    -3.029435     0.374877
  H     -1.122540    -3.029877    -0.374424
  C     -5.164764    -1.150476     0.389823
  H     -3.570245     0.187957     1.034147
  H     -3.901051     0.247123    -0.701735
  H     -5.969183    -0.431860     0.564700
  H     -5.428204    -1.751486    -0.482076
  H     -5.100839    -1.806901     1.259249
  C      5.165172    -1.148961    -0.389843
  H      3.570233     0.188812    -1.034499
  H      3.901021     0.248513     0.701368
  H      5.969364    -0.430137    -0.564900
  H      5.428800    -1.749670     0.482206
  H      5.101451    -1.805623    -1.259105
  C     -0.109204    -2.049233    -1.995454
  C      0.109894    -2.048703     1.995666
  C     -0.761768    -3.264891     2.318066
  C      1.306996    -1.982005     2.947686
  H     -0.475676    -1.134085     2.141103
  C     -1.306324    -1.983150    -2.947493
  H      0.476079    -1.134468    -2.141117
  C      0.762841    -3.265228    -2.317547
  H      0.961256    -2.002353     3.983534
  H      1.981014    -2.832039     2.798851
  H      1.879491    -1.059331     2.821687
  H     -1.044516    -3.244405     3.373493
  H     -1.684913    -3.290920     1.735508
  H     -0.215126    -4.197587     2.140490
  H     -0.960575    -2.003643    -3.983336
  H     -1.980072    -2.833361    -2.798450
  H     -1.879112    -1.060627    -2.821722
  H      1.045583    -3.244920    -3.372979
  H      1.685995    -3.290820    -1.734983
  H      0.216494    -4.198052    -2.139735
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PBE1.ML10
  Ti     0.030260     0.115499     1.038466
  Cl     2.230432    -0.168255     0.717474
  Cl    -1.421935    -0.798138    -0.426752
  Cl    -0.175347    -1.527831     2.538044
  Cl    -0.680903     1.736341     2.411511
  O      0.194250     1.652322    -0.442873
  C     -0.758901     2.778786    -0.613638
  C     -0.312684     3.461579    -1.893584
  C      0.219064     2.298009    -2.736386
  C      0.934201     1.429432    -1.715991
  H     -1.759452     2.348222    -0.694705
  H     -0.688954     3.391482     0.279926
  H      0.481891     4.182872    -1.686678
  H     -1.136554     3.988943    -2.376066
  H      0.893010     2.623110    -3.530022
  H     -0.608164     1.748380    -3.191872
  H      0.896258     0.364986    -1.938138
  H      1.964818     1.732570    -1.534019
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PBE1.ML10-cis
  Ti     0.000001     0.000000     0.875250
  Cl     2.316411    -0.003746     0.628408
  Cl    -2.316410     0.003746     0.628411
  Cl     0.003368    -1.711325     2.358578
  Cl    -0.003365     1.711326     2.358577
  O     -0.024626     1.407513    -0.738536
  O      0.024625    -1.407513    -0.738536
  C     -0.971965     2.552064    -0.812227
  C     -0.340409     3.505794    -1.811869
  C      0.417865     2.566122    -2.756200
  C      0.997778     1.538137    -1.801556
  C      0.971964    -2.552065    -0.812227
  C      0.340407    -3.505794    -1.811869
  C     -0.417865    -2.566121    -2.756200
  C     -0.997778    -1.538136    -1.801556
  H     -1.928253     2.150337    -1.146117
  H     -1.074463     2.947166     0.195485
  H      0.355761     4.183043    -1.310925
  H     -1.092558     4.106435    -2.325101
  H      1.198825     3.074939    -3.323036
  H     -0.270676     2.098460    -3.465868
  H      1.152280     0.547440    -2.223226
  H      1.920315     1.873989    -1.329345
  H      1.928252    -2.150340    -1.146116
  H      1.074461    -2.947168     0.195485
  H      1.092556    -4.106437    -2.325101
  H     -0.355764    -4.183042    -1.310925
  H      0.270676    -2.098460    -3.465867
  H     -1.198825    -3.074937    -3.323037
  H     -1.152279    -0.547439    -2.223227
  H     -1.920315    -1.873987    -1.329346
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PBE1.ML11
  Ti    -1.166654    -1.972503     0.204662
  Cl    -3.274750    -1.280475     0.825008
  Cl    -1.045478    -3.697630     1.631349
  Cl    -1.843927    -2.992741    -1.678504
  Cl     1.107616    -2.037228    -0.373024
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  O     -0.492775    -0.608123     1.724822
  C     -0.785603     0.789108     1.435108
  O     -1.040106     0.003437    -0.782045
  C     -0.391852     1.040086     0.002809
  H     -1.855887     0.920854     1.585055
  H     -0.225629     1.429629     2.118438
  H     -0.747411     2.017456    -0.334809
  H      0.689984     0.962845    -0.143092
  C     -0.841550     0.167828    -2.216952
  H     -1.125629     1.184817    -2.493040
  H      0.202632    -0.031193    -2.466325
  H     -1.487927    -0.551351    -2.707316
  C      0.598864    -0.851720     2.658756
  H      1.539391    -0.499776     2.232380
  H      0.369625    -0.344795     3.597005
  H      0.641464    -1.925200     2.810555
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PBE1.ML12
  Ti    -1.062026    -1.899286     0.165703
  Cl    -2.406906    -0.007764     0.346551
  Cl    -1.621395    -2.689381     2.201543
  Cl    -2.559095    -3.044998    -1.070210
  Cl     0.654908    -3.437524    -0.158582
  O      0.484702    -0.672208     1.052226
  C      0.717916     0.731730     0.702301
  O     -0.283921    -0.963199    -1.623182
  C      1.107874     0.858008    -0.757234
  H     -0.198341     1.276695     0.930752
  H      1.522686     1.097371     1.343032
  H      1.361601     1.908303    -0.944331
  H      2.008268     0.267551    -0.951757
  C     -0.119176    -1.697408    -2.873915
  H      0.890314    -1.529738    -3.253148
  H     -0.258425    -2.749334    -2.654393
  H     -0.870242    -1.356774    -3.588408
  C      1.318253    -1.149616     2.151219
  C      0.017413     0.466700    -1.734976
  H      0.342894     0.651389    -2.760560
  H     -0.911790     1.006442    -1.550776
  H      1.030848    -0.631532     3.067534
  H      1.145716    -2.214685     2.251265
  H      2.366000    -0.966333     1.906976
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PBE1.ML13
  Ti    -0.652986    -2.181032     0.037663
  Cl    -2.574361    -1.055951     0.711812
  Cl    -0.451168    -3.401183     1.925865
  Cl    -1.765767    -3.746810    -1.147857
  Cl     1.450201    -2.746799    -0.779409
  O      0.382654    -0.540184     1.020174
  C      1.528559     0.224813     0.500331
  O     -0.720318    -0.861303    -1.689907
  C      1.175788     0.964266    -0.786938
  H      1.791831     0.936793     1.285516
  H      2.351938    -0.474577     0.359647
  H      1.849223     1.823707    -0.858800
  H      1.394165     0.324190    -1.643177
  C     -0.566591    -1.422241    -3.032532
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  H     -0.114502    -2.401374    -2.932234
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  H     -1.548942    -1.505155    -3.499562
  C      0.130651    -0.272417     2.436343
  C     -0.291352     1.423926    -0.825694
  H     -0.363934     2.444682    -1.213227
  H     -0.709890     1.441395     0.181617
  H      0.046855     0.806120     2.580765
  H     -0.802825    -0.753033     2.702505
  H      0.949809    -0.682501     3.028583
  C     -1.159969     0.543952    -1.718396
  H     -2.208119     0.565944    -1.421687
  H     -1.073964     0.861477    -2.759901
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PBE1.ML14
  Ti    -1.224288    -1.643317     0.433528
  Cl    -1.749504     0.615585     0.683130
  Cl    -1.582050    -2.141423     2.604267
  Cl    -3.281820    -2.143888    -0.351417
  Cl    -0.332860    -3.720543    -0.110859
  O      0.791496    -1.078693     0.893945
  C      1.432210     0.150289     0.410550
  O     -0.493984    -1.085919    -1.547215
  C      1.635204     0.128276    -1.108027
  H      0.791437     0.974879     0.717765
  H      2.390985     0.236205     0.922841
  C      2.363813     1.445503    -1.492036
  C      2.489317    -1.117166    -1.512627
  C     -1.202642    -1.612752    -2.712261
  H     -0.541980    -1.566301    -3.578050
  H     -1.453099    -2.645322    -2.491711
  H     -2.108540    -1.031251    -2.885792
  C      1.570360    -1.804607     1.894552
  C      0.277578     0.134059    -1.815287
  H      0.422339     0.196482    -2.895059
  H     -0.332898     0.974984    -1.488017
  H      1.552616    -1.248881     2.833059
  H      1.106679    -2.776006     2.023457
  H      2.589622    -1.926942     1.528022
  H      2.747248     1.332664    -2.510350
  C      1.557432     2.748553    -1.400771
  H      3.247101     1.539276    -0.849018
  C      2.433388     4.011726    -1.448502
  H      0.831489     2.807179    -2.221794
  H      0.971700     2.775610    -0.474983
  C      1.572628     5.260012    -1.240182
  H      3.150351     3.949724    -0.616709
  C      3.226564     4.117491    -2.754029
  H      2.187662     6.163952    -1.219652
  H      0.846625     5.370051    -2.052994
  H      1.016128     5.209623    -0.299923
  H      3.809834     5.042121    -2.779617
  H      3.924379     3.286284    -2.884120
  H      2.549596     4.128690    -3.615773
  C      2.527507    -1.383838    -3.022023
  C      3.934654    -1.045855    -0.997824
  H      1.999731    -1.980344    -1.049318
  H      3.212795    -2.210238    -3.228057
  H      1.555899    -1.675921    -3.421294
  H      2.887455    -0.518789    -3.588105
  H      4.415584    -2.019657    -1.122030
  H      4.524837    -0.317936    -1.562025
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  H      4.010893    -0.782113     0.059963
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PBE1.ML15
  Ti    -0.923611    -2.101546     0.276890
  Cl    -2.304094    -0.231926     0.448022
  Cl    -1.230328    -2.686826     2.431410
  Cl    -2.522385    -3.353562    -0.700299
  Cl     0.743950    -3.696113    -0.071125
  O      0.701667    -0.784803     0.825324
  C      0.792781     0.613261     0.397366
  O     -0.315718    -1.311205    -1.642583
  C      0.984964     0.739440    -1.116527
  H     -0.121491     1.109295     0.720820
  H      1.650200     1.060321     0.902101
  C      1.041594     2.226541    -1.456970
  C      2.355469     0.260687    -1.579105
  C     -0.322583    -2.141736    -2.846754
  H      0.562326    -1.903516    -3.437752
  H     -0.287132    -3.176029    -2.523649
  H     -1.238020    -1.950704    -3.408449
  C      1.634774    -1.129243     1.898040
  C     -0.162126     0.119112    -1.919072
  H      0.048419     0.231386    -2.983434
  H     -1.111907     0.596844    -1.681787
  H      1.329858    -0.622124     2.814487
  H      1.590688    -2.204522     2.029374
  H      2.638427    -0.830005     1.594381
  C      2.280373     2.551073    -2.036457
  C      2.548776     3.860051    -2.425993
  C      1.570492     4.834748    -2.230627
  C      0.341684     4.509126    -1.654969
  C      0.067859     3.196012    -1.262362
  H      3.499717     4.124291    -2.874045
  H      1.766600     5.857730    -2.529367
  H     -0.406327     5.279398    -1.510855
  H     -0.890104     2.951849    -0.815549
  C      2.901058    -1.015337    -1.531660
  C      4.195748    -1.210395    -2.023263
  C      4.927717    -0.146591    -2.551580
  C      4.381801     1.135586    -2.600200
  C      3.093977     1.335497    -2.112461
  H      2.342319    -1.848540    -1.123900
  H      4.633007    -2.201511    -1.991973
  H      5.929514    -0.317929    -2.927601
  H      4.955627     1.958035    -3.011921
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B3LYP.M
  Ti    -0.000006     0.000034    -0.000066
  Cl     1.730406    -1.128606     0.777907
  Cl    -1.301878    -1.355208    -1.158414
  Cl     0.712264     1.631130    -1.306057
  Cl    -1.140796     0.852656     1.686650
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B3LYP.L01
  O      1.247069     1.358606     0.000000
  C      1.073308     0.137970     0.000000
  O     -0.175252    -0.436491     0.000000
  C      2.156694    -0.900243     0.000000
  C     -1.344421     0.473542     0.000001
  C     -2.585357    -0.397673     0.000000
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  H     -1.281926     1.109999     0.883171
  H     -1.281925     1.110001    -0.883168
  H     -3.478646     0.231837     0.000001
  H     -2.615343    -1.035210    -0.884507
  H     -2.615343    -1.035213     0.884504
  H      3.125827    -0.409006    -0.000015
  H      2.067999    -1.540164     0.879467
  H      2.067981    -1.540185    -0.879449
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B3LYP.L02
  O     -1.456951     0.159660     1.069866
  C     -0.327221     0.127838     1.574644
  O     -0.131759     0.162327     2.933555
  C      0.938161     0.050206     0.806298
  C     -1.336951     0.240064     3.787084
  C      0.860090     0.009206    -0.593760
  H     -0.113894     0.035512    -1.062344
  C      2.191692     0.017175     1.434948
  C      3.353263    -0.056186     0.666987
  C      3.271674    -0.096903    -0.727660
  C      2.023453    -0.064093    -1.356634
  H      1.958886    -0.095559    -2.436491
  H      4.175420    -0.153868    -1.321075
  H      4.319402    -0.081551     1.154222
  H      2.246626     0.048940     2.512904
  C     -0.861663     0.265868     5.226875
  H     -1.891382     1.138761     3.515300
  H     -1.965408    -0.624476     3.571352
  H     -1.722436     0.323405     5.897652
  H     -0.298617    -0.636312     5.469529
  H     -0.224293     1.131224     5.413291
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B3LYP.L03
  O     -0.912713     1.086611     0.373962
  C     -0.052368     0.320651     0.818804
  O     -0.303283    -0.553985     1.845476
  C      1.363804     0.278571     0.367152
  C     -1.666017    -0.543679     2.419691
  C      1.717134     0.668448    -0.939833
  C      0.721612     0.955056    -2.014083
  O      0.763591     1.945710    -2.747807
  O     -0.188634    -0.052434    -2.157653
  C     -1.297314     0.170050    -3.110189
  C      2.374400    -0.040172     1.284188
  C      3.717659     0.050948     0.923120
  C      4.065719     0.470175    -0.361495
  C      3.067669     0.778695    -1.285117
  H      3.324193     1.100954    -2.285016
  H      5.106547     0.554600    -0.645136
  H      4.486561    -0.192810     1.644405
  H      2.096812    -0.340212     2.283497
  C     -2.167855    -1.083450    -3.120193
  H     -1.850371     1.047530    -2.773038
  H     -0.873504     0.378755    -4.094489
  C     -3.423187    -0.821430    -3.975320
  C     -1.393436    -2.313850    -3.622352
  H     -2.485889    -1.267524    -2.088470
  C     -1.724831    -1.597878     3.522350
  H     -1.871313     0.458250     2.803030
  H     -2.373384    -0.756398     1.617498
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  C     -3.178041    -1.727967     4.019843
  H     -1.425410    -2.553166     3.077830
  C     -0.765199    -1.273688     4.679743
  H     -2.022063    -3.207148    -3.587289
  H     -1.071455    -2.172412    -4.659204
  H     -0.507067    -2.496488    -3.013927
  H     -4.077879    -1.695610    -3.970552
  H     -3.997058     0.029070    -3.598665
  H     -3.154742    -0.614182    -5.015746
  H     -0.804035    -2.054155     5.443409
  H      0.264318    -1.193798     4.329251
  H     -1.037299    -0.326263     5.155930
  H     -3.250533    -2.500622     4.788018
  H     -3.529658    -0.789630     4.459339
  H     -3.859658    -1.997555     3.209078
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B3LYP.L04
  O     -1.162364     0.994539     0.465073
  C     -0.299538     0.237246     0.920246
  O     -0.526568    -0.570461     2.005874
  C      1.096540     0.137750     0.418981
  C     -1.862815    -0.488687     2.637924
  C      1.408661     0.460823    -0.916330
  C      0.380032     0.730384    -1.963503
  O      0.413227     1.694248    -2.732629
  O     -0.552975    -0.263901    -2.040354
  C     -1.685931    -0.052439    -2.969928
  C      2.133153    -0.170274     1.310530
  C      3.463127    -0.132795     0.895011
  C      3.771759     0.221042    -0.419049
  C      2.747080     0.517809    -1.316993
  H      2.973308     0.789228    -2.339058
  H      4.802611     0.263634    -0.745314
  H      4.252903    -0.367545     1.596447
  H      1.885964    -0.420437     2.331415
  C     -2.569509    -1.281032    -2.879850
  H     -2.202050     0.856569    -2.660200
  H     -1.284020     0.100757    -3.971598
  H     -3.422736    -1.171335    -3.553878
  H     -2.020729    -2.179776    -3.164840
  H     -2.948304    -1.414231    -1.865997
  C     -1.861090    -1.453139     3.807862
  H     -2.031852     0.543425     2.946624
  H     -2.610111    -0.746217     1.887188
  H     -2.834841    -1.432496     4.303279
  H     -1.668185    -2.473038     3.473104
  H     -1.099693    -1.180760     4.539961
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B3LYP.L05
  O      1.199940     0.161574     0.995430
  C      0.766624     1.210988     1.484107
  O      0.812012     1.469363     2.831571
  C      0.151019     2.314046     0.704727
  C      1.409277     0.428888     3.698170
  C      0.048646     2.166185    -0.682162
  H      0.413146     1.266163    -1.156414
  C     -0.322978     3.483546     1.317940
  C     -0.893730     4.493129     0.543935
  C     -0.996514     4.347254    -0.838909
  C     -0.524051     3.179745    -1.457087
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  C     -0.610294     2.976481    -2.924873
  H     -1.437687     5.126211    -1.442679
  H     -1.258655     5.394261     1.018751
  H     -0.241018     3.591795     2.389158
  C      1.342355     0.943633     5.122776
  H      0.845240    -0.494042     3.561201
  H      2.432744     0.254237     3.365417
  H      1.774607     0.204180     5.801310
  H      1.901658     1.873959     5.229988
  H      0.310238     1.123782     5.426257
  O     -1.189635     4.035909    -3.577890
  O     -0.210296     1.969578    -3.519841
  C     -1.322494     3.931083    -5.048151
  C     -1.984603     5.208081    -5.527566
  H     -0.327294     3.792902    -5.471464
  H     -1.914343     3.043905    -5.274703
  H     -2.103621     5.175024    -6.613284
  H     -2.971456     5.329991    -5.079149
  H     -1.380496     6.080890    -5.276413
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B3LYP.L06
  O      1.094179     0.221289     0.863432
  C      0.696057     1.242837     1.436633
  O      0.829151     1.427830     2.788106
  C      0.033869     2.384471     0.756096
  C      1.478477     0.344093     3.559609
  C     -0.157408     2.306546    -0.630820
  H      0.180915     1.424240    -1.155641
  C     -0.397937     3.520835     1.455832
  C     -1.013277     4.564811     0.773390
  C     -1.204555     4.486886    -0.613525
  C     -0.772748     3.350522    -1.313262
  H     -0.921570     3.293735    -2.380943
  C     -1.866742     5.628520    -1.294063
  H     -1.351600     5.447118     1.298211
  H     -0.249115     3.577623     2.523514
  C      1.501325     0.783064     5.010597
  H      0.905637    -0.571346     3.409391
  H      2.478849     0.189865     3.154336
  H      1.974639     0.009966     5.620779
  H      2.066857     1.707861     5.131375
  H      0.490453     0.944527     5.387072
  O     -1.999836     5.443528    -2.645536
  O     -2.264864     6.650069    -0.720862
  C     -2.649161     6.527265    -3.417038
  C     -2.672010     6.088293    -4.868027
  H     -3.649533     6.681493    -3.011766
  H     -2.076320     7.442704    -3.266821
  H     -3.145323     6.861392    -5.478209
  H     -1.661138     5.926830    -5.244502
  H     -3.237542     5.163497    -4.988804
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B3LYP.L07
  C     -5.377384     0.643779     0.338980
  C     -4.315528    -0.345973    -0.098455
  O     -3.002732     0.317485     0.084809
  C     -1.881193    -0.394202    -0.251413
  O     -1.924363    -1.555558    -0.667568
  O      1.924238     1.554183    -0.671105
  C      1.881146     0.393679    -0.252575
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  C      0.633000    -0.429346    -0.068244
  C     -0.633011     0.429192    -0.068986
  H     -0.585697     1.162876    -0.879122
  O      3.002748    -0.317317     0.084898
  C      4.315509     0.345772    -0.099955
  C      5.377447    -0.643072     0.339330
  H      0.585527    -1.164660    -0.876892
  H      0.724694    -1.010835     0.850363
  H     -0.724526     1.012530     0.848466
  H     -4.412553    -0.624944    -1.148091
  H     -4.322847    -1.258015     0.498884
  H      4.412351     0.622587    -1.150178
  H      4.322924     1.259040     0.495508
  H     -6.368124     0.198397     0.219635
  H     -5.248623     0.917829     1.386794
  H     -5.335406     1.552954    -0.261958
  H      6.368163    -0.197930     0.218898
  H      5.248870    -0.914969     1.387727
  H      5.335371    -1.553481    -0.259731
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B3LYP.L08
  C      0.769433     0.868344    -2.724040
  C     -0.520525     1.635243    -2.506587
  O     -0.151149     2.962730    -1.958623
  C     -1.174567     3.832011    -1.684400
  O     -2.355931     3.537896    -1.893970
  C     -0.737911     5.170446    -1.106335
  C     -1.100629     5.279461     0.427891
  C     -2.597431     5.076437     0.625221
  O     -3.145763     4.196730     1.290509
  C      0.718708     5.584166    -1.458510
  C      0.882753     5.708144    -2.989316
  C      1.115664     6.923973    -0.804820
  C     -0.209725     4.488430     1.429320
  C     -0.323065     2.950744     1.383497
  C     -0.444339     5.002282     2.867144
  O     -3.307318     6.056449    -0.024907
  C     -4.781920     5.931274    -0.031104
  C     -5.323476     7.081133    -0.858308
  H      1.311279     0.738445    -1.786400
  H      1.420653     1.386963    -3.428889
  H      0.544822    -0.121286    -3.129318
  H     -1.183528     1.146323    -1.792475
  H     -1.075438     1.791829    -3.431844
  H     -1.404272     5.890540    -1.589505
  H     -0.945230     6.337965     0.652974
  H      1.401339     4.806913    -1.106897
  H      1.911895     5.976584    -3.239888
  H      0.650094     4.775612    -3.502221
  H      0.229403     6.492432    -3.384458
  H      2.102896     7.230534    -1.158275
  H      0.409562     7.716428    -1.072272
  H      1.164885     6.867906     0.283394
  H      0.821963     4.744130     1.164644
  H      0.341678     2.518984     2.136965
  H     -1.338914     2.624759     1.599776
  H     -0.020208     2.549567     0.417539
  H      0.283375     4.557470     3.550204
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  H     -5.031658     4.958771    -0.455117
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  H     -4.950782     7.033213    -1.882193
  H     -6.414849     7.031750    -0.888415
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B3LYP.L09
  C     -1.488048     0.678004     0.805556
  H     -1.823842     1.348721     1.595840
  H     -0.458483     0.388986     1.014803
  H     -2.117244    -0.216152     0.825544
  C     -1.597852     1.341944    -0.558958
  H     -1.303892     0.671860    -1.363679
  H     -2.600847     1.724898    -0.743947
  O     -0.641006     2.469201    -0.691216
  C     -1.001631     3.688547    -0.186920
  C      0.092316     4.730907    -0.339026
  O     -2.103060     3.902604     0.330170
  C      0.681500     4.768419    -1.782100
  H     -0.408608     5.686141    -0.179575
  C      1.151996     4.612517     0.821083
  H      1.878737     5.405540     0.639297
  C      0.565627     4.832732     2.249421
  C      1.910704     3.296809     0.766222
  C      1.723861     5.891445    -1.945947
  H      1.166690     3.811795    -1.982899
  C     -0.453898     4.960268    -2.809605
  H     -0.047844     4.977541    -3.823719
  H     -1.190651     4.156567    -2.763451
  H     -0.975594     5.907876    -2.643479
  H      2.027649     5.966812    -2.993003
  H      1.306851     6.861340    -1.654807
  H      2.622610     5.708121    -1.358368
  O      3.017067     3.379652    -0.047623
  O      1.615847     2.271353     1.383271
  C      3.857157     2.167561    -0.205886
  C      3.352888     1.297454    -1.347499
  H      4.848077     2.569016    -0.405395
  H      3.859582     1.628132     0.740010
  H      4.012918     0.434736    -1.471273
  H      2.346627     0.931619    -1.143866
  H      3.339505     1.853977    -2.285791
  C      1.708777     4.902975     3.284224
  C     -0.297999     6.105556     2.344266
  H     -0.059277     3.970108     2.494535
  H      1.300361     5.021316     4.290371
  H      2.320256     3.999857     3.283113
  H      2.359139     5.761471     3.086905
  H     -0.566382     6.290086     3.387158
  H      0.249933     6.984192     1.986853
  H     -1.226372     6.018769     1.781055
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B3LYP.L10
  O      0.000000    -1.279549    -0.000099
  C      1.196723    -0.427310     0.131178
  C      0.738715     0.993894    -0.225067
  C     -0.738713     0.993862     0.225209
  C     -1.196724    -0.427291    -0.131238
  H      1.556770    -0.487913     1.162192
  H      1.962048    -0.822095    -0.536125
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  H      0.805438     1.158926    -1.303192
  H      1.330989     1.761772     0.274237
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  H     -0.805437     1.158741     1.303358
  H     -1.962043    -0.822173     0.536015
  H     -1.556781    -0.487744    -1.162258
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B3LYP.L11
  C      0.052749    -0.091340     0.090434
  H     -0.000966     0.001521     1.172196
  H      1.102855    -0.124434    -0.221084
  H     -0.443652    -1.017251    -0.221239
  O     -0.618571     1.071589    -0.454390
  C     -0.636143     1.101859    -1.906541
  C     -1.367326     2.368251    -2.310125
  H      0.385175     1.112793    -2.302933
  H     -1.156311     0.222806    -2.302806
  O     -1.384898     2.398521    -3.762276
  H     -2.388644     2.357317    -1.913734
  H     -0.847158     3.247304    -1.913860
  C     -2.056218     3.561450    -4.307100
  H     -2.002503     3.468589    -5.388862
  H     -3.106324     3.594544    -3.995582
  H     -1.559817     4.487362    -3.995427
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B3LYP.L12
  C      0.019855    -0.034595     0.230442
  H     -0.075835     0.130982     1.300586
  H      1.081893    -0.088150    -0.035913
  H     -0.464659    -0.981157    -0.036031
  O     -0.628233     1.087903    -0.417453
  C     -0.588201     1.018858    -1.868697
  C     -1.299596     2.251286    -2.411901
  H      0.457440     0.986085    -2.205769
  H     -1.082682     0.097009    -2.205968
  C     -1.318510     2.283993    -3.934599
  H     -2.325035     2.268328    -2.038977
  H     -0.801508     3.147787    -2.038969
  O     -2.016064     3.491899    -4.343092
  H     -0.297682     2.294261    -4.341881
  H     -1.837666     1.404947    -4.341812
  C     -2.105563     3.646689    -5.781083
  H     -2.641964     4.575633    -5.957488
  H     -1.110471     3.708968    -6.236765
  H     -2.657025     2.815964    -6.236627
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B3LYP.L13
  C      0.077903    -0.135025     0.187630
  H      0.013189    -0.023177     1.267143
  H      1.131794    -0.175020    -0.111383
  H     -0.414604    -1.067542    -0.111615
  O     -0.587208     1.017492    -0.385730
  C     -0.589155     1.020794    -1.840411
  C     -1.313697     2.275537    -2.307999
  H      0.445273     1.007537    -2.210248
  H     -1.094816     0.118253    -2.210168
  C     -1.373309     2.378494    -3.842001
  H     -2.323941     2.267264    -1.888453
  H     -0.801422     3.146383    -1.888616
  C     -2.097850     3.633236    -4.309589
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  H     -0.363064     2.386766    -4.261547
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  H     -3.132278     3.646493    -3.939751
  H     -1.592189     4.535777    -3.939832
  C     -2.764909     4.789055    -6.337630
  H     -2.700195     4.677208    -7.417143
  H     -3.818799     4.829050    -6.038617
  H     -2.272401     5.721572    -6.038385
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B3LYP.L14
  C      0.492830    -0.003947     0.024852
  H      0.820272     0.256683     1.028439
  H      1.365130    -0.254209    -0.590484
  H     -0.171517    -0.874684     0.072415
  O     -0.199349     1.156152    -0.497310
  C     -0.685526     0.961578    -1.853535
  C     -1.416831     2.223446    -2.367808
  H      0.172269     0.729191    -2.499734
  H     -1.355068     0.093129    -1.874229
  C     -1.404089     2.095866    -3.907443
  C     -2.906940     2.306429    -1.854704
  C     -0.664519     3.521667    -1.945718
  O     -2.146859     3.197018    -4.494663
  H     -0.373367     2.117964    -4.278609
  H     -1.849541     1.145118    -4.226166
  C     -2.159430     3.170307    -5.942942
  H     -2.733333     4.036454    -6.263417
  H     -1.143299     3.235004    -6.348759
  H     -2.636410     2.257239    -6.318010
  H     -3.272008     3.272194    -2.215260
  C     -3.840261     1.231215    -2.452008
  C     -3.043813     2.296276    -0.317041
  H     -4.084597     2.493131    -0.044221
  H     -2.761635     1.330335     0.105796
  H     -2.425960     3.053638     0.163784
  H     -4.843185     1.344667    -2.032415
  H     -3.931675     1.321394    -3.534802
  H     -3.508079     0.215661    -2.215536
  H     -1.261847     4.363063    -2.301637
  H     -0.649852     3.565134    -0.856986
  C      0.784555     3.672612    -2.444735
  C      1.557515     4.833193    -1.772644
  H      1.338334     2.748307    -2.251778
  H      0.802771     3.835186    -3.528909
  C      3.039117     4.809436    -2.194419
  C      0.933298     6.208598    -2.076829
  H      1.513484     4.671891    -0.687733
  H      3.606420     5.597602    -1.691885
  H      3.505778     3.851288    -1.949668
  H      3.138565     4.964682    -3.273833
  H      1.509613     7.010091    -1.606500
  H      0.919473     6.395870    -3.155691
  H     -0.092990     6.281058    -1.712585
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B3LYP.L15
  C     -0.531365    -0.000097     0.000030
  C     -1.410231     0.174169     1.253878
  C      0.438178    -1.170447     0.202191
  C      0.437591     1.170731    -0.202175
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  O     -2.301875     1.305143     1.053816
  H     -2.002863    -0.730222     1.416156
  H     -0.774972     0.352798     2.128577
  C     -3.199373     1.525003     2.169498
  H     -3.817718     2.380103     1.906723
  H     -3.837613     0.650626     2.338532
  H     -2.642002     1.746054     3.086670
  C      1.774956    -0.723103     0.128457
  C      2.832447    -1.619711     0.289910
  C      2.545971    -2.967457     0.526855
  C      1.220877    -3.411002     0.597877
  C      0.156756    -2.513200     0.434814
  H      3.860584    -1.283489     0.234305
  H      3.356553    -3.674049     0.654675
  H      1.014796    -4.458764     0.777458
  H     -0.865956    -2.860681     0.469879
  C      1.774594     0.724047    -0.128502
  C      2.831635     1.621177    -0.290005
  C      2.544482     2.968781    -0.526939
  C      1.219167     3.411672    -0.597901
  C      0.155496     2.513345    -0.434787
  H      3.859940     1.285462    -0.234447
  H      3.354710     3.675772    -0.654798
  H      1.012560     4.459332    -0.777475
  H     -0.867389     2.860322    -0.469806
  C     -1.410202    -0.174797    -1.253778
  O     -2.301280    -1.306208    -1.053673
  H     -2.003284     0.729302    -1.416033
  H     -0.774894    -0.353117    -2.128505
  C     -3.198717    -1.526517    -2.169317
  H     -3.816630    -2.381920    -1.906511
  H     -2.641276    -1.747298    -3.086511
  H     -3.837396    -0.652455    -2.338328
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B3LYP.ML01
  Ti     0.086526     0.043831     1.386767
  Cl     1.146039     1.515498     2.760314
  Cl     1.327864    -1.488990     0.296042
  Cl    -2.012891     0.476492     0.625105
  Cl    -0.588475    -1.315992     3.047236
  O      0.686046     1.383126    -0.150967
  C      0.651380     2.532119    -0.659296
  O      1.326330     2.795843    -1.779962
  C     -0.112535     3.677282    -0.093384
  C      2.126871     1.699595    -2.422482
  C      2.768101     2.295573    -3.656076
  H      2.852181     1.353689    -1.687808
  H      1.440240     0.885253    -2.647976
  H      3.363206     1.528646    -4.156930
  H      2.015266     2.655274    -4.357745
  H      3.427798     3.123938    -3.397045
  H     -1.168985     3.408611    -0.028785
  H      0.232379     3.872385     0.924181
  H      0.009425     4.565447    -0.704928
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B3LYP.ML01-cis
  Ti     0.000000     0.000001     1.245528
  Cl     0.633700     1.595231     2.751181
  Cl     2.176859    -0.839744     0.919116
  Cl    -2.176860     0.839745     0.919115
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  Cl    -0.633700    -1.595228     2.751182
  O      0.531986     1.294226    -0.357681
  C      0.590194     2.477525    -0.770052
  O      1.307330     2.773718    -1.864591
  C     -0.082581     3.639501    -0.131204
  C      2.082289     1.682864    -2.536009
  C      2.983383     2.350558    -3.552670
  H      2.630129     1.141932    -1.766537
  H      1.359534     1.007037    -2.992394
  H      3.564164     1.587951    -4.076762
  H      2.404622     2.907963    -4.289793
  H      3.680127     3.034919    -3.068235
  H     -1.139519     3.411418     0.012856
  H      0.340109     3.793298     0.864435
  H      0.042964     4.535743    -0.730366
  O     -0.531986    -1.294226    -0.357680
  C     -0.590194    -2.477525    -0.770050
  O     -1.307330    -2.773719    -1.864590
  C     -2.082289    -1.682864    -2.536008
  C     -2.983383    -2.350559    -3.552669
  H     -2.630129    -1.141932    -1.766536
  H     -1.359533    -1.007038    -2.992394
  H     -3.564163    -1.587952    -4.076761
  H     -2.404622    -2.907965    -4.289791
  H     -3.680127    -3.034920    -3.068233
  C      0.082581    -3.639500    -0.131202
  H      1.139518    -3.411417     0.012858
  H     -0.340110    -3.793297     0.864437
  H     -0.042964    -4.535743    -0.730363
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B3LYP.ML02
  Cl    -1.929987    -2.705995    -1.343121
  Ti     0.000508    -2.464048    -0.147498
  Cl     0.140701    -4.664776     0.325050
  Cl     2.109813    -2.378931    -1.018474
  Cl    -0.225909    -1.792564     1.996403
  H     -0.393451     0.838076     1.369723
  C     -0.432876     1.804539     0.889113
  C     -0.325796     1.892780    -0.509232
  C     -0.161645     0.663081    -1.292469
  O     -0.109739    -0.486209    -0.771602
  O     -0.069237     0.843009    -2.614673
  C      0.101038    -0.322962    -3.541667
  C     -0.588992     2.963002     1.645188
  C     -0.639029     4.209730     1.015502
  C     -0.532672     4.300449    -0.376571
  C     -0.376481     3.148744    -1.140928
  H     -0.293746     3.210932    -2.215575
  H     -0.571690     5.266586    -0.861520
  H     -0.760465     5.108367     1.606341
  H     -0.671267     2.893213     2.721330
  C      0.170760     0.246659    -4.941771
  H      1.013122    -0.840363    -3.251111
  H     -0.752454    -0.982207    -3.396726
  H      0.295240    -0.572020    -5.654172
  H     -0.743734     0.782952    -5.196366
  H      1.017825     0.924348    -5.051080
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B3LYP.ML03
  Ti    -0.076373    -1.795684     0.000000
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Cl	-2.233854	-0.848223	0.000000
Cl	-0.462398	-3.173487	1.755377
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Cl	2.254162	-2.071844	0.000001
O	0.396380	-0.184064	1.318081
C	0.379464	1.037132	1.566471
O	0.871674	1.486543	2.735175
C	-0.177490	2.117159	0.709699
C	1.386211	0.474187	3.713789
C	-0.177489	2.117159	-0.709700
C	0.379465	1.037132	-1.566472
O	0.396380	-0.184064	-1.318081
O	0.871674	1.486542	-2.735176
C	1.386211	0.474186	-3.713789
C	-0.732527	3.214520	1.385777
C	-1.309999	4.276966	0.696162
C	-1.309999	4.276965	-0.696165
C	-0.732526	3.214519	-1.385779
H	-0.714130	3.219861	-2.464294
H	-1.751519	5.097041	-1.245843
H	-1.751519	5.097042	1.245840
H	-0.714131	3.219862	2.464292
C	1.924848	1.229806	-4.922408
H	2.156347	-0.109499	-3.209355
H	0.555008	-0.182982	-3.967040
C	2.310689	0.205974	-6.009721
H	1.114671	1.855454	-5.312868
C	3.114153	2.132871	-4.553614
C	1.924850	1.229809	4.922406
H	0.555006	-0.182979	3.967042
H	2.156345	-0.109499	3.209355
C	2.310690	0.205977	6.009720
C	3.114156	2.132870	4.553610
H	1.114674	1.855458	5.312866
H	3.466568	2.679488	5.431124
H	3.949659	1.537160	4.173636
H	2.841228	2.860943	3.788548
H	2.672213	0.721314	6.901488
H	1.460209	-0.414165	6.302481
H	3.108370	-0.456326	5.662023
H	2.672210	0.721311	-6.901491
H	3.108370	-0.456327	-5.662024
H	1.460208	-0.414170	-6.302481
H	3.466563	2.679487	-5.431130
H	2.841225	2.860943	-3.788553
H	3.949657	1.537161	-4.173640

B3LYP.ML04

Cl	-2.319287	-0.830230	0.000001
Ti	-0.174307	-1.803172	0.000000
Cl	-0.574666	-3.175828	1.755817
Cl	-0.574667	-3.175828	-1.755817
Cl	2.153413	-2.103636	-0.000001
O	0.316572	-0.195671	1.317246
C	0.319796	1.025108	1.567275
O	0.813904	1.462819	2.740764
C	-0.211531	2.117159	0.709875
C	1.312032	0.435807	3.715234
C	-0.211531	2.117159	-0.709875
C	0.319795	1.025108	-1.567276

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  O      0.316571    -0.195671    -1.317247
  O      0.813903     1.462819    -2.740765
  C      1.312031     0.435807    -3.715234
  C     -0.740701     3.227354     1.385735
  C     -1.293563     4.302827     0.696133
  C     -1.293563     4.302827    -0.696133
  C     -0.740702     3.227354    -1.385735
  H     -0.721158     3.232723    -2.464180
  H     -1.715355     5.133142    -1.245885
  H     -1.715354     5.133142     1.245885
  H     -0.721157     3.232723     2.464180
  C      1.820096     1.192333    -4.922963
  H      2.087896    -0.139186    -3.212991
  H      0.479347    -0.227518    -3.944429
  H      2.200845     0.478644    -5.657013
  H      1.024488     1.771145    -5.393296
  H      2.631791     1.868358    -4.652766
  C      1.820095     1.192334     4.922963
  H      0.479349    -0.227518     3.944428
  H      2.087899    -0.139184     3.212991
  H      2.200845     0.478645     5.657014
  H      2.631790     1.868360     4.652767
  H      1.024486     1.771144     5.393296
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B3LYP.ML05
  Cl    -1.926573    -2.643722    -1.434659
  Ti     0.002762    -2.442027    -0.232938
  Cl     0.143988    -4.652877     0.177347
  Cl     2.105436    -2.325938    -1.111652
  Cl    -0.218163    -1.828308     1.929024
  H     -0.392342     0.814212     1.387884
  C     -0.435079     1.796066     0.939368
  C     -0.331406     1.930514    -0.455506
  C     -0.166129     0.725720    -1.280250
  O     -0.110875    -0.437300    -0.794490
  O     -0.077522     0.950653    -2.594399
  C      0.093390    -0.182646    -3.562017
  C     -0.592127     2.929110     1.733563
  C     -0.646395     4.192847     1.148347
  C     -0.543277     4.332667    -0.244440
  C     -0.385799     3.201794    -1.047100
  H     -0.306635     3.308624    -2.116616
  C     -0.606990     5.702241    -0.818373
  H     -0.767956     5.081925     1.751485
  H     -0.671904     2.825233     2.806788
  C      0.157990     0.435533    -4.941456
  H      1.007535    -0.707023    -3.291115
  H     -0.758217    -0.848417    -3.437188
  H      0.282776    -0.357741    -5.681993
  H     -0.758479     0.977958    -5.174781
  H      1.002868     1.118971    -5.029069
  O     -0.495696     5.716089    -2.181575
  O     -0.745749     6.729954    -0.145765
  C     -0.547241     7.036750    -2.854080
  C     -0.402831     6.784730    -4.341602
  H     -1.496309     7.508925    -2.599913
  H      0.258732     7.651889    -2.453735
  H     -0.435559     7.735604    -4.878698
  H      0.546987     6.298219    -4.566841
  H     -1.211979     6.154918    -4.713346
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B3LYP.ML06
  Cl    -1.925600    -2.695145    -1.419902
  Ti     0.006612    -2.505072    -0.220632
  Cl     0.148317    -4.718495     0.171875
  Cl     2.108633    -2.379761    -1.099942
  Cl    -0.211213    -1.902254     1.941691
  H     -0.387883     0.759413     1.413996
  C     -0.430878     1.740337     0.964182
  C     -0.328231     1.875332    -0.429981
  C     -0.163220     0.670087    -1.257118
  O     -0.107494    -0.493037    -0.774361
  O     -0.075695     0.899005    -2.571244
  C      0.094544    -0.232413    -3.541530
  C     -0.587331     2.869995     1.758310
  C     -0.642819     4.141877     1.172310
  C     -0.540227     4.276922    -0.220190
  C     -0.383755     3.150600    -1.018574
  H     -0.304452     3.249766    -2.090482
  H     -0.583802     5.259654    -0.664145
  C     -0.811525     5.319470     2.067510
  H     -0.667876     2.783181     2.832378
  C      0.158080     0.387938    -4.920023
  H      1.008869    -0.757204    -3.272074
  H     -0.756944    -0.898388    -3.417032
  H      0.282247    -0.404187    -5.661867
  H     -0.758655     0.930479    -5.152239
  H      1.003136     1.071222    -5.007674
  O     -0.852286     6.504432     1.386605
  O     -0.906005     5.247443     3.297304
  C     -1.018231     7.742327     2.186706
  C     -1.032457     8.903503     1.212913
  H     -1.946962     7.657527     2.751143
  H     -0.191708     7.799781     2.895136
  H     -1.153414     9.840082     1.762344
  H     -0.099327     8.955925     0.650704
  H     -1.858466     8.813392     0.506409
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B3LYP.ML07
  Cl    -2.067923    -0.896732    -0.168694
  Ti     0.118452    -1.748477     0.000527
  Cl    -0.293648    -3.126982     1.748562
  Cl    -0.053797    -3.233479    -1.694458
  Cl     2.459540    -1.800161     0.170616
  O      0.360359    -0.097986     1.363853
  C      0.775158     1.048653     1.613586
  O      1.003735     1.449809     2.870035
  C      1.078569     2.099783     0.581312
  C      0.811426     0.452581     3.978890
  C      0.144633     2.077569    -0.653333
  C      0.491062     1.027097    -1.670442
  O      0.552382    -0.196919    -1.440465
  O      0.736180     1.512184    -2.895011
  C      1.041823     0.536761    -3.996222
  H      1.017412     3.073176     1.065107
  H      0.177247     3.047530    -1.143503
  C      1.245258     1.350403    -5.255173
  H      1.927898    -0.021269    -3.698106
  H      0.200495    -0.151164    -4.061713
  H      1.469696     0.676400    -6.084938
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  H      0.348366     1.916006    -5.508947
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  C      1.200712     1.149150     5.263785
  H     -0.232581     0.144370     3.957575
  H      1.436413    -0.409167     3.751139
  H      1.074422     0.456158     6.098645
  H      2.243365     1.467013     5.240219
  H      0.573087     2.021719     5.447185
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  H      2.122951     1.967441     0.279053
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B3LYP.ML08
  Ti     0.079264    -1.666915     0.354971
  Cl    -2.208524    -1.100245     0.449366
  Cl     0.054813    -2.962467     2.202501
  Cl    -0.197449    -3.240406    -1.259136
  Cl     2.418507    -1.585092     0.140412
  O      0.411583     0.067320     1.598451
  C      0.316115     1.314989     1.568181
  O      1.045262     2.061863     2.410379
  C     -0.592794     2.075588     0.625211
  C      1.960137     1.358952     3.371036
  C      0.087776     2.331467    -0.764488
  C      0.183938     1.056009    -1.572840
  O      0.157682    -0.102359    -1.112918
  O      0.292913     1.264265    -2.894275
  C      0.398477     0.063525    -3.792289
  H     -1.424736     1.391026     0.441231
  C      1.454248     3.117467    -0.712758
  C      0.516360     0.585042    -5.207608
  H      1.267859    -0.507979    -3.471674
  H     -0.493247    -0.539957    -3.631999
  H      0.587593    -0.260474    -5.895487
  H     -0.356540     1.176913    -5.484630
  H      1.408621     1.199648    -5.330908
  C      2.702495     2.434365     4.134154
  H      1.337778     0.734751     4.010632
  H      2.615655     0.714315     2.788257
  H      3.376147     1.963374     4.853577
  H      3.300372     3.053284     3.464389
  H      2.014349     3.078281     4.682697
  H     -0.611504     2.955228    -1.320260
  C     -1.193361     3.355524     1.286574
  C      1.561938     4.122808    -1.875015
  H      1.424429     3.687119     0.219905
  C      2.697047     2.207465    -0.670726
  H      3.587964     2.809246    -0.479545
  H      2.644623     1.438200     0.099481
  H      2.847960     1.698502    -1.625955
  H      2.488889     4.695268    -1.793503
  H      1.564375     3.611731    -2.839241
  H      0.730633     4.832414    -1.869533
  C     -2.107339     4.134976     0.319548
  C     -2.001853     2.963227     2.542693
  H     -0.375536     4.010181     1.597143
  H     -2.620529     4.930839     0.863036
  H     -1.560544     4.609379    -0.496844
  H     -2.874502     3.485207    -0.111973
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  H     -1.394344     2.438638     3.281065
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B3LYP.ML09
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  Ti    -0.000271     1.909974    -0.000388
  Cl     1.706520     3.362610     0.335857
  Cl    -1.707517     3.361993    -0.336994
  Cl    -0.447470     1.597331     2.289063
  O      1.339295     0.254066     0.227086
  C      1.588487    -0.968559     0.253610
  O      2.844255    -1.406850     0.069598
  C      0.591189    -2.075762     0.513012
  C      3.922367    -0.387133    -0.163435
  C     -0.590495    -2.076072    -0.512799
  C     -1.588136    -0.969116    -0.253672
  O     -1.339325     0.253592    -0.227451
  O     -2.843767    -1.407753    -0.069551
  C     -3.922197    -0.388315     0.163230
  H      1.133161    -3.008227     0.358542
  H     -1.132177    -3.008667    -0.358099
  C     -5.211440    -1.154451     0.364110
  H     -3.631976     0.199529     1.032266
  H     -3.944748     0.265195    -0.707530
  H     -6.026009    -0.446929     0.534507
  H     -5.457297    -1.752594    -0.513835
  H     -5.148073    -1.814817     1.229520
  C      5.211852    -1.152915    -0.364106
  H      3.631969     0.200396    -1.032625
  H      3.944704     0.266608     0.707157
  H      6.026199    -0.445180    -0.534678
  H      5.457890    -1.750753     0.513996
  H      5.148701    -1.813524    -1.229346
  C     -0.130145    -2.062106    -2.013700
  C      0.130838    -2.061564     2.013909
  C     -0.736749    -3.294938     2.330224
  C      1.341286    -2.005622     2.965779
  H     -0.458527    -1.156620     2.181298
  C     -1.340608    -2.006781    -2.965586
  H      0.458935    -1.157018    -2.181313
  C      0.737831    -3.295285    -2.329704
  H      0.999535    -2.039098     4.001699
  H      2.013920    -2.852983     2.804172
  H      1.913211    -1.083347     2.848660
  H     -1.007572    -3.289699     3.388029
  H     -1.665058    -3.317614     1.758479
  H     -0.188756    -4.221949     2.134151
  H     -0.998844    -2.040400    -4.001497
  H     -2.012972    -2.854318    -2.803774
  H     -1.912828    -1.084660    -2.848692
  H      1.008653    -3.290228    -3.387509
  H      1.666147    -3.317524    -1.757952
  H      0.190131    -4.222419    -2.133396
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B3LYP.ML10
  Ti     0.032247     0.096116     1.070868
  Cl     2.248521    -0.191604     0.724979
  Cl    -1.453399    -0.843390    -0.375461
  Cl    -0.154955    -1.544139     2.606685
  Cl    -0.657280     1.749350     2.449436
  O      0.177500     1.635192    -0.453620
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  C     -0.780234     2.778988    -0.625857
  C     -0.315145     3.477967    -1.899041
  C      0.236896     2.322141    -2.757101
  C      0.931976     1.421008    -1.739247
  H     -1.778389     2.350602    -0.721030
  H     -0.715107     3.379526     0.274007
  H      0.471658     4.200388    -1.673617
  H     -1.133912     4.006103    -2.387502
  H      0.929765     2.664661    -3.525582
  H     -0.579195     1.787560    -3.246224
  H      0.877573     0.362557    -1.976454
  H      1.962770     1.705286    -1.540545
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B3LYP.ML10-cis
  Ti     0.000000     0.000000     0.889954
  Cl     2.340071    -0.001236     0.637493
  Cl    -2.340072     0.001236     0.637493
  Cl     0.003390    -1.723981     2.391122
  Cl    -0.003391     1.723981     2.391122
  O     -0.026157     1.434804    -0.741730
  O      0.026156    -1.434804    -0.741730
  C     -0.979293     2.597349    -0.808901
  C     -0.346418     3.558515    -1.812265
  C      0.431426     2.624818    -2.762178
  C      1.008475     1.578227    -1.814084
  C      0.979293    -2.597349    -0.808902
  C      0.346419    -3.558514    -1.812266
  C     -0.431427    -2.624818    -2.762178
  C     -1.008476    -1.578227    -1.814083
  H     -1.935616     2.197605    -1.138149
  H     -1.071814     2.988205     0.199194
  H      0.338412     4.243645    -1.309156
  H     -1.101322     4.150115    -2.330221
  H      1.216989     3.144391    -3.311047
  H     -0.245033     2.165973    -3.487048
  H      1.155798     0.593543    -2.247170
  H      1.928942     1.902838    -1.334746
  H      1.935616    -2.197604    -1.138150
  H      1.071814    -2.988205     0.199193
  H      1.101323    -4.150114    -2.330221
  H     -0.338411    -4.243645    -1.309156
  H      0.245032    -2.165972    -3.487049
  H     -1.216990    -3.144391    -3.311046
  H     -1.155799    -0.593543    -2.247169
  H     -1.928942    -1.902839    -1.334745
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B3LYP.ML11
  Ti    -1.154346    -2.000541     0.196374
  Cl    -3.281485    -1.290764     0.825139
  Cl    -1.043522    -3.738948     1.640032
  Cl    -1.847503    -3.028942    -1.700858
  Cl     1.139871    -2.078788    -0.390108
  O     -0.462979    -0.608278     1.722776
  C     -0.755010     0.802879     1.430729
  O     -1.027033     0.003966    -0.802406
  C     -0.377633     1.054964    -0.013502
  H     -1.820021     0.941883     1.598157
  H     -0.179363     1.439193     2.102734
  H     -0.749153     2.026737    -0.346177
  H      0.701394     0.991390    -0.171209
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  C     -0.869978     0.188228    -2.254062
  H     -1.195521     1.196200    -2.511851
  H      0.172489     0.027444    -2.530578
  H     -1.504601    -0.548536    -2.730101
  C      0.591123    -0.860056     2.717829
  H      1.550650    -0.515968     2.332914
  H      0.322283    -0.347065     3.640666
  H      0.614737    -1.931670     2.874341
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B3LYP.ML12
  Ti    -1.079028    -1.919686     0.172909
  Cl    -2.438275    -0.008836     0.353341
  Cl    -1.643604    -2.715876     2.227216
  Cl    -2.588260    -3.076717    -1.074622
  Cl     0.659926    -3.467564    -0.155605
  O      0.491456    -0.671818     1.069617
  C      0.726963     0.744683     0.708457
  O     -0.284677    -0.967270    -1.640750
  C      1.116990     0.866653    -0.759808
  H     -0.187763     1.287697     0.937742
  H      1.532606     1.110785     1.344749
  H      1.371600     1.916204    -0.947117
  H      2.016225     0.276615    -0.953066
  C     -0.127570    -1.701404    -2.909859
  H      0.876912    -1.526772    -3.295221
  H     -0.261639    -2.752481    -2.692864
  H     -0.885497    -1.357580    -3.613509
  C      1.331659    -1.145763     2.184831
  C      0.023503     0.477028    -1.747357
  H      0.354056     0.662388    -2.769280
  H     -0.905073     1.014797    -1.566402
  H      1.038749    -0.623093     3.095228
  H      1.161285    -2.208899     2.287434
  H      2.377529    -0.958678     1.941568
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B3LYP.ML13
  Ti    -0.782398    -2.239256     0.148349
  Cl    -2.615322    -0.880343     0.706018
  Cl    -0.760927    -3.313362     2.148643
  Cl    -2.069159    -3.699825    -1.032859
  Cl     1.241268    -3.196189    -0.572917
  O      0.461628    -0.641294     0.951206
  C      1.499082     0.050572     0.148302
  O     -0.540180    -0.935806    -1.682677
  C      0.992695     1.401532    -0.374156
  H      2.380441     0.159486     0.782841
  H      1.733046    -0.637640    -0.652923
  H      1.164177     2.185057     0.368877
  H      1.602605     1.668265    -1.244232
  C     -0.448351    -1.613504    -2.995174
  H      0.244476    -1.054845    -3.624850
  H     -0.070548    -2.611435    -2.821290
  H     -1.438666    -1.654190    -3.448350
  C      0.365314    -0.151204     2.336064
  C     -0.503985     1.409624    -0.733527
  H     -0.776938     2.420567    -1.056343
  H     -1.097382     1.202088     0.153319
  H      0.311030     0.937083     2.332122
  H     -0.538573    -0.564760     2.764500
  H      1.240207    -0.494141     2.887976
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C	-0.943671	0.489312	-1.864653
H	-2.029477	0.506845	-1.970845
H	-0.485958	0.804607	-2.805177

B3LYP.ML14

Ti	-1.263360	-1.671534	0.446434
Cl	-1.796945	0.610092	0.698278
Cl	-1.637590	-2.168310	2.636247
Cl	-3.332042	-2.181038	-0.361641
Cl	-0.352216	-3.768295	-0.088857
O	0.785654	-1.096616	0.908781
C	1.430603	0.144994	0.413324
O	-0.513266	-1.106302	-1.558398
C	1.636282	0.122982	-1.115507
H	0.786701	0.964417	0.718931
H	2.385614	0.233437	0.926804
C	2.368943	1.454119	-1.501027
C	2.502320	-1.128966	-1.528729
C	-1.205429	-1.649208	-2.744579
H	-0.524589	-1.617339	-3.593001
H	-1.465895	-2.675324	-2.515753
H	-2.101527	-1.063152	-2.943445
C	1.551857	-1.797900	1.957819
C	0.268509	0.127225	-1.825856
H	0.406363	0.191996	-2.903715
H	-0.344823	0.960791	-1.494380
H	1.481769	-1.233584	2.887069
H	1.109283	-2.778360	2.075852
H	2.585763	-1.893810	1.632025
H	2.730948	1.350240	-2.525699
C	1.572776	2.773041	-1.381795
H	3.262224	1.535074	-0.873989
C	2.458842	4.039657	-1.472746
H	0.812897	2.832528	-2.168949
H	1.031182	2.807929	-0.432076
C	1.618253	5.299437	-1.191771
H	3.225175	3.964402	-0.689474
C	3.176211	4.160021	-2.831188
H	2.240690	6.197492	-1.203948
H	0.838848	5.424313	-1.949859
H	1.129016	5.242753	-0.216140
H	3.768379	5.077283	-2.875563
H	3.853926	3.324201	-3.017312
H	2.449840	4.194634	-3.649778
C	2.573485	-1.376875	-3.050712
C	3.947160	-1.083109	-0.979522
H	2.001727	-1.994822	-1.089820
H	3.229938	-2.227262	-3.247864
H	1.604991	-1.622623	-3.483721
H	2.984032	-0.520843	-3.592819
H	4.420000	-2.057444	-1.120921
H	4.556502	-0.346848	-1.508916
H	4.002452	-0.851977	0.085539

B3LYP.ML15

Ti	-0.949260	-2.133417	0.293778
Cl	-2.344469	-0.244413	0.466592
Cl	-1.261075	-2.724730	2.467413
Cl	-2.563052	-3.396922	-0.691460
Cl	0.739347	-3.737497	-0.060398

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  O      0.701040    -0.795700     0.845663
  C      0.794661     0.614975     0.405232
  O     -0.327543    -1.327931    -1.651610
  C      0.990580     0.740651    -1.118384
  H     -0.119539     1.107305     0.726595
  H      1.648577     1.060719     0.912338
  C      1.047459     2.239073    -1.461427
  C      2.371580     0.263592    -1.585771
  C     -0.352323    -2.160005    -2.872744
  H      0.520196    -1.913706    -3.475728
  H     -0.306867    -3.193338    -2.554469
  H     -1.277139    -1.967717    -3.415684
  C      1.632274    -1.133210     1.942593
  C     -0.165557     0.118144    -1.925563
  H      0.041477     0.229314    -2.988488
  H     -1.113436     0.593058    -1.685908
  H      1.307821    -0.629283     2.852445
  H      1.597484    -2.207235     2.070642
  H      2.634398    -0.821602     1.652454
  C      2.289900     2.563467    -2.043305
  C      2.559596     3.875590    -2.434652
  C      1.580660     4.855043    -2.239667
  C      0.348858     4.530132    -1.661996
  C      0.073680     3.213585    -1.267552
  H      3.509540     4.138374    -2.882720
  H      1.778209     5.876302    -2.539072
  H     -0.398054     5.299799    -1.517915
  H     -0.883651     2.973443    -0.821167
  C      2.925736    -1.012495    -1.541417
  C      4.224064    -1.203034    -2.036431
  C      4.952816    -0.133320    -2.565935
  C      4.399113     1.149599    -2.611675
  C      3.107875     1.344885    -2.120609
  H      2.374225    -1.848283    -1.135077
  H      4.664243    -2.191553    -2.006687
  H      5.953651    -0.299385    -2.943495
  H      4.968468     1.973848    -3.022814
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TPSS.M
  Ti     0.000017     0.000055    -0.000135
  Cl     1.732375    -1.129915     0.778866
  Cl    -1.303423    -1.356803    -1.159713
  Cl     0.713098     1.633083    -1.307574
  Cl    -1.142077     0.853587     1.688578
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TPSS.L01
  O      1.235328     1.367778     0.000001
  C      1.075374     0.134635     0.000000
  O     -0.178770    -0.462256    -0.000001
  C      2.171001    -0.901820     0.000000
  C     -1.349095     0.473870     0.000001
  C     -2.600399    -0.394925    -0.000001
  H     -1.272915     1.107133     0.888915
  H     -1.272915     1.107138    -0.888909
  H     -3.490684     0.246294     0.000000
  H     -2.633087    -1.033149    -0.889148
  H     -2.633087    -1.033153     0.889143
  H      3.138528    -0.397828    -0.000019
  H      2.085705    -1.542960     0.884215
  H      2.085681    -1.542987    -0.884192
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TPSS.L02
  O     -1.463405     0.159956     1.080874
  C     -0.319385     0.127416     1.581193
  O     -0.110560     0.161717     2.953605
  C      0.945075     0.049786     0.808203
  C     -1.345409     0.240212     3.794030
  C      0.858830     0.009517    -0.598144
  H     -0.122832     0.036668    -1.060579
  C      2.208259     0.015778     1.432917
  C      3.370671    -0.057774     0.655316
  C      3.279851    -0.097682    -0.745545
  C      2.022538    -0.063941    -1.371249
  H      1.951804    -0.094825    -2.455472
  H      4.184062    -0.154786    -1.346563
  H      4.343951    -0.083916     1.138938
  H      2.267969     0.047034     2.514940
  C     -0.882424     0.267942     5.245351
  H     -1.891752     1.143499     3.507034
  H     -1.965428    -0.631388     3.564477
  H     -1.756860     0.325545     5.905594
  H     -0.320263    -0.638130     5.494551
  H     -0.246599     1.138609     5.437072
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TPSS.L03
  O     -0.907627     1.099267     0.408283
  C     -0.036285     0.315591     0.831262
  O     -0.279359    -0.589263     1.854511
  C      1.379006     0.276989     0.371876
  C     -1.661830    -0.558237     2.426126
  C      1.724013     0.673657    -0.942431
  C      0.719863     0.950340    -2.013290
  O      0.757360     1.937363    -2.771311
  O     -0.202574    -0.069162    -2.132818
  C     -1.305602     0.166266    -3.115843
  C      2.401776    -0.031465     1.289582
  C      3.748224     0.075779     0.921136
  C      4.088078     0.502431    -0.370963
  C      3.078418     0.801712    -1.294197
  H      3.325353     1.126452    -2.300378
  H      5.131175     0.599274    -0.659839
  H      4.526234    -0.160479     1.642146
  H      2.128643    -0.333254     2.294569
  C     -2.189037    -1.084847    -3.128056
  H     -1.851604     1.054337    -2.783509
  H     -0.854390     0.364512    -4.094098
  C     -3.428658    -0.813581    -4.016838
  C     -1.414466    -2.330451    -3.614395
  H     -2.530672    -1.259249    -2.098393
  C     -1.733519    -1.614846     3.533265
  H     -1.849980     0.452548     2.804929
  H     -2.362759    -0.767935     1.612361
  C     -3.196820    -1.716150     4.032418
  H     -1.448672    -2.579702     3.091107
  C     -0.769433    -1.297189     4.698349
  H     -2.057102    -3.219233    -3.585963
  H     -1.072258    -2.192463    -4.649705
  H     -0.537899    -2.516825    -2.985172
  H     -4.094983    -1.684519    -4.015011
  H     -3.999324     0.051695    -3.656661
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  H     -3.131989    -0.619905    -5.056626
  H     -0.826610    -2.076525     5.468142
  H      0.265800    -1.236558     4.346836
  H     -1.030994    -0.338043     5.166598
  H     -3.281498    -2.490701     4.803755
  H     -3.529023    -0.766127     4.472376
  H     -3.883154    -1.973940     3.215909
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TPSS.L04
  O     -1.161452     1.003067     0.485322
  C     -0.288868     0.230763     0.926631
  O     -0.510636    -0.600357     2.015591
  C      1.107513     0.132243     0.422090
  C     -1.867798    -0.496392     2.639572
  C      1.416296     0.459703    -0.919944
  C      0.382899     0.719477    -1.967059
  O      0.413525     1.678825    -2.760198
  O     -0.561446    -0.285659    -2.022842
  C     -1.686555    -0.060743    -2.985654
  C      2.153130    -0.166487     1.317270
  C      3.487913    -0.115984     0.898119
  C      3.793299     0.243297    -0.422770
  C      2.760324     0.531675    -1.323416
  H      2.980920     0.804299    -2.350976
  H      4.827737     0.296249    -0.751451
  H      4.284179    -0.343806     1.601674
  H      1.906516    -0.416515     2.343165
  C     -2.604090    -1.271104    -2.871246
  H     -2.178581     0.873135    -2.699369
  H     -1.257050     0.053846    -3.985108
  H     -3.445873    -1.157480    -3.565829
  H     -2.069352    -2.193164    -3.122698
  H     -3.002440    -1.362445    -1.855671
  C     -1.883424    -1.469588     3.811436
  H     -2.017483     0.542671     2.947645
  H     -2.607764    -0.745319     1.873441
  H     -2.865535    -1.436557     4.299347
  H     -1.699688    -2.493883     3.471177
  H     -1.121161    -1.204876     4.551749
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TPSS.L05
  O      1.201712     0.160339     1.004649
  C      0.763171     1.220237     1.494588
  O      0.807043     1.485567     2.856198
  C      0.145939     2.325952     0.716826
  C      1.417326     0.413682     3.704385
  C      0.043670     2.176828    -0.676358
  H      0.410022     1.273723    -1.152439
  C     -0.331266     3.501165     1.333139
  C     -0.905335     4.515880     0.556714
  C     -1.007749     4.368333    -0.832454
  C     -0.532197     3.195248    -1.454079
  C     -0.616994     2.989224    -2.923386
  H     -1.450702     5.149180    -1.439958
  H     -1.272499     5.420798     1.033757
  H     -0.248432     3.608119     2.408633
  C      1.361798     0.912439     5.142772
  H      0.841638    -0.503841     3.551626
  H      2.439786     0.248454     3.352438
  H      1.800200     0.156974     5.806680
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  H      1.927634     1.842936     5.257131
  H      0.327790     1.089774     5.456542
  O     -1.202859     4.062728    -3.579619
  O     -0.214495     1.974529    -3.526823
  C     -1.321954     3.925256    -5.065461
  C     -1.984041     5.201549    -5.568968
  H     -0.316265     3.781291    -5.470991
  H     -1.915033     3.029910    -5.273332
  H     -2.093933     5.148328    -6.659284
  H     -2.978062     5.327993    -5.127374
  H     -1.377570     6.080150    -5.325400
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TPSS.L06
  O      1.102736     0.209610     0.883082
  C      0.697697     1.244625     1.452011
  O      0.827150     1.442651     2.817500
  C      0.035437     2.384665     0.766303
  C      1.486837     0.332508     3.575066
  C     -0.152824     2.297612    -0.627796
  H      0.190249     1.407514    -1.145568
  C     -0.400992     3.530096     1.463144
  C     -1.017860     4.573746     0.770367
  C     -1.206121     4.486693    -0.623733
  C     -0.769693     3.341262    -1.320573
  H     -0.917261     3.280000    -2.392600
  C     -1.868382     5.626733    -1.309441
  H     -1.360933     5.463844     1.288139
  H     -0.253423     3.591358     2.535170
  C      1.516106     0.760904     5.036593
  H      0.903155    -0.578155     3.411831
  H      2.486745     0.188154     3.155515
  H      1.993414    -0.024426     5.635862
  H      2.087085     1.686678     5.162432
  H      0.502408     0.919300     5.419007
  O     -1.997835     5.428707    -2.674929
  O     -2.273420     6.661748    -0.740512
  C     -2.657522     6.538849    -3.432496
  C     -2.686791     6.110454    -4.894023
  H     -3.657430     6.683203    -3.012944
  H     -2.073840     7.449513    -3.269260
  H     -3.164099     6.895784    -5.493291
  H     -1.673093     5.952058    -5.276437
  H     -3.257769     5.184680    -5.019862
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TPSS.L07
  C     -5.386250     0.611488     0.449602
  C     -4.326064    -0.324364    -0.116369
  O     -3.002078     0.340851     0.114630
  C     -1.888842    -0.349389    -0.333452
  O     -1.958887    -1.470984    -0.869795
  O      1.958726     1.469208    -0.873152
  C      1.888782     0.348702    -0.334522
  C      0.624010    -0.449834    -0.108630
  C     -0.624028     0.449601    -0.109411
  H     -0.538200     1.189698    -0.916564
  O      3.002100    -0.340626     0.114757
  C      4.326043     0.324121    -0.117834
  C      5.386330    -0.610555     0.449887
  H      0.538023    -1.191550    -0.914280
  H      0.716885    -1.016478     0.823127
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  H     -0.716722     1.018114     0.821225
  H     -4.435569    -0.487526    -1.192505
  H     -4.304971    -1.295719     0.386177
  H      4.435367     0.485065    -1.194322
  H      4.305028     1.296510     0.382712
  H     -6.379234     0.167963     0.304458
  H     -5.232540     0.773840     1.521458
  H     -5.362434     1.581494    -0.057615
  H      6.379287    -0.167324     0.303661
  H      5.232802    -0.770697     1.522101
  H      5.362436    -1.581605    -0.055324
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TPSS.L08
  C      0.747421     0.854372    -2.787576
  C     -0.537792     1.629309    -2.525624
  O     -0.129515     2.966053    -1.980048
  C     -1.169798     3.825970    -1.664177
  O     -2.362510     3.507885    -1.834982
  C     -0.727225     5.173225    -1.100917
  C     -1.092118     5.298140     0.436619
  C     -2.592201     5.092983     0.635525
  O     -3.150543     4.222609     1.324727
  C      0.738625     5.576422    -1.445902
  C      0.901638     5.719993    -2.981835
  C      1.142775     6.914190    -0.776856
  C     -0.199382     4.505885     1.441470
  C     -0.328641     2.963113     1.405140
  C     -0.436451     5.031106     2.881810
  O     -3.303674     6.070309    -0.047842
  C     -4.792576     5.920046    -0.030719
  C     -5.354505     7.041888    -0.894995
  H      1.316238     0.713931    -1.862579
  H      1.381140     1.377797    -3.511165
  H      0.500065    -0.133810    -3.195039
  H     -1.181900     1.148598    -1.783663
  H     -1.121723     1.804157    -3.433929
  H     -1.393856     5.894475    -1.592058
  H     -0.931497     6.362869     0.652947
  H      1.416308     4.786729    -1.099881
  H      1.938751     5.979438    -3.228660
  H      0.652328     4.791680    -3.504242
  H      0.253124     6.521204    -3.362838
  H      2.137002     7.217111    -1.127516
  H      0.436362     7.713362    -1.041303
  H      1.186287     6.843159     0.315792
  H      0.836820     4.756215     1.169989
  H      0.342518     2.529733     2.158363
  H     -1.351489     2.651601     1.632616
  H     -0.038513     2.555965     0.432455
  H      0.284263     4.575784     3.572389
  H     -0.312844     6.121422     2.934191
  H     -1.444999     4.778056     3.226928
  H     -5.025238     4.926306    -0.423147
  H     -5.126227     5.979521     1.009538
  H     -5.073808     8.022992    -0.496972
  H     -4.987058     6.961925    -1.923266
  H     -6.449663     6.975535    -0.912606
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TPSS.L09
  C     -1.477101     0.628789     0.758620
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  H     -1.738109     1.289834     1.589832
  H     -0.445540     0.290708     0.892898
  H     -2.144136    -0.242948     0.785549
  C     -1.646164     1.345492    -0.580244
  H     -1.407862     0.701893    -1.429132
  H     -2.646183     1.772946    -0.692143
  O     -0.655119     2.464550    -0.724963
  C     -1.003454     3.679623    -0.164453
  C      0.084596     4.731472    -0.336369
  O     -2.092493     3.874444     0.410159
  C      0.671976     4.759719    -1.784574
  H     -0.422406     5.689123    -0.175227
  C      1.159265     4.628592     0.819442
  H      1.883070     5.427595     0.623695
  C      0.572372     4.848720     2.252051
  C      1.918032     3.309273     0.772572
  C      1.723106     5.883208    -1.953120
  H      1.149494     3.794467    -1.985782
  C     -0.473738     4.964308    -2.808092
  H     -0.071790     4.969759    -3.828793
  H     -1.222069     4.166235    -2.745742
  H     -0.980297     5.924549    -2.638830
  H      2.020019     5.957540    -3.006876
  H      1.308402     6.856603    -1.654332
  H      2.626678     5.690115    -1.367069
  O      3.046207     3.399513    -0.035356
  O      1.611988     2.271942     1.386967
  C      3.874979     2.156323    -0.170404
  C      3.373958     1.294896    -1.329142
  H      4.879015     2.546318    -0.346378
  H      3.832354     1.622357     0.782185
  H      4.023849     0.417029    -1.438083
  H      2.352968     0.948885    -1.142010
  H      3.391745     1.856574    -2.269240
  C      1.726384     4.927979     3.283624
  C     -0.296402     6.126008     2.342236
  H     -0.050096     3.979758     2.499298
  H      1.319419     5.048371     4.294971
  H      2.340498     4.020807     3.276484
  H      2.374878     5.790779     3.075640
  H     -0.565261     6.312473     3.389328
  H      0.254040     7.005516     1.977777
  H     -1.226929     6.029135     1.774687
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TPSS.L10
  O      0.000001    -1.293780    -0.000104
  C      1.203115    -0.425506     0.135588
  C      0.739678     0.995944    -0.231990
  C     -0.739677     0.995911     0.232133
  C     -1.203117    -0.425487    -0.135648
  H      1.554177    -0.480833     1.174425
  H      1.972111    -0.826336    -0.530022
  H      0.796710     1.150436    -1.316351
  H      1.334802     1.770685     0.262269
  H     -1.334800     1.770723    -0.262016
  H     -0.796708     1.150249     1.316515
  H     -1.972103    -0.826414     0.529914
  H     -1.554193    -0.480662    -1.174488
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TPSS.L11
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  C      0.057920    -0.100316     0.097297
  H      0.005002    -0.008741     1.183253
  H      1.109566    -0.125898    -0.223412
  H     -0.445821    -1.023796    -0.223484
  O     -0.624094     1.081152    -0.436861
  C     -0.634646     1.099304    -1.905741
  C     -1.368823     2.370806    -2.310925
  H      0.393359     1.110259    -2.294596
  H     -1.158108     0.214446    -2.294500
  O     -1.379375     2.388958    -3.779805
  H     -2.396828     2.359851    -1.922070
  H     -0.845361     3.255664    -1.922166
  C     -2.061389     3.570426    -4.313963
  H     -2.008471     3.478851    -5.399920
  H     -3.113035     3.596008    -3.993254
  H     -1.557648     4.493906    -3.993182
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TPSS.L12
  C      0.026844    -0.046626     0.236852
  H     -0.066761     0.115431     1.311799
  H      1.090426    -0.092710    -0.040745
  H     -0.464925    -0.990799    -0.040800
  O     -0.633154     1.096456    -0.398779
  C     -0.587381     1.017399    -1.865715
  C     -1.302811     2.256718    -2.407437
  H      0.463839     0.986221    -2.196868
  H     -1.085990     0.091477    -2.197024
  C     -1.319671     2.285935    -3.937169
  H     -2.332706     2.270044    -2.035210
  H     -0.799350     3.155247    -2.035166
  O     -2.026477     3.510024    -4.340011
  H     -0.296529     2.303400    -4.347766
  H     -1.846290     1.408543    -4.347738
  C     -2.106226     3.647931    -5.796337
  H     -2.644164     4.579640    -5.978204
  H     -1.102393     3.705183    -6.242914
  H     -2.657790     2.807175    -6.242764
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TPSS.L13
  C      0.084710    -0.146858     0.196718
  H      0.021690    -0.037810     1.280657
  H      1.139975    -0.179136    -0.112678
  H     -0.415304    -1.076663    -0.112804
  O     -0.591564     1.025092    -0.364476
  C     -0.587551     1.018108    -1.835392
  C     -1.315524     2.278706    -2.303499
  H      0.452956     1.005668    -2.198657
  H     -1.096893     0.110684    -2.198602
  C     -1.371481     2.375324    -3.846501
  H     -2.330932     2.268344    -1.886482
  H     -0.798917     3.153013    -1.886647
  C     -2.099454     3.635922    -4.314608
  H     -0.356074     2.385687    -4.263518
  H     -1.888089     1.501017    -4.263353
  O     -2.095442     3.628938    -5.785524
  H     -3.139961     3.648362    -3.951343
  H     -1.590112     4.543346    -3.951397
  C     -2.771716     4.800888    -6.346718
  H     -2.708695     4.691840    -7.430656
  H     -3.826980     4.833166    -6.037321
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  H     -2.271701     5.730693    -6.037195
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TPSS.L14
  C      0.516499     0.001327     0.022102
  H      0.864427     0.266748     1.021821
  H      1.375478    -0.251045    -0.617612
  H     -0.160979    -0.863542     0.080219
  O     -0.183640     1.182556    -0.486936
  C     -0.692903     0.964303    -1.848105
  C     -1.425752     2.229322    -2.362947
  H      0.162264     0.723291    -2.502100
  H     -1.370719     0.096449    -1.842919
  C     -1.407269     2.097695    -3.905137
  C     -2.918325     2.311900    -1.853445
  C     -0.673498     3.531866    -1.939568
  O     -2.163669     3.211340    -4.490723
  H     -0.371809     2.130762    -4.275952
  H     -1.856431     1.145052    -4.227725
  C     -2.161939     3.165508    -5.954930
  H     -2.744536     4.028054    -6.283098
  H     -1.137231     3.235817    -6.348403
  H     -2.630083     2.238956    -6.319190
  H     -3.283287     3.285319    -2.207437
  C     -3.847545     1.233348    -2.466723
  C     -3.054682     2.281170    -0.309754
  H     -4.101650     2.467584    -0.034852
  H     -2.762391     1.306850     0.098697
  H     -2.436609     3.041854     0.176931
  H     -4.854924     1.336279    -2.043351
  H     -3.934211     1.341543    -3.553061
  H     -3.502583     0.214281    -2.241354
  H     -1.269652     4.374901    -2.308929
  H     -0.663813     3.577540    -0.845648
  C      0.784250     3.667262    -2.437388
  C      1.562615     4.831800    -1.764134
  H      1.330399     2.735967    -2.231520
  H      0.806015     3.825817    -3.526444
  C      3.049664     4.801450    -2.192210
  C      0.940180     6.212861    -2.081516
  H      1.517138     4.675262    -0.674943
  H      3.620753     5.594032    -1.690944
  H      3.513050     3.837901    -1.942501
  H      3.144812     4.953152    -3.276822
  H      1.519705     7.017609    -1.610483
  H      0.932412     6.391142    -3.166251
  H     -0.092083     6.285642    -1.720074
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TPSS.L15
  C     -0.530744    -0.000099     0.000032
  C     -1.412333     0.170580     1.258407
  C      0.439423    -1.172982     0.203998
  C      0.438834     1.173264    -0.203979
  O     -2.311729     1.312852     1.045368
  H     -2.010774    -0.735515     1.417797
  H     -0.777176     0.358289     2.135661
  C     -3.207286     1.521102     2.185377
  H     -3.832020     2.377492     1.925388
  H     -3.837870     0.635928     2.352007
  H     -2.634539     1.741027     3.098052
  C      1.782662    -0.724088     0.129758
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  C      2.844066    -1.626844     0.294211
  C      2.552789    -2.979192     0.534252
  C      1.220612    -3.422947     0.606394
  C      0.152523    -2.520346     0.441244
  H      3.877082    -1.291611     0.238724
  H      3.365640    -3.689958     0.664126
  H      1.012316    -4.474547     0.788821
  H     -0.875139    -2.867140     0.478375
  C      1.782298     0.725034    -0.129803
  C      2.843248     1.628316    -0.294309
  C      2.551289     2.980518    -0.534338
  C      1.218890     3.423614    -0.606417
  C      0.151256     2.520485    -0.441213
  H      3.876433     1.293593    -0.238872
  H      3.363783     3.691687    -0.664253
  H      1.010065     4.475111    -0.788835
  H     -0.876580     2.866771    -0.478295
  C     -1.412304    -0.171212    -1.258305
  O     -2.311136    -1.313918    -1.045224
  H     -2.011191     0.734592    -1.417673
  H     -0.777093    -0.358616    -2.135585
  C     -3.206634    -1.522614    -2.185198
  H     -3.830941    -2.379306    -1.925178
  H     -2.633813    -1.742268    -3.097892
  H     -3.837655    -0.637749    -2.351812
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TPSS.ML01
  Ti     0.083408     0.051457     1.386702
  Cl     1.155886     1.529038     2.745761
  Cl     1.317689    -1.516251     0.338405
  Cl    -2.005345     0.485651     0.592614
  Cl    -0.628583    -1.266465     3.069280
  O      0.709636     1.356197    -0.166555
  C      0.655811     2.524918    -0.656699
  O      1.328467     2.815258    -1.787633
  C     -0.118987     3.660560    -0.071269
  C      2.136043     1.701645    -2.433302
  C      2.772890     2.303684    -3.675000
  H      2.864018     1.364971    -1.691518
  H      1.439760     0.888915    -2.652744
  H      3.369314     1.531692    -4.176076
  H      2.011656     2.660336    -4.375730
  H      3.434197     3.136172    -3.415517
  H     -1.176916     3.379352    -0.013756
  H      0.227695     3.839656     0.953007
  H      0.000127     4.560834    -0.673706
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TPSS.ML01-cis
  Ti     0.000001     0.000001     1.244620
  Cl     0.662814     1.580618     2.755645
  Cl     2.157078    -0.873744     0.917464
  Cl    -2.157077     0.873745     0.917466
  Cl    -0.662810    -1.580615     2.755647
  O      0.556453     1.279527    -0.362751
  C      0.609323     2.486962    -0.738806
  O      1.290456     2.812389    -1.864551
  C     -0.017008     3.645438    -0.036379
  C      2.018027     1.698863    -2.587503
  C      2.907403     2.371689    -3.621773
  H      2.574345     1.131068    -1.838425
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  H      1.253042     1.057391    -3.033420
  H      3.451411     1.600376    -4.180576
  H      2.316326     2.961278    -4.329781
  H      3.639180     3.027818    -3.140442
  H     -1.056798     3.400594     0.203066
  H      0.500004     3.803241     0.918079
  H      0.046882     4.545554    -0.648106
  O     -0.556454    -1.279527    -0.362749
  C     -0.609324    -2.486962    -0.738803
  O     -1.290457    -2.812389    -1.864548
  C     -2.018027    -1.698863    -2.587502
  C     -2.907401    -2.371690    -3.621772
  H     -2.574345    -1.131068    -1.838424
  H     -1.253041    -1.057393    -3.033418
  H     -3.451409    -1.600377    -4.180576
  H     -2.316324    -2.961280    -4.329780
  H     -3.639180    -3.027819    -3.140442
  C      0.017006    -3.645438    -0.036375
  H      1.056795    -3.400594     0.203072
  H     -0.500008    -3.803241     0.918082
  H     -0.046883    -4.545554    -0.648102
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TPSS.ML02
  Cl    -1.946479    -2.692585    -1.335863
  Ti     0.004248    -2.450349    -0.166733
  Cl     0.170137    -4.662005     0.256939
  Cl     2.135133    -2.321534    -0.989030
  Cl    -0.238484    -1.821410     1.987892
  H     -0.404772     0.829148     1.365627
  C     -0.439689     1.805181     0.893814
  C     -0.329238     1.903988    -0.510422
  C     -0.168359     0.676392    -1.299142
  O     -0.120734    -0.485221    -0.777740
  O     -0.072967     0.862162    -2.633706
  C      0.095587    -0.340496    -3.542392
  C     -0.592636     2.963537     1.661166
  C     -0.635935     4.220426     1.035879
  C     -0.526245     4.321999    -0.362042
  C     -0.373295     3.169929    -1.137420
  H     -0.287675     3.236957    -2.215824
  H     -0.560081     5.296043    -0.842021
  H     -0.754752     5.119317     1.635064
  H     -0.677530     2.886715     2.741293
  C      0.172741     0.209121    -4.957591
  H      1.008903    -0.851665    -3.230983
  H     -0.768867    -0.987730    -3.380441
  H      0.295297    -0.629361    -5.653752
  H     -0.742914     0.746395    -5.223795
  H      1.028445     0.881436    -5.074681
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TPSS.ML03
  Ti    -0.119686    -1.765351     0.000000
  Cl    -2.230618    -0.727020     0.000000
  Cl    -0.569189    -3.127000     1.757188
  Cl    -0.569189    -3.127001    -1.757187
  Cl     2.191341    -2.140334     0.000001
  O      0.424265    -0.192151     1.327758
  C      0.382283     1.043322     1.565601
  O      0.877671     1.512966     2.741424
  C     -0.197048     2.113176     0.712322
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  C      1.405505     0.476092     3.714757
  C     -0.197048     2.113176    -0.712324
  C      0.382283     1.043321    -1.565602
  O      0.424266    -0.192152    -1.327758
  O      0.877672     1.512964    -2.741425
  C      1.405505     0.476091    -3.714758
  C     -0.773477     3.205858     1.392349
  C     -1.372652     4.262363     0.699873
  C     -1.372651     4.262363    -0.699876
  C     -0.773477     3.205858    -1.392351
  H     -0.755434     3.207045    -2.475441
  H     -1.830738     5.077623    -1.252180
  H     -1.830739     5.077623     1.252177
  H     -0.755434     3.207046     2.475438
  C      1.947940     1.227531    -4.930992
  H      2.176843    -0.095503    -3.190886
  H      0.568782    -0.182771    -3.961261
  C      2.353394     0.183250    -6.003123
  H      1.134858     1.844278    -5.339000
  C      3.137762     2.142479    -4.562919
  C      1.947941     1.227533     4.930991
  H      0.568782    -0.182769     3.961261
  H      2.176843    -0.095502     3.190885
  C      2.353396     0.183252     6.003121
  C      3.137763     2.142481     4.562916
  H      1.134860     1.844281     5.338999
  H      3.494673     2.679732     5.449659
  H      3.973097     1.549144     4.167011
  H      2.852105     2.880784     3.805912
  H      2.718275     0.692807     6.902236
  H      1.505057    -0.449495     6.291120
  H      3.157107    -0.467156     5.634314
  H      2.718272     0.692805    -6.902238
  H      3.157105    -0.467158    -5.634316
  H      1.505054    -0.449498    -6.291121
  H      3.494670     2.679730    -5.449663
  H      2.852104     2.880782    -3.805915
  H      3.973096     1.549143    -4.167015
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TPSS.ML04
  Cl    -2.292285    -0.709039     0.000001
  Ti    -0.196222    -1.775806     0.000000
  Cl    -0.662549    -3.130536     1.757688
  Cl    -0.662551    -3.130536    -1.757687
  Cl     2.109671    -2.178350    -0.000001
  O      0.367532    -0.207935     1.326845
  C      0.343964     1.027328     1.566821
  O      0.838691     1.484950     2.749059
  C     -0.209389     2.109684     0.712543
  C      1.344806     0.434024     3.719902
  C     -0.209390     2.109684    -0.712543
  C      0.343963     1.027328    -1.566822
  O      0.367531    -0.207935    -1.326845
  O      0.838690     1.484950    -2.749060
  C      1.344805     0.434023    -3.719902
  C     -0.759588     3.216064     1.392190
  C     -1.333685     4.286411     0.699834
  C     -1.333685     4.286411    -0.699834
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  H     -0.740835     3.216942    -2.475187
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  H     -1.772082     5.112340    -1.252189
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  C      1.831684     1.188053    -4.946864
  H      2.135934    -0.118472    -3.208314
  H      0.510698    -0.240702    -3.926862
  H      2.218548     0.464144    -5.674173
  H      1.017577     1.747569    -5.418716
  H      2.637814     1.882431    -4.689717
  C      1.831683     1.188054     4.946864
  H      0.510700    -0.240702     3.926860
  H      2.135936    -0.118471     3.208314
  H      2.218547     0.464145     5.674174
  H      2.637813     1.882432     4.689719
  H      1.017575     1.747569     5.418715
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TPSS.ML05
  Cl    -1.924915    -2.663613    -1.407199
  Ti     0.024296    -2.436880    -0.235821
  Cl     0.210845    -4.653634     0.138709
  Cl     2.146123    -2.265820    -1.069197
  Cl    -0.215336    -1.855126     1.932524
  H     -0.408966     0.801997     1.380612
  C     -0.449155     1.790849     0.936466
  C     -0.341690     1.928847    -0.464929
  C     -0.176690     0.721910    -1.288439
  O     -0.121160    -0.450537    -0.796033
  O     -0.087859     0.946394    -2.616032
  C      0.083549    -0.228517    -3.560839
  C     -0.605920     2.927015     1.736907
  C     -0.655530     4.197119     1.149568
  C     -0.548280     4.340499    -0.249662
  C     -0.391495     3.206192    -1.059102
  H     -0.309130     3.314291    -2.132243
  C     -0.606773     5.714936    -0.817680
  H     -0.776348     5.090663     1.753698
  H     -0.688706     2.821024     2.814393
  C      0.142220     0.362677    -4.959927
  H      1.004565    -0.739081    -3.271861
  H     -0.773361    -0.888194    -3.409324
  H      0.266427    -0.454315    -5.680907
  H     -0.781044     0.898275    -5.201950
  H      0.990104     1.046707    -5.065004
  O     -0.489146     5.727097    -2.195102
  O     -0.745939     6.752360    -0.139322
  C     -0.538170     7.079476    -2.842045
  C     -0.388026     6.850852    -4.340053
  H     -1.493394     7.541107    -2.576310
  H      0.273049     7.679729    -2.420415
  H     -0.418188     7.817315    -4.858075
  H      0.566571     6.366182    -4.569568
  H     -1.201299     6.227347    -4.725631
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TPSS.ML06
  Cl    -1.927093    -2.702065    -1.406861
  Ti     0.022731    -2.491131    -0.232878
  Cl     0.205682    -4.711380     0.119369
  Cl     2.147540    -2.312730    -1.057938
  Cl    -0.219812    -1.924880     1.936449
  H     -0.408670     0.754292     1.400396
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  C     -0.447585     1.742282     0.954471
  C     -0.338407     1.881483    -0.446178
  C     -0.172473     0.675112    -1.271670
  O     -0.118589    -0.497935    -0.782460
  O     -0.080667     0.903383    -2.599186
  C      0.092390    -0.269829    -3.546097
  C     -0.604286     2.875499     1.752588
  C     -0.653057     4.154717     1.164231
  C     -0.544050     4.293529    -0.234982
  C     -0.387732     3.163492    -1.037853
  H     -0.303104     3.261056    -2.113963
  H     -0.582726     5.282035    -0.677266
  C     -0.820836     5.330244     2.064145
  H     -0.690118     2.790640     2.830800
  C      0.157539     0.323409    -4.943992
  H      1.011322    -0.782566    -3.254286
  H     -0.766219    -0.928273    -3.398798
  H      0.282944    -0.492575    -5.665866
  H     -0.763815     0.860919    -5.189143
  H      1.007313     1.005723    -5.045161
  O     -0.851453     6.527580     1.374249
  O     -0.923510     5.258889     3.304835
  C     -1.017426     7.759646     2.214120
  C     -1.018525     8.943093     1.256018
  H     -1.955066     7.659870     2.768319
  H     -0.188370     7.789875     2.926846
  H     -1.138140     9.871285     1.828241
  H     -0.076784     8.999526     0.700387
  H     -1.844969     8.869518     0.541621
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TPSS.ML07
  Cl    -2.111793    -0.835612    -0.102380
  Ti     0.056833    -1.734320     0.013105
  Cl    -0.348486    -3.101040     1.776929
  Cl    -0.196346    -3.225322    -1.669440
  Cl     2.392688    -1.840453     0.130270
  O      0.366255    -0.095913     1.359116
  C      0.754057     1.074064     1.597895
  O      1.013137     1.482645     2.860219
  C      0.984223     2.146101     0.561130
  C      0.874934     0.440481     3.959934
  C      0.023821     2.054279    -0.660257
  C      0.427475     1.015653    -1.673647
  O      0.499542    -0.222991    -1.460821
  O      0.723088     1.524978    -2.892329
  C      1.099588     0.530813    -3.978488
  H      0.864025     3.118292     1.045950
  H     -0.011783     3.024247    -1.159196
  C      1.363109     1.348595    -5.232331
  H      1.976469    -0.014201    -3.621434
  H      0.260601    -0.161478    -4.079457
  H      1.635895     0.667557    -6.047472
  H      0.471498     1.907290    -5.533771
  H      2.187934     2.051945    -5.080054
  C      1.286499     1.126721     5.251813
  H     -0.166979     0.111998     3.954688
  H      1.519993    -0.397541     3.686651
  H      1.197289     0.408765     6.075989
  H      2.325130     1.468644     5.203969
  H      0.640021     1.982967     5.468775
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  H     -0.986899     1.795186    -0.320531
  H      2.031957     2.077440     0.237537
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TPSS.ML08
  Ti     0.072597    -1.645030     0.348693
  Cl    -2.203987    -1.049062     0.447514
  Cl     0.034429    -2.941390     2.199628
  Cl    -0.233064    -3.226620    -1.257367
  Cl     2.407294    -1.595051     0.124257
  O      0.439238     0.064969     1.604555
  C      0.323703     1.322697     1.562275
  O      1.048683     2.090012     2.412367
  C     -0.595664     2.074156     0.620186
  C      1.976363     1.362309     3.369439
  C      0.088924     2.347896    -0.769055
  C      0.187615     1.070843    -1.578252
  O      0.167972    -0.099957    -1.118137
  O      0.291905     1.282169    -2.913008
  C      0.396567     0.047157    -3.794418
  H     -1.419834     1.373746     0.429439
  C      1.462598     3.128800    -0.693669
  C      0.512130     0.550830    -5.223896
  H      1.271812    -0.513064    -3.457982
  H     -0.501743    -0.547872    -3.615260
  H      0.584546    -0.312058    -5.896875
  H     -0.367171     1.137288    -5.508746
  H      1.407569     1.166487    -5.356474
  C      2.727954     2.438099     4.137172
  H      1.346185     0.736863     4.006383
  H      2.624505     0.722090     2.766869
  H      3.403374     1.955307     4.853707
  H      3.328205     3.058237     3.463665
  H      2.039543     3.082765     4.692945
  H     -0.609374     2.982485    -1.323192
  C     -1.206091     3.353368     1.285003
  C      1.579529     4.154393    -1.845899
  H      1.428170     3.680920     0.254607
  C      2.700198     2.200963    -0.668531
  H      3.599957     2.791138    -0.458551
  H      2.628206     1.411635     0.086429
  H      2.843720     1.712066    -1.640425
  H      2.517201     4.716304    -1.755423
  H      1.575245     3.651510    -2.819866
  H      0.750222     4.872832    -1.826105
  C     -2.129697     4.126574     0.311403
  C     -2.020190     2.945833     2.540577
  H     -0.389286     4.014692     1.599808
  H     -2.655625     4.917040     0.859530
  H     -1.579214     4.609818    -0.503866
  H     -2.887502     3.462612    -0.125508
  H     -2.427895     3.838970     3.028573
  H     -2.858386     2.294383     2.262951
  H     -1.404842     2.416268     3.275710
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TPSS.ML09
  Cl     0.349296     1.574612    -2.301161
  Ti    -0.000271     1.887183    -0.000373
  Cl     1.716968     3.348209     0.262657
  Cl    -1.717967     3.347605    -0.263768
  Cl    -0.349738     1.575077     2.300492
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  O      1.355858     0.249466     0.174252
  C      1.595097    -0.985652     0.232652
  O      2.864050    -1.438034     0.068886
  C      0.596408    -2.089778     0.510456
  C      3.937232    -0.391039    -0.176637
  C     -0.595707    -2.090090    -0.510226
  C     -1.594740    -0.986208    -0.232698
  O     -1.355882     0.248998    -0.174588
  O     -2.863554    -1.438943    -0.068835
  C     -3.937063    -0.392223     0.176425
  H      1.134889    -3.030923     0.362031
  H     -1.133896    -3.031366    -0.361569
  C     -5.243727    -1.151316     0.343439
  H     -3.641065     0.166738     1.066987
  H     -3.932406     0.278108    -0.686304
  H     -6.051849    -0.430430     0.516432
  H     -5.483032    -1.728902    -0.555146
  H     -5.199483    -1.831187     1.200305
  C      5.244128    -1.149767    -0.343495
  H      3.641046     0.167622    -1.067325
  H      3.932382     0.279491     0.685935
  H      6.052023    -0.428671    -0.516670
  H      5.483627    -1.727068     0.555222
  H      5.200080    -1.829853    -1.200201
  C     -0.132555    -2.051688    -2.014647
  C      0.133249    -2.051142     2.014868
  C     -0.750344    -3.279254     2.339475
  C      1.349290    -1.999778     2.969766
  H     -0.448256    -1.133094     2.167143
  C     -1.348606    -2.000942    -2.969564
  H      0.448665    -1.133497    -2.167148
  C      0.751424    -3.279606    -2.338940
  H      1.003466    -2.019882     4.009325
  H      2.014820    -2.858984     2.812000
  H      1.929116    -1.079211     2.837555
  H     -1.029826    -3.255242     3.399424
  H     -1.676505    -3.297331     1.754852
  H     -0.204314    -4.215034     2.156975
  H     -1.002770    -2.021192    -4.009115
  H     -2.013866    -2.860320    -2.811591
  H     -1.928723    -1.080526    -2.837581
  H      1.030900    -3.255777    -3.398894
  H      1.677589    -3.297245    -1.754311
  H      0.205687    -4.215511    -2.156202
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TPSS.ML10
  Ti     0.037240     0.108290     1.059101
  Cl     2.251587    -0.204719     0.705254
  Cl    -1.436908    -0.819647    -0.408882
  Cl    -0.167160    -1.543120     2.585487
  Cl    -0.682056     1.751463     2.440011
  O      0.207173     1.656369    -0.424071
  C     -0.781223     2.789005    -0.615442
  C     -0.317341     3.480314    -1.898835
  C      0.229268     2.310981    -2.754369
  C      0.944019     1.418685    -1.733761
  H     -1.771526     2.333028    -0.710355
  H     -0.721188     3.395469     0.285574
  H      0.475488     4.204042    -1.679908
  H     -1.142909     4.003207    -2.390250
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  H      0.916544     2.650793    -3.534610
  H     -0.595270     1.766456    -3.226881
  H      0.875282     0.351926    -1.947437
  H      1.980269     1.705770    -1.545931
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TPSS.ML10-cis
  Ti     0.000000     0.000000     0.848836
  Cl     2.337087    -0.010370     0.593179
  Cl    -2.337087     0.010369     0.593180
  Cl     0.001658    -1.721656     2.359694
  Cl    -0.001657     1.721655     2.359694
  O     -0.025878     1.428843    -0.761268
  O      0.025878    -1.428843    -0.761268
  C     -0.993478     2.596746    -0.817428
  C     -0.341073     3.589527    -1.785114
  C      0.456418     2.679114    -2.752450
  C      1.037239     1.615230    -1.817307
  C      0.993478    -2.596746    -0.817428
  C      0.341072    -3.589527    -1.785113
  C     -0.456418    -2.679114    -2.752450
  C     -1.037240    -1.615229    -1.817307
  H     -1.939856     2.190972    -1.179961
  H     -1.102064     2.953352     0.206203
  H      0.338048     4.260845    -1.248182
  H     -1.092440     4.193031    -2.302803
  H      1.247351     3.221127    -3.279323
  H     -0.212341     2.227310    -3.494610
  H      1.200287     0.635528    -2.265194
  H      1.942373     1.944879    -1.303766
  H      1.939855    -2.190972    -1.179961
  H      1.102064    -2.953352     0.206203
  H      1.092439    -4.193032    -2.302803
  H     -0.338049    -4.260845    -1.248181
  H      0.212340    -2.227310    -3.494610
  H     -1.247352    -3.221126    -3.279323
  H     -1.200287    -0.635527    -2.265195
  H     -1.942373    -1.944878    -1.303766
------------------------------------------------
TPSS.ML11
  Ti    -1.186798    -1.980600     0.208630
  Cl    -3.315180    -1.292187     0.838133
  Cl    -1.046469    -3.729186     1.641455
  Cl    -1.864519    -3.005033    -1.699534
  Cl     1.110495    -2.026098    -0.376622
  O     -0.526194    -0.617069     1.755709
  C     -0.818553     0.808320     1.455332
  O     -1.078823     0.013214    -0.783536
  C     -0.399378     1.059045     0.017607
  H     -1.894476     0.924992     1.589765
  H     -0.264269     1.441202     2.153797
  H     -0.743194     2.039221    -0.331385
  H      0.682471     0.953333    -0.123729
  C     -0.817975     0.165174    -2.241417
  H     -1.064928     1.193698    -2.521733
  H      0.231229    -0.069959    -2.444162
  H     -1.476591    -0.544031    -2.736031
  C      0.635450    -0.852249     2.654854
  H      1.553609    -0.513846     2.166927
  H      0.444496    -0.317237     3.589498
  H      0.663996    -1.927376     2.817286
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TPSS.ML12
  Ti    -1.053460    -1.905513     0.163653
  Cl    -2.392084     0.021865     0.340050
  Cl    -1.635497    -2.684335     2.225118
  Cl    -2.583897    -3.042586    -1.084981
  Cl     0.649348    -3.491547    -0.151342
  O      0.515390    -0.687848     1.042365
  C      0.742433     0.750789     0.708278
  O     -0.252365    -0.978397    -1.627803
  C      1.126653     0.890464    -0.766426
  H     -0.181153     1.280900     0.952143
  H      1.556658     1.099892     1.350136
  H      1.353210     1.951798    -0.946999
  H      2.039517     0.317449    -0.966828
  C     -0.145276    -1.720721    -2.913492
  H      0.820097    -1.480940    -3.369180
  H     -0.196842    -2.776655    -2.662134
  H     -0.979629    -1.428935    -3.557867
  C      1.316833    -1.162965     2.203065
  C      0.033048     0.482802    -1.756201
  H      0.365863     0.650905    -2.784675
  H     -0.909686     1.004873    -1.576894
  H      0.924337    -0.701173     3.113684
  H      1.201490    -2.243104     2.232283
  H      2.363083    -0.892609     2.031679
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TPSS.ML13
  Ti    -0.778214    -2.227906     0.132594
  Cl    -2.600204    -0.856284     0.699201
  Cl    -0.777961    -3.315048     2.131886
  Cl    -2.081039    -3.671721    -1.059164
  Cl     1.233392    -3.206324    -0.588214
  O      0.470901    -0.667388     0.942055
  C      1.525252     0.028155     0.140087
  O     -0.518966    -0.940863    -1.662516
  C      1.023873     1.391173    -0.374925
  H      2.403278     0.124782     0.787763
  H      1.745272    -0.668096    -0.664733
  H      1.212379     2.173063     0.371631
  H      1.622502     1.651839    -1.259349
  C     -0.447932    -1.620807    -2.991773
  H      0.216784    -1.035175    -3.634460
  H     -0.038359    -2.610649    -2.812079
  H     -1.455903    -1.683746    -3.411781
  C      0.325723    -0.119607     2.315255
  C     -0.485597     1.408479    -0.709402
  H     -0.759804     2.425694    -1.024555
  H     -1.067010     1.189842     0.188903
  H      0.106795     0.950700     2.255515
  H     -0.500936    -0.653791     2.775913
  H      1.260374    -0.304520     2.853351
  C     -0.948972     0.491478    -1.841057
  H     -2.041031     0.491079    -1.915659
  H     -0.510164     0.802890    -2.796243
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TPSS.ML14
  Ti    -1.248641    -1.655862     0.442880
  Cl    -1.750843     0.634058     0.687676
  Cl    -1.626478    -2.138727     2.639906
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  Cl    -3.331688    -2.135232    -0.359220
  Cl    -0.377873    -3.771201    -0.080586
  O      0.781894    -1.109372     0.900934
  C      1.444189     0.144185     0.417382
  O     -0.502368    -1.118097    -1.542675
  C      1.644744     0.121486    -1.114381
  H      0.795947     0.964550     0.729738
  H      2.404777     0.210259     0.934444
  C      2.382547     1.455621    -1.497158
  C      2.505557    -1.133771    -1.529444
  C     -1.219639    -1.658642    -2.733196
  H     -0.542765    -1.612052    -3.590238
  H     -1.466803    -2.690396    -2.492641
  H     -2.123929    -1.069722    -2.907018
  C      1.546397    -1.828188     1.958649
  C      0.274434     0.133136    -1.823400
  H      0.404782     0.185551    -2.907736
  H     -0.345469     0.963825    -1.480366
  H      1.445634    -1.278724     2.898698
  H      1.103169    -2.817838     2.035879
  H      2.589659    -1.896488     1.640420
  H      2.757921     1.345603    -2.522062
  C      1.567287     2.771194    -1.391361
  H      3.268663     1.541731    -0.851868
  C      2.451748     4.047469    -1.464845
  H      0.821251     2.823120    -2.198110
  H      1.007501     2.798887    -0.446593
  C      1.587961     5.307045    -1.215955
  H      3.200854     3.981926    -0.659139
  C      3.202153     4.164425    -2.813633
  H      2.207819     6.212433    -1.217465
  H      0.827388     5.418364    -2.000947
  H      1.071240     5.249242    -0.249635
  H      3.791833     5.088855    -2.847967
  H      3.889883     3.325604    -2.976215
  H      2.489506     4.188730    -3.650089
  C      2.564461    -1.377281    -3.058583
  C      3.960256    -1.076398    -0.991303
  H      2.004255    -2.001325    -1.082397
  H      3.222760    -2.230029    -3.263306
  H      1.584828    -1.621279    -3.480100
  H      2.970041    -0.511971    -3.599685
  H      4.441931    -2.049790    -1.143508
  H      4.555678    -0.325555    -1.525764
  H      4.017018    -0.847843     0.079612
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TPSS.ML15
  Ti    -0.934649    -2.122903     0.286194
  Cl    -2.319074    -0.225701     0.453388
  Cl    -1.254060    -2.709651     2.464853
  Cl    -2.560005    -3.382649    -0.695654
  Cl     0.740490    -3.740667    -0.061063
  O      0.699145    -0.807299     0.835968
  C      0.794796     0.621335     0.406249
  O     -0.321788    -1.335518    -1.640120
  C      0.993160     0.744252    -1.121288
  H     -0.128702     1.105536     0.728668
  H      1.655945     1.055455     0.919682
  C      1.047332     2.245761    -1.463821
  C      2.375156     0.266188    -1.588397
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  C     -0.363679    -2.179310    -2.869560
  H      0.493949    -1.911477    -3.492324
  H     -0.289714    -3.210130    -2.532341
  H     -1.311644    -2.001779    -3.384828
  C      1.628260    -1.150551     1.951516
  C     -0.168048     0.122941    -1.929583
  H      0.041364     0.219385    -2.997535
  H     -1.122071     0.591619    -1.681530
  H      1.271856    -0.668139     2.865796
  H      1.602295    -2.233244     2.045781
  H      2.628977    -0.808397     1.674817
  C      2.296127     2.572690    -2.047495
  C      2.563933     3.892812    -2.439050
  C      1.577393     4.872821    -2.241724
  C      0.339822     4.543807    -1.662134
  C      0.065216     3.220540    -1.267151
  H      3.516885     4.160318    -2.888301
  H      1.773552     5.899202    -2.541135
  H     -0.411694     5.315239    -1.517060
  H     -0.895292     2.975467    -0.819341
  C      2.925967    -1.017747    -1.540999
  C      4.230574    -1.211588    -2.036084
  C      4.965887    -0.138136    -2.567400
  C      4.414292     1.152169    -2.615860
  C      3.115890     1.352137    -2.124618
  H      2.366267    -1.853648    -1.132536
  H      4.670818    -2.205017    -2.005152
  H      5.971342    -0.307491    -2.944624
  H      4.989295     1.977491    -3.028281
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M06L.M
  Ti     0.000476    -0.000265    -0.000326
  Cl     1.728071    -1.127007     0.777194
  Cl    -1.300399    -1.352897    -1.156451
  Cl     0.710781     1.628929    -1.303789
  Cl    -1.138938     0.851248     1.683393
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M06L.L01
  O      1.210085     1.355343     0.000002
  C      1.056848     0.131252     0.000000
  O     -0.180693    -0.462206    -0.000001
  C      2.144586    -0.890819     0.000000
  C     -1.331663     0.460157     0.000001
  C     -2.575548    -0.391094    -0.000001
  H     -1.255763     1.099456     0.879987
  H     -1.255764     1.099460    -0.879982
  H     -3.461138     0.243625     0.000001
  H     -2.612858    -1.028611    -0.881631
  H     -2.612858    -1.028615     0.881627
  H      3.108880    -0.395107    -0.000018
  H      2.063287    -1.532523     0.875703
  H      2.063265    -1.532548    -0.875682
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M06L.L02
  O     -1.449367     0.160936     1.092983
  C     -0.314351     0.127785     1.588153
  O     -0.104700     0.160345     2.943674
  C      0.939613     0.050649     0.819693
  C     -1.319532     0.237594     3.772222
  C      0.854212     0.010758    -0.577808
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  H     -0.124819     0.038154    -1.035181
  C      2.194826     0.016620     1.440637
  C      3.350223    -0.056721     0.668550
  C      3.259419    -0.096275    -0.723578
  C      2.010350    -0.062499    -1.346194
  H      1.940783    -0.093110    -2.425087
  H      4.159289    -0.153253    -1.321512
  H      4.318878    -0.082973     1.149304
  H      2.250774     0.047783     2.518364
  C     -0.867648     0.266521     5.210120
  H     -1.872664     1.131816     3.483993
  H     -1.944723    -0.625496     3.542209
  H     -1.732565     0.324304     5.870225
  H     -0.306449    -0.631676     5.462111
  H     -0.233455     1.129973     5.403667
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M06L.L03
  O     -0.751229     1.302055     0.110934
  C      0.091552     0.510746     0.546909
  O     -0.204282    -0.472019     1.451622
  C      1.536658     0.549431     0.228438
  C     -1.617170    -0.566250     1.856341
  C      1.982533     0.766345    -1.087833
  C      1.073087     0.712384    -2.252743
  O      1.193577     1.390818    -3.277441
  O      0.112590    -0.243197    -2.077340
  C     -0.993454    -0.291879    -3.042734
  C      2.467881     0.499034     1.269053
  C      3.822446     0.699674     1.014977
  C      4.257776     0.956927    -0.284136
  C      3.339680     0.986682    -1.329592
  H      3.657396     1.163594    -2.347716
  H      5.307416     1.123343    -0.483097
  H      4.533178     0.664490     1.829279
  H      2.117114     0.322023     2.276163
  C     -2.251385    -0.683255    -2.282111
  H     -1.080204     0.685415    -3.516774
  H     -0.734848    -1.029607    -3.806409
  C     -3.438558    -0.699395    -3.248254
  C     -2.082045    -2.034020    -1.583222
  H     -2.416723     0.087979    -1.523095
  C     -1.801421    -1.881951     2.590311
  H     -1.850271     0.293179     2.490389
  H     -2.234130    -0.501872     0.959057
  C     -3.285768    -2.064492     2.920254
  H     -1.491910    -2.681225     1.909045
  C     -0.937278    -1.947056     3.850622
  H     -2.970619    -2.285986    -1.001135
  H     -1.927814    -2.832048    -2.314236
  H     -1.221869    -2.025857    -0.913706
  H     -4.360876    -0.945548    -2.722044
  H     -3.578020     0.267965    -3.732277
  H     -3.296068    -1.449371    -4.030404
  H     -1.058458    -2.904754     4.357176
  H      0.117440    -1.818582     3.611440
  H     -1.223189    -1.160541     4.553934
  H     -3.455131    -3.017336     3.421154
  H     -3.637992    -1.274605     3.587996
  H     -3.903793    -2.043672     2.021242
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M06L.L04

O	-1.145384	0.946385	0.357187
C	-0.278986	0.197006	0.823811
O	-0.515726	-0.628987	1.891222
C	1.126533	0.129430	0.372092
C	-1.877628	-0.564310	2.451765
C	1.469470	0.448006	-0.954891
C	0.457235	0.653917	-2.016048
O	0.488963	1.565221	-2.849019
O	-0.485425	-0.331843	-2.009632
C	-1.649936	-0.107457	-2.884053
C	2.142537	-0.128002	1.299012
C	3.480301	-0.043095	0.925071
C	3.817399	0.310624	-0.380584
C	2.813898	0.555797	-1.313425
H	3.055780	0.822454	-2.332869
H	4.855541	0.391221	-0.672161
H	4.255762	-0.239696	1.652610
H	1.868347	-0.372598	2.314534
C	-2.673172	-1.151198	-2.516406
H	-2.002779	0.908904	-2.708049
H	-1.320038	-0.178962	-3.920777
H	-3.562952	-1.036164	-3.134705
H	-2.281191	-2.156187	-2.664469
H	-2.965899	-1.046784	-1.472694
C	-1.920524	-1.526085	3.611401
H	-2.076102	0.466653	2.745852
H	-2.581225	-0.824310	1.660467
H	-2.913449	-1.522974	4.059831
H	-1.696120	-2.540311	3.286145
H	-1.200172	-1.247763	4.378782

M06L.L05

O	1.194097	0.179207	0.998314
C	0.759178	1.231268	1.482429
O	0.799920	1.496744	2.827330
C	0.148490	2.327905	0.708454
C	1.398337	0.442051	3.664467
C	0.045633	2.179954	-0.675842
H	0.408830	1.279258	-1.150121
C	-0.323554	3.497286	1.320296
C	-0.892611	4.507345	0.549754
C	-0.995026	4.359259	-0.830596
C	-0.525183	3.192452	-1.449063
C	-0.611949	2.989766	-2.907136
H	-1.434570	5.135590	-1.438425
H	-1.255826	5.408618	1.024344
H	-0.238697	3.600574	2.391504
C	1.338810	0.927456	5.090244
H	0.835445	-0.477979	3.505916
H	2.417396	0.270009	3.317485
H	1.770383	0.179723	5.754814
H	1.897279	1.853953	5.212345
H	0.310631	1.105501	5.400621
O	-1.191862	4.052227	-3.551925
O	-0.214270	1.983795	-3.507359
C	-1.311735	3.917692	-5.014427
C	-1.975246	5.174138	-5.517486
H	-0.312414	3.772329	-5.425179
H	-1.890182	3.018351	-5.226607

H	-2.088002	5.125913	-6.600061
H	-2.963386	5.298151	-5.077738
H	-1.381572	6.054206	-5.276199

M06L.L06

O	1.090352	0.234390	0.881384
C	0.687939	1.261321	1.444342
O	0.813941	1.459868	2.793453
C	0.031071	2.391766	0.762045
C	1.463855	0.367691	3.539626
C	-0.155444	2.304328	-0.623498
H	0.187691	1.416188	-1.134978
C	-0.402468	3.530159	1.454823
C	-1.015241	4.567029	0.766068
C	-1.201756	4.479592	-0.619475
C	-0.768217	3.341198	-1.312253
H	-0.916692	3.283697	-2.379771
C	-1.858624	5.610037	-1.301771
H	-1.358376	5.455170	1.277548
H	-0.253993	3.587661	2.522341
C	1.496558	0.785019	4.987504
H	0.890681	-0.544705	3.373843
H	2.458136	0.214601	3.119540
H	1.970739	0.008137	5.586322
H	2.061256	1.706647	5.116918
H	0.490689	0.944564	5.371963
O	-1.984625	5.411490	-2.650882
O	-2.261037	6.636967	-0.738814
C	-2.634539	6.503667	-3.397056
C	-2.667243	6.086339	-4.844934
H	-3.628821	6.656757	-2.976970
H	-2.061365	7.416063	-3.231273
H	-3.141423	6.863221	-5.443751
H	-1.661373	5.926794	-5.229393
H	-3.231940	5.164710	-4.974348

M06L.L07

C	-5.348379	0.627051	0.346968
C	-4.275714	-0.330570	-0.104437
O	-2.981870	0.350700	0.095327
C	-1.871036	-0.366516	-0.253929
O	-1.926910	-1.522233	-0.687232
O	1.926792	1.520800	-0.690754
C	1.870991	0.366014	-0.254970
C	0.621798	-0.437463	-0.063795
C	-0.621818	0.437382	-0.064712
H	-0.554825	1.169149	-0.873851
O	2.981881	-0.350465	0.095615
C	4.275697	0.330368	-0.105814
C	5.348443	-0.626400	0.347208
H	0.554715	-1.171065	-0.871261
H	0.705787	-1.024663	0.850170
H	-0.705699	1.026660	0.847924
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M06L.L08
  C      0.564190     0.977898    -2.842032
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  O     -0.241460     3.090272    -2.054687
  C     -1.218791     3.898071    -1.540191
  O     -2.401216     3.538977    -1.481151
  C     -0.723063     5.234997    -1.035642
  C     -1.056581     5.374895     0.485565
  C     -2.540840     5.185799     0.715011
  O     -3.076868     4.400548     1.500411
  C      0.740271     5.572392    -1.392148
  C      0.895512     5.735531    -2.910171
  C      1.206581     6.863194    -0.707600
  C     -0.166813     4.542177     1.434136
  C     -0.318458     3.022781     1.291050
  C     -0.376883     4.980735     2.888712
  O     -3.258220     6.058278    -0.061244
  C     -4.716329     5.852360    -0.063314
  C     -5.282280     6.744406    -1.138568
  H      1.240493     0.899106    -1.992133
  H      1.097222     1.466428    -3.656154
  H      0.300805    -0.029512    -3.162396
  H     -1.222731     1.295505    -1.635674
  H     -1.378817     1.853214    -3.298848
  H     -1.366558     5.970599    -1.530650
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M06L.L09
  C     -1.218805     0.763639     0.863810
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  C     -1.358603     1.327811    -0.532086
  H     -1.028299     0.632563    -1.299913
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M06L.L10

O	0.000001	-1.274062	-0.000103
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C	-0.731902	0.988420	0.230119
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H	1.958941	-0.819196	-0.521456
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M06L.L11

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M06L.L12
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  O     -0.636720     1.103847    -0.420612
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  C     -0.598737     1.037311    -1.839379
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M06L.L14
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M06L.L15

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  O      0.742510     1.357798    -0.185977
  C      0.677198     2.518770    -0.663778
  O      1.334176     2.814616    -1.785974
  C     -0.096342     3.627358    -0.066345
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  C      0.614693     2.444122    -0.734555
  O      1.289282     2.768618    -1.846154
  C      0.000670     3.582221    -0.022218
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H	2.684117	0.632248	6.857365
H	1.538976	-0.532595	6.194622
H	3.181856	-0.445325	5.557491
H	2.684115	0.632245	-6.857367
H	3.181855	-0.445328	-5.557492
H	1.538975	-0.532598	-6.194622
H	3.388151	2.682606	-5.485332
H	2.743852	2.916823	-3.859466
H	3.906321	1.626592	-4.173458

M06L.ML04

Cl	-2.230898	-0.585688	-0.000001
Ti	-0.174969	-1.742456	-0.000001
Cl	-0.678203	-3.052848	1.770200
Cl	-0.678202	-3.052846	-1.770202
Cl	2.113016	-2.183792	0.000000
O	0.420071	-0.183306	1.311873
C	0.370545	1.038844	1.558321
O	0.839143	1.488546	2.737005
C	-0.190946	2.106105	0.708696
C	1.344192	0.443543	3.678336
C	-0.190945	2.106106	-0.708695
C	0.370546	1.038844	-1.558321
O	0.420072	-0.183305	-1.311873
O	0.839145	1.488546	-2.737005
C	1.344194	0.443543	-3.678335
C	-0.752246	3.198649	1.383376
C	-1.336066	4.255093	0.695366
C	-1.336065	4.255093	-0.695365
C	-0.752245	3.198649	-1.383376
H	-0.733169	3.198127	-2.461731
H	-1.783388	5.071185	-1.244643
H	-1.783389	5.071184	1.244644
H	-0.733171	3.198126	2.461731
C	1.798916	1.164734	-4.917265
H	2.143726	-0.092253	-3.168570
H	0.528915	-0.256865	-3.855583
H	2.186666	0.440888	-5.632507
H	0.977204	1.699754	-5.389575

H	2.590761	1.876468	-4.692147
C	1.798918	1.164735	4.917264
H	0.528913	-0.256864	3.855586
H	2.143723	-0.092254	3.168570
H	2.186668	0.440889	5.632506
H	2.590763	1.876468	4.692144
H	0.977207	1.699757	5.389575

M06L.ML05

Cl	-1.845042	-2.702391	-1.539402
Ti	0.012374	-2.407011	-0.265379
Cl	0.253244	-4.600050	0.175708
Cl	2.121569	-2.185194	-1.088923
Cl	-0.324723	-1.784203	1.874383
H	-0.405176	0.811302	1.337286
C	-0.440002	1.801415	0.903741
C	-0.343334	1.943236	-0.489370
C	-0.197761	0.744132	-1.307214
O	-0.171865	-0.417261	-0.818252
O	-0.095650	0.959653	-2.621115
C	0.049588	-0.221325	-3.524452
C	-0.578912	2.927796	1.706118
C	-0.623040	4.191902	1.126120
C	-0.528379	4.340152	-0.264779
C	-0.387395	3.214585	-1.074808
H	-0.313957	3.325710	-2.144590
C	-0.584688	5.706168	-0.822962
H	-0.731060	5.082631	1.728936
H	-0.652656	2.819043	2.778496
C	0.177551	0.322549	-4.920638
H	0.929120	-0.774740	-3.197183
H	-0.831786	-0.845674	-3.384620
H	0.285132	-0.505781	-5.619286
H	-0.703867	0.893775	-5.205057
H	1.052127	0.962762	-5.016757
O	-0.490151	5.720096	-2.186083
O	-0.705187	6.734004	-0.145171
C	-0.541821	7.054200	-2.816244
C	-0.423304	6.841641	-4.303166
H	-1.480719	7.526925	-2.528105
H	0.271560	7.652516	-2.405877
H	-0.456508	7.801643	-4.816880
H	0.516137	6.353415	-4.556230
H	-1.240193	6.227525	-4.678038

M06L.ML06

Cl	-1.844218	-2.731217	-1.518834
Ti	0.020646	-2.450612	-0.251684
Cl	0.258042	-4.646826	0.172927
Cl	2.127080	-2.226191	-1.081701
Cl	-0.305891	-1.837413	1.890044
H	-0.417500	0.768780	1.365901
C	-0.450503	1.758577	0.931984
C	-0.344017	1.904632	-0.459433
C	-0.192271	0.707416	-1.280434
O	-0.161707	-0.454897	-0.795853
O	-0.090454	0.928184	-2.594127
C	0.060486	-0.249739	-3.500818
C	-0.597095	2.881415	1.731123
C	-0.639661	4.155521	1.151791

C	-0.532594	4.300777	-0.238261
C	-0.384764	3.181017	-1.042168
H	-0.301188	3.279021	-2.113867
H	-0.567010	5.289201	-0.669735
C	-0.800262	5.319425	2.049392
H	-0.681150	2.796655	2.804856
C	0.165280	0.296766	-4.897887
H	0.950822	-0.791379	-3.183267
H	-0.810690	-0.886240	-3.351792
H	0.276337	-0.529429	-5.598484
H	-0.727315	0.855535	-5.172102
H	1.029825	0.948981	-5.003742
O	-0.837681	6.503906	1.369626
O	-0.892807	5.245360	3.280409
C	-0.998705	7.712869	2.202112
C	-1.029297	8.891063	1.263654
H	-1.917017	7.604160	2.779092
H	-0.166777	7.750058	2.905421
H	-1.147310	9.812640	1.832295
H	-0.106164	8.961161	0.691116
H	-1.860489	8.814554	0.564951

M06L.ML07

Cl	-1.443374	-0.808870	-1.165737
Ti	0.521414	-1.440206	-0.037964
Cl	-0.476683	-2.799501	1.460300
Cl	1.209807	-2.934854	-1.580583
Cl	2.571366	-1.279511	1.101457
O	0.043029	0.260420	1.188505
C	0.690057	1.253903	1.594164
O	0.922522	1.455949	2.886515
C	1.263126	2.296785	0.690756
C	0.516923	0.347175	3.814990
C	0.561480	2.380798	-0.665232
C	0.926997	1.270809	-1.596087
O	1.357947	0.156539	-1.217591
O	0.754752	1.552621	-2.882995
C	0.940751	0.412937	-3.843086
H	1.236330	3.257540	1.200507
H	0.770335	3.331404	-1.151151
C	0.546529	0.926647	-5.199296
H	1.983518	0.106408	-3.776166
H	0.314787	-0.404213	-3.485653
H	0.667692	0.131054	-5.932996
H	-0.494833	1.241447	-5.211622
H	1.167068	1.767392	-5.503766
C	1.009146	0.731087	5.182009
H	-0.566100	0.255419	3.748254
H	0.967870	-0.566129	3.427939
H	0.734958	-0.046973	5.892941
H	2.092271	0.832853	5.194351
H	0.568416	1.668257	5.516792
H	-0.524662	2.328486	-0.539836
H	2.320333	2.044118	0.562649

M06L.ML08

Ti	-0.124039	-1.618544	0.327276
Cl	-2.360575	-1.033797	0.686247
Cl	0.067233	-2.963601	2.119780
Cl	-0.545186	-3.119183	-1.314897

Cl	2.189554	-1.473276	-0.112422
O	0.331979	0.074841	1.572585
C	0.232742	1.322185	1.528771
O	1.018379	2.080984	2.308222
C	-0.711943	2.085064	0.643173
C	2.039278	1.363272	3.129795
C	-0.068375	2.373220	-0.741269
C	0.024167	1.110101	-1.546720
O	-0.167313	-0.037871	-1.099316
O	0.338076	1.300653	-2.832956
C	0.560868	0.064800	-3.650554
H	-1.549045	1.402647	0.468599
C	1.297301	3.131991	-0.674354
C	1.085786	0.525446	-4.982308
H	1.259899	-0.563640	-3.098714
H	-0.392312	-0.458058	-3.712078
H	1.270445	-0.339897	-5.617001
H	0.372405	1.172935	-5.488716
H	2.023543	1.067138	-4.868191
C	2.957295	2.418284	3.683661
H	1.501725	0.806372	3.896005
H	2.539669	0.647976	2.476838
H	3.725200	1.947788	4.295803
H	3.451725	2.965148	2.882079
H	2.416441	3.130672	4.303788
H	-0.770477	3.014060	-1.278785
C	-1.264137	3.344927	1.354384
C	1.447186	4.114443	-1.837581
H	1.262698	3.704536	0.258707
C	2.499383	2.183306	-0.611002
H	3.407953	2.738299	-0.378243
H	2.389577	1.394572	0.134679
H	2.657210	1.686367	-1.571137
H	2.381399	4.669678	-1.749907
H	1.458707	3.587041	-2.792298
H	0.628805	4.836106	-1.859504
C	-2.180857	4.160803	0.439311
C	-2.031310	2.911948	2.610092
H	-0.420609	3.970850	1.660315
H	-2.672397	4.947525	1.010994
H	-1.641837	4.646396	-0.374962
H	-2.963155	3.533440	0.005081
H	-2.411426	3.780184	3.147527
H	-2.881783	2.281261	2.342708
H	-1.403258	2.347026	3.299678

M06L.ML09

Cl	0.760995	1.487418	-2.202354
Ti	-0.000251	1.817140	-0.000357
Cl	1.654437	3.245940	0.568473
Cl	-1.655376	3.245312	-0.569496
Cl	-0.761388	1.487659	2.201717
O	1.282027	0.173494	0.404224
C	1.539852	-1.046112	0.321374
O	2.782180	-1.458593	0.044766
C	0.552943	-2.153317	0.548318
C	3.791066	-0.381668	-0.221064
C	-0.552254	-2.153598	-0.548147
C	-1.539488	-1.046638	-0.321435
O	-1.282028	0.173025	-0.404578

O	-2.781683	-1.459427	-0.044691
C	-3.790883	-0.382748	0.220938
H	1.101007	-3.092084	0.449730
H	-1.100039	-3.092506	-0.449359
C	-5.053231	-1.075744	0.653609
H	-3.367517	0.273726	0.980884
H	-3.899566	0.187088	-0.701260
H	-5.822669	-0.331626	0.853773
H	-5.422670	-1.747866	-0.118614
H	-4.893956	-1.650275	1.564345
C	5.053641	-1.074377	-0.653531
H	3.367531	0.274511	-0.981170
H	3.899541	0.188405	0.701013
H	5.822862	-0.330070	-0.853828
H	5.423252	-1.746217	0.118855
H	4.894577	-1.649157	-1.564147
C	0.020253	-2.070415	-1.990277
C	-0.019583	-2.070000	1.990434
C	-0.914924	-3.275840	2.282385
C	1.111038	-1.968208	3.017150
H	-0.613177	-1.151096	2.060672
C	-1.110396	-1.969244	-3.017022
H	0.613531	-1.151323	-2.060718
C	0.916011	-3.276013	-2.281947
H	0.704312	-1.943571	4.027119
H	1.787137	-2.824166	2.946447
H	1.695135	-1.055691	2.886519
H	-1.281670	-3.226744	3.307444
H	-1.784367	-3.318999	1.626495
H	-0.358331	-4.210442	2.175433
H	-0.703673	-1.944684	-4.026993
H	-1.786197	-2.825422	-2.946136
H	-1.694814	-1.056902	-2.886592
H	1.282735	-3.227031	-3.307019
H	1.785472	-3.318717	-1.626051
H	0.359743	-4.210783	-2.174772

M06L.ML10

Ti	0.018904	0.107987	1.022524
Cl	2.228943	-0.216060	0.722066
Cl	-1.423711	-0.676726	-0.546418
Cl	-0.282027	-1.602953	2.452542
Cl	-0.708669	1.720482	2.415135
O	0.280632	1.717252	-0.395387
C	-0.715860	2.811215	-0.583555
C	-0.345008	3.441003	-1.913160
C	0.193580	2.253718	-2.719078
C	0.984204	1.465389	-1.691282
H	-1.703954	2.346915	-0.598257
H	-0.627461	3.462748	0.278719
H	0.429008	4.196876	-1.776715
H	-1.202608	3.913802	-2.385335
H	0.814520	2.558606	-3.557887
H	-0.630181	1.650939	-3.102946
H	0.984486	0.391438	-1.858537
H	2.006495	1.815681	-1.557734

M06L.ML10-cis

Ti	0.000000	0.000000	0.956480
Cl	2.329013	-0.019387	0.673194

Cl	-2.329013	0.019387	0.673190
Cl	0.005763	-1.749370	2.413324
Cl	-0.005766	1.749369	2.413325
O	-0.009791	1.378527	-0.689386
O	0.009792	-1.378525	-0.689388
C	-0.965046	2.516815	-0.811892
C	-0.351520	3.413360	-1.873495
C	0.393168	2.421311	-2.776762
C	0.998092	1.453696	-1.776776
C	0.965047	-2.516813	-0.811894
C	0.351521	-3.413360	-1.873495
C	-0.393170	-2.421311	-2.776762
C	-0.998092	-1.453697	-1.776776
H	-1.922748	2.090046	-1.107501
H	-1.056240	2.957113	0.177427
H	0.350577	4.116625	-1.424734
H	-1.109883	3.982348	-2.405814
H	1.155160	2.897307	-3.389259
H	-0.306879	1.909008	-3.439848
H	1.150917	0.437847	-2.134065
H	1.925110	1.817381	-1.336560
H	1.922749	-2.090045	-1.107504
H	1.056242	-2.957111	0.177426
H	1.109883	-3.982348	-2.405814
H	-0.350576	-4.116625	-1.424732
H	0.306876	-1.909009	-3.439849
H	-1.155162	-2.897309	-3.389257
H	-1.150919	-0.437847	-2.134066
H	-1.925110	-1.817381	-1.336558

M06L.ML11

Ti	-1.216704	-1.987295	0.215490
Cl	-3.324169	-1.278579	0.844677
Cl	-1.043835	-3.712062	1.656255
Cl	-1.877306	-2.980207	-1.701815
Cl	1.082303	-1.978837	-0.365589
O	-0.561051	-0.612863	1.769641
C	-0.847827	0.790767	1.458176
O	-1.099865	0.022740	-0.765270
C	-0.412926	1.033434	0.037699
H	-1.921869	0.909796	1.574602
H	-0.316835	1.431165	2.160250
H	-0.713513	2.022184	-0.312163
H	0.666148	0.902429	-0.088728
C	-0.786370	0.149471	-2.190457
H	-0.972493	1.178629	-2.494954
H	0.253764	-0.130502	-2.361284
H	-1.449521	-0.528594	-2.712358
C	0.636274	-0.827926	2.583486
H	1.518255	-0.454662	2.063426
H	0.492808	-0.325926	3.538987
H	0.719130	-1.899835	2.720770

M06L.ML12

Ti	-1.134529	-1.903423	0.187102
Cl	-2.495551	-0.021124	0.376392
Cl	-1.627429	-2.755222	2.228765
Cl	-2.578184	-3.112071	-1.074204
Cl	0.703390	-3.326593	-0.187297
O	0.363604	-0.620049	1.122414

C	0.637978	0.767511	0.713260
O	-0.427808	-0.919171	-1.628871
C	1.062519	0.834860	-0.741940
H	-0.282323	1.321438	0.891534
H	1.419593	1.146476	1.370633
H	1.394169	1.855347	-0.948500
H	1.917631	0.176645	-0.915972
C	0.003992	-1.696740	-2.792413
H	1.089563	-1.792559	-2.790554
H	-0.452385	-2.674879	-2.706210
H	-0.347572	-1.192289	-3.691438
C	1.381204	-1.172505	2.018913
C	-0.058319	0.503934	-1.709648
H	0.238536	0.699228	-2.739402
H	-0.964586	1.063625	-1.484316
H	1.514787	-0.483537	2.851922
H	1.006329	-2.124536	2.373465
H	2.313465	-1.319957	1.473999

M06L.ML13

Ti	-0.650400	-2.179674	0.037406
Cl	-2.556432	-1.001080	0.716822
Cl	-0.429522	-3.400631	1.940441
Cl	-1.769664	-3.752050	-1.161414
Cl	1.472293	-2.683209	-0.812936
O	0.402146	-0.542493	1.035305
C	1.538635	0.248977	0.517005
O	-0.753482	-0.860465	-1.701897
C	1.167963	0.927740	-0.794960
H	1.755748	0.990984	1.286895
H	2.388365	-0.423169	0.412362
H	1.850948	1.767983	-0.928509
H	1.353937	0.237747	-1.617789
C	-0.574131	-1.421237	-3.045508
H	0.106835	-0.780407	-3.605556
H	-0.145948	-2.408200	-2.931483
H	-1.544230	-1.483272	-3.537208
C	0.138798	-0.278995	2.454076
C	-0.298768	1.401996	-0.816386
H	-0.369002	2.434947	-1.160471
H	-0.717450	1.376459	0.189509
H	0.063133	0.798183	2.601841
H	-0.800827	-0.754631	2.702454
H	0.947026	-0.698882	3.051751
C	-1.169357	0.558587	-1.738780
H	-2.222831	0.598878	-1.468151
H	-1.049353	0.873160	-2.776576

M06L.ML14

Ti	-1.221670	-1.673484	0.441060
Cl	-1.805666	0.585548	0.665698
Cl	-1.582209	-2.220649	2.612129
Cl	-3.247640	-2.260086	-0.402065
Cl	-0.181743	-3.692294	-0.144567
O	0.760007	-1.009027	0.960998
C	1.394469	0.214772	0.436777
O	-0.477496	-1.074387	-1.545887
C	1.611109	0.164582	-1.079940
H	0.731809	1.029454	0.719313
H	2.344111	0.328625	0.959349

C	2.362216	1.463992	-1.473620
C	2.437976	-1.105739	-1.457487
C	-1.173922	-1.613636	-2.717354
H	-0.531168	-1.500759	-3.589218
H	-1.353734	-2.663837	-2.514147
H	-2.116668	-1.087479	-2.862444
C	1.656510	-1.868656	1.740412
C	0.262127	0.172805	-1.802943
H	0.413788	0.242101	-2.881237
H	-0.366096	1.000378	-1.474659
H	2.222090	-1.240303	2.427329
H	1.029644	-2.560061	2.290620
H	2.318301	-2.416919	1.071676
H	2.752087	1.337723	-2.487711
C	1.556549	2.767714	-1.398869
H	3.240953	1.556918	-0.825546
C	2.435356	4.028936	-1.445559
H	0.839391	2.816890	-2.226680
H	0.958638	2.796429	-0.482074
C	1.570027	5.282108	-1.294089
H	3.127015	3.981537	-0.594338
C	3.264481	4.098533	-2.731709
H	2.181304	6.185104	-1.278324
H	0.871026	5.371376	-2.129357
H	0.985148	5.255406	-0.373762
H	3.849612	5.017773	-2.769415
H	3.959713	3.262675	-2.819416
H	2.612754	4.085631	-3.609586
C	2.492213	-1.375425	-2.964850
C	3.869197	-1.060772	-0.906295
H	1.910605	-1.952592	-1.005529
H	3.151120	-2.220212	-3.165038
H	1.516191	-1.632901	-3.372921
H	2.882987	-0.520723	-3.522835
H	4.345641	-2.033702	-1.030649
H	4.478193	-0.330202	-1.442693
H	3.915128	-0.811650	0.155083

M06L.ML15

Ti	-0.917342	-2.125229	0.282385
Cl	-2.302139	-0.240453	0.455327
Cl	-1.179838	-2.706426	2.458779
Cl	-2.507306	-3.386803	-0.729287
Cl	0.789129	-3.696098	-0.093229
O	0.707517	-0.781037	0.811916
C	0.779039	0.629876	0.398743
O	-0.310354	-1.304196	-1.638528
C	0.967025	0.757876	-1.115712
H	-0.138343	1.112422	0.731401
H	1.633841	1.077650	0.904934
C	1.034749	2.241846	-1.460172
C	2.333084	0.266252	-1.572662
C	-0.299862	-2.138268	-2.844794
H	0.573772	-1.875791	-3.440070
H	-0.233336	-3.167666	-2.513905
H	-1.221919	-1.976265	-3.401551
C	1.659665	-1.132999	1.870641
C	-0.179520	0.135163	-1.917301
H	0.025724	0.246320	-2.981745
H	-1.134475	0.599863	-1.676884

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  H      1.337529    -0.682324     2.808407
  H      1.656692    -2.213665     1.948139
  H      2.647689    -0.779012     1.579398
  C      2.281225     2.555641    -2.036611
  C      2.556735     3.865126    -2.428135
  C      1.580976     4.845154    -2.238452
  C      0.346381     4.528105    -1.666333
  C      0.063903     3.215995    -1.270988
  H      3.509110     4.123087    -2.872241
  H      1.783339     5.864493    -2.538481
  H     -0.396460     5.301602    -1.527732
  H     -0.894851     2.973898    -0.827249
  C      2.862253    -1.016627    -1.516759
  C      4.158965    -1.227964    -2.000714
  C      4.905659    -0.171898    -2.528542
  C      4.374857     1.117603    -2.585568
  C      3.084247     1.335768    -2.105745
  H      2.288108    -1.838637    -1.108043
  H      4.584571    -2.221688    -1.963562
  H      5.906102    -0.355165    -2.897136
  H      4.959421     1.930593    -2.996012
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M06.M
  Ti     0.000117    -0.000037    -0.000183
  Cl     1.718752    -1.120988     0.772812
  Cl    -1.293234    -1.346031    -1.150548
  Cl     0.707344     1.620207    -1.297127
  Cl    -1.132988     0.846856     1.675067
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M06.L01
  O      1.228257     1.351593     0.000000
  C      1.056593     0.137629     0.000000
  O     -0.178884    -0.434366     0.000000
  C      2.130510    -0.894374     0.000000
  C     -1.328692     0.467056     0.000000
  C     -2.561356    -0.396999     0.000000
  H     -1.267609     1.107939     0.880720
  H     -1.267609     1.107940    -0.880719
  H     -3.456511     0.225469     0.000001
  H     -2.586250    -1.034986    -0.882553
  H     -2.586250    -1.034987     0.882553
  H      3.099842    -0.406614    -0.000012
  H      2.039320    -1.533757     0.877315
  H      2.039305    -1.533774    -0.877300
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M06.L02
  O     -1.445313     0.160660     1.080429
  C     -0.322646     0.128888     1.583145
  O     -0.127365     0.162661     2.928465
  C      0.936167     0.051492     0.819944
  C     -1.319478     0.238829     3.765962
  C      0.854661     0.010006    -0.572828
  H     -0.122037     0.036475    -1.035858
  C      2.183876     0.018858     1.444706
  C      3.339005    -0.054818     0.678340
  C      3.254228    -0.096174    -0.709914
  C      2.011091    -0.063698    -1.334975
  H      1.945519    -0.095843    -2.413759
  H      4.156237    -0.153681    -1.304260
  H      4.305500    -0.080133     1.162703
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H	2.238617	0.051237	2.522668
C	-0.849510	0.263688	5.195989
H	-1.878361	1.135406	3.494179
H	-1.952077	-0.623092	3.549175
H	-1.704688	0.320343	5.869914
H	-0.284531	-0.636829	5.433661
H	-0.210800	1.126962	5.378856

M06.L03

O	-0.866723	1.045906	0.173366
C	-0.015711	0.290300	0.635800
O	-0.294140	-0.627602	1.596449
C	1.421760	0.313018	0.284964
C	-1.666231	-0.682243	2.083652
C	1.841813	0.694914	-0.996048
C	0.898952	0.898098	-2.119681
O	0.956163	1.831057	-2.913543
O	-0.002772	-0.107050	-2.204371
C	-1.155056	0.103163	-3.069953
C	2.375388	0.069562	1.271804
C	3.727790	0.230349	1.000462
C	4.138975	0.643816	-0.260759
C	3.196278	0.876408	-1.253473
H	3.497003	1.192589	-2.242979
H	5.190156	0.781207	-0.472755
H	4.457487	0.043902	1.776130
H	2.044796	-0.227481	2.256639
C	-2.181963	-0.956591	-2.733125
H	-1.537857	1.109849	-2.888121
H	-0.835656	0.034362	-4.114257
C	-3.457411	-0.678237	-3.524902
C	-1.652985	-2.356244	-3.026539
H	-2.396324	-0.866280	-1.662335
C	-1.730076	-1.713794	3.189877
H	-1.952974	0.308852	2.448531
H	-2.322776	-0.938023	1.249090
C	-3.184038	-1.872042	3.629553
H	-1.373774	-2.664778	2.780739
C	-0.848172	-1.315719	4.368566
H	-2.393153	-3.114309	-2.763775
H	-1.433395	-2.459579	-4.093822
H	-0.738232	-2.559928	-2.470917
H	-4.223884	-1.419017	-3.293049
H	-3.863136	0.310628	-3.303862
H	-3.259885	-0.731611	-4.599693
H	-0.899170	-2.064206	5.160988
H	0.193625	-1.206425	4.067829
H	-1.184948	-0.362046	4.786505
H	-3.268095	-2.622186	4.416691
H	-3.568062	-0.928548	4.028224
H	-3.827766	-2.176470	2.802141

M06.L04

O	-1.144640	0.937684	0.330388
C	-0.289268	0.202873	0.819505
O	-0.536207	-0.596265	1.888782
C	1.118490	0.130210	0.373046
C	-1.883975	-0.547296	2.449550
C	1.460536	0.445179	-0.948795
C	0.448047	0.676282	-2.005926

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  O      0.465823     1.622546    -2.785768
  O     -0.464390    -0.321543    -2.054859
  C     -1.654200    -0.085555    -2.867431
  C      2.129051    -0.139749     1.294459
  C      3.463489    -0.070860     0.917109
  C      3.800026     0.277347    -0.385263
  C      2.799335     0.536425    -1.312673
  H      3.042825     0.804762    -2.331648
  H      4.838097     0.344372    -0.679813
  H      4.238470    -0.277127     1.642163
  H      1.857540    -0.384486     2.310633
  C     -2.625534    -1.187098    -2.538163
  H     -2.042894     0.900907    -2.609372
  H     -1.364968    -0.075593    -3.919012
  H     -3.543437    -1.065187    -3.113788
  H     -2.200596    -2.163514    -2.768251
  H     -2.877230    -1.161516    -1.477965
  C     -1.906987    -1.496070     3.617874
  H     -2.101994     0.481556     2.739364
  H     -2.591868    -0.829253     1.668779
  H     -2.898030    -1.506130     4.072086
  H     -1.664811    -2.508719     3.298291
  H     -1.185649    -1.195294     4.376695
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M06.L05
  O      1.190820     0.178698     0.986458
  C      0.759707     1.221039     1.473957
  O      0.803731     1.477642     2.808237
  C      0.147017     2.318636     0.700767
  C      1.394772     0.448438     3.658204
  C      0.045560     2.170782    -0.679379
  H      0.410387     1.269989    -1.154122
  C     -0.324602     3.482357     1.311358
  C     -0.892990     4.488424     0.541876
  C     -0.994573     4.342048    -0.834922
  C     -0.524331     3.180035    -1.449802
  C     -0.608998     2.976370    -2.908986
  H     -1.435284     5.119724    -1.440838
  H     -1.257593     5.388695     1.016294
  H     -0.241645     3.588432     2.382793
  C      1.331183     0.958585     5.073030
  H      0.834279    -0.477370     3.521852
  H      2.417401     0.268421     3.324021
  H      1.761595     0.224499     5.754539
  H      1.888409     1.889028     5.175099
  H      0.300144     1.141635     5.373139
  O     -1.181798     4.026551    -3.554811
  O     -0.211459     1.974417    -3.498946
  C     -1.309829     3.917950    -5.004958
  C     -1.967099     5.184957    -5.483171
  H     -0.315627     3.776026    -5.430738
  H     -1.898321     3.028822    -5.235102
  H     -2.087752     5.157352    -6.566353
  H     -2.951109     5.305450    -5.031713
  H     -1.363649     6.055110    -5.227632
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M06.L06
  O      1.083885     0.241035     0.860301
  C      0.688211     1.256388     1.430364
  O      0.818732     1.441879     2.768552
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C	0.029685	2.392169	0.754009
C	1.459507	0.370505	3.525949
C	-0.157456	2.310966	-0.626353
H	0.183911	1.426416	-1.145478
C	-0.400914	3.522252	1.450871
C	-1.013233	4.560390	0.768924
C	-1.200373	4.479187	-0.611438
C	-0.769775	3.349103	-1.308300
H	-0.918255	3.293983	-2.376113
C	-1.858899	5.614969	-1.287793
H	-1.354600	5.444940	1.288050
H	-0.252433	3.577372	2.518684
C	1.483664	0.806454	4.966447
H	0.889950	-0.547651	3.375954
H	2.459315	0.210233	3.120207
H	1.954731	0.039066	5.581070
H	2.046645	1.731746	5.082100
H	0.473285	0.971281	5.338556
O	-1.989418	5.429478	-2.625982
O	-2.254572	6.630321	-0.717730
C	-2.630190	6.500854	-3.383379
C	-2.654345	6.064906	-4.823878
H	-3.629998	6.661126	-2.977639
H	-2.060632	7.419009	-3.233382
H	-3.125409	6.832295	-5.438501
H	-1.643965	5.900078	-5.195984
H	-3.217327	5.139615	-4.939532

M06.L07

C	-5.341744	0.681921	-0.000208
C	-4.267940	-0.372952	0.000779
O	-2.985481	0.327990	-0.000064
C	-1.861900	-0.433842	0.000617
O	-1.885782	-1.661238	0.001889
O	1.885782	1.661239	-0.001914
C	1.861900	0.433842	-0.000626
C	0.633002	-0.416345	0.000381
C	-0.633002	0.416346	-0.000382
H	-0.666372	1.080690	-0.866439
O	2.985481	-0.327990	0.000069
C	4.267940	0.372952	-0.000781
C	5.341744	-0.681922	0.000222
H	0.666216	-1.082515	-0.864279
H	0.666374	-1.080688	0.866439
H	-0.666218	1.082512	0.864279
H	-4.312199	-1.015788	-0.879489
H	-4.312033	-1.013972	0.882380
H	4.312035	1.013960	-0.882391
H	4.312198	1.015800	0.879479
H	-6.326743	0.214507	0.000375
H	-5.261397	1.316222	0.881587
H	-5.261572	1.314393	-0.883332
H	6.326742	-0.214507	-0.000365
H	5.261570	-1.314381	0.883355
H	5.261398	-1.316234	-0.881564

M06.L08

C	0.651596	0.933101	-2.652816
C	-0.618391	1.706417	-2.418875
O	-0.221059	3.059528	-2.030414

C	-1.207724	3.889642	-1.609136
O	-2.392564	3.561947	-1.638176
C	-0.732375	5.219902	-1.077467
C	-1.071990	5.323503	0.442005
C	-2.554788	5.123609	0.656423
O	-3.089342	4.281259	1.368031
C	0.717105	5.593766	-1.430049
C	0.865014	5.746378	-2.946389
C	1.132167	6.909964	-0.769947
C	-0.181580	4.493750	1.385556
C	-0.299130	2.974773	1.236210
C	-0.413632	4.914073	2.838897
O	-3.265725	6.054505	-0.034700
C	-4.713061	5.870785	-0.078685
C	-5.263960	6.942328	-0.981342
H	1.254266	0.903809	-1.745084
H	1.246489	1.389241	-3.443207
H	0.419231	-0.091435	-2.943902
H	-1.223400	1.285727	-1.613341
H	-1.246663	1.770246	-3.307916
H	-1.383800	5.957836	-1.561192
H	-0.902445	6.377235	0.690667
H	1.385238	4.795577	-1.092989
H	1.894825	5.998207	-3.205690
H	0.598820	4.834934	-3.478694
H	0.224846	6.558473	-3.304616
H	2.113924	7.216257	-1.134879
H	0.423044	7.704304	-1.023784
H	1.193376	6.845298	0.317415
H	0.850345	4.766880	1.134982
H	0.281072	2.488560	2.023271
H	-1.334764	2.650073	1.332859
H	0.098471	2.627145	0.281818
H	0.329167	4.449121	3.489624
H	-0.329934	5.997988	2.956854
H	-1.401809	4.605148	3.180085
H	-4.908334	4.865129	-0.454659
H	-5.105909	5.935692	0.936804
H	-5.023249	7.934161	-0.599700
H	-4.848803	6.850129	-1.984202
H	-6.348642	6.854288	-1.049487

M06.L09

C	-1.247560	0.786582	0.899356
H	-1.671759	1.521562	1.583088
H	-0.226360	0.578036	1.214721
H	-1.837012	-0.128196	0.973027
C	-1.268344	1.303068	-0.519706
H	-0.853825	0.585943	-1.224796
H	-2.272023	1.587238	-0.836181
O	-0.393547	2.469287	-0.651326
C	-0.882265	3.677365	-0.269607
C	0.168442	4.748867	-0.353046
O	-2.041784	3.850104	0.095869
C	0.788623	4.835900	-1.763370
H	-0.365568	5.689205	-0.195263
C	1.167592	4.610533	0.831881
H	1.901331	5.414480	0.709831
C	0.508285	4.787912	2.214833
C	1.924587	3.306499	0.772780

C	1.757859	6.011002	-1.861877
H	1.328170	3.909495	-1.969080
C	-0.328902	5.002486	-2.794372
H	0.087633	5.092153	-3.798853
H	-1.019825	4.157506	-2.795242
H	-0.906971	5.908562	-2.588769
H	2.080256	6.147326	-2.895769
H	1.269488	6.938167	-1.543397
H	2.651155	5.862442	-1.256276
O	2.909707	3.341084	-0.165351
O	1.719523	2.325261	1.480273
C	3.661309	2.107027	-0.392885
C	2.888952	1.174615	-1.296589
H	4.589508	2.445361	-0.846502
H	3.873940	1.646336	0.571598
H	3.477058	0.279834	-1.503919
H	1.953482	0.873610	-0.825994
H	2.655857	1.661475	-2.243629
C	1.589054	4.883683	3.293585
C	-0.373676	6.034398	2.277257
H	-0.107394	3.903931	2.414636
H	1.134239	4.975450	4.281009
H	2.237876	4.008710	3.307269
H	2.205049	5.773557	3.128325
H	-0.670857	6.224622	3.309852
H	0.177292	6.914049	1.926445
H	-1.284449	5.934743	1.687827

M06.L10

O	0.000001	-1.260554	-0.000099
C	1.179554	-0.422022	0.137338
C	0.728901	0.985590	-0.234889
C	-0.728899	0.985557	0.235030
C	-1.179555	-0.422002	-0.137398
H	1.529095	-0.463745	1.173371
H	1.958792	-0.819616	-0.511144
H	0.774606	1.127653	-1.316637
H	1.329729	1.759917	0.239317
H	-1.329728	1.759952	-0.239065
H	-0.774604	1.127466	1.316799
H	-1.958786	-0.819690	0.511036
H	-1.529108	-0.463574	-1.173432

M06.L11

C	0.035858	-0.062091	0.063022
H	-0.009482	0.016323	1.145256
H	1.084309	-0.096805	-0.253083
H	-0.458329	-0.987423	-0.253112
O	-0.627548	1.087056	-0.469294
C	-0.639850	1.108288	-1.901748
C	-1.363619	2.361823	-2.314918
H	0.381603	1.115423	-2.300946
H	-1.156754	0.227232	-2.300860
O	-1.375921	2.383054	-3.747372
H	-2.385072	2.354687	-1.915720
H	-0.846715	3.242878	-1.915806
C	-2.039327	3.532201	-4.279688
H	-1.993987	3.453787	-5.361922
H	-3.087778	3.566915	-3.963583
H	-1.545140	4.457533	-3.963555

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M06.L12
  C      0.011965    -0.019818     0.176004
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  H      1.069763    -0.071134    -0.106252
  H     -0.473070    -0.961734    -0.104695
  O     -0.634716     1.099502    -0.434641
  C     -0.603916     1.044846    -1.866527
  C     -1.310920     2.269595    -2.396692
  H      0.438989     1.013403    -2.216722
  H     -1.098714     0.125970    -2.215979
  C     -1.324821     2.294354    -3.906700
  H     -2.335847     2.287112    -2.023901
  H     -0.813705     3.165827    -2.023493
  O     -2.010465     3.481493    -4.324835
  H     -0.299615     2.294521    -4.307027
  H     -1.836942     1.406444    -4.307471
  C     -2.082291     3.607321    -5.747144
  H     -2.614795     4.529786    -5.959213
  H     -1.082487     3.657528    -6.193360
  H     -2.625187     2.766751    -6.194275
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M06.L13
  C      0.057941    -0.100294     0.144147
  H      0.005354    -0.008668     1.225153
  H      1.109118    -0.140162    -0.163455
  H     -0.433369    -1.030622    -0.162950
  O     -0.601440     1.041668    -0.407893
  C     -0.602739     1.043759    -1.842363
  C     -1.319785     2.285642    -2.314305
  H      0.430945     1.028730    -2.218483
  H     -1.106545     0.141002    -2.218381
  C     -1.367221     2.368389    -3.835695
  H     -2.332148     2.282022    -1.900436
  H     -0.810755     3.160555    -1.900114
  C     -2.084267     3.610272    -4.307637
  H     -0.354857     2.372008    -4.249564
  H     -1.876251     1.493475    -4.249886
  O     -2.085565     3.612362    -5.742107
  H     -3.117951     3.625300    -3.931517
  H     -1.580460     4.513028    -3.931619
  C     -2.744946     4.754324    -6.294147
  H     -2.692360     4.662698    -7.375152
  H     -3.796123     4.794192    -5.986545
  H     -2.253636     5.684652    -5.987050
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M06.L14
  C      0.426151     0.097289     0.062613
  H      0.815682     0.381766     1.035824
  H      1.242302    -0.298116    -0.553135
  H     -0.329737    -0.686932     0.190026
  O     -0.143926     1.269673    -0.523061
  C     -0.669706     1.022090    -1.834793
  C     -1.397081     2.256596    -2.379472
  H      0.160756     0.738051    -2.499532
  H     -1.356615     0.163696    -1.796804
  C     -1.371486     2.104490    -3.900305
  C     -2.872964     2.327253    -1.877942
  C     -0.666906     3.555221    -1.982767
  O     -2.091609     3.186768    -4.502858
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H	-0.334975	2.107162	-4.263722
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H	-2.717696	3.933218	-6.289649
H	-1.170989	3.056410	-6.377535
H	-2.699428	2.154338	-6.215886
H	-3.237307	3.308650	-2.198594
C	-3.793945	1.280657	-2.509472
C	-3.000830	2.246255	-0.355274
H	-4.035799	2.441847	-0.065634
H	-2.734785	1.252124	0.012687
H	-2.365159	2.964748	0.159618
H	-4.789519	1.355196	-2.067281
H	-3.903418	1.422841	-3.585171
H	-3.439070	0.261432	-2.328217
H	-1.270841	4.387546	-2.352740
H	-0.649748	3.621238	-0.893120
C	0.764407	3.697796	-2.495024
C	1.568238	4.774523	-1.758797
H	1.299849	2.747690	-2.388441
H	0.763039	3.946346	-3.565085
C	3.003325	4.806824	-2.278079
C	0.927994	6.153886	-1.899264
H	1.585866	4.502159	-0.695380
H	3.606782	5.537820	-1.735873
H	3.483754	3.830640	-2.182352
H	3.014567	5.084597	-3.336819
H	1.545683	6.921362	-1.427819
H	0.821986	6.411677	-2.958128
H	-0.062260	6.195172	-1.444040

M06.L15

C	-0.534781	-0.000068	0.000035
C	-1.399120	0.176376	1.244500
C	0.423694	-1.161720	0.203174
C	0.423126	1.162044	-0.203156
O	-2.288449	1.283014	1.042370
H	-1.979390	-0.735626	1.424922
H	-0.751825	0.364240	2.111801
C	-3.159102	1.496077	2.156487
H	-3.794309	2.342417	1.910963
H	-3.783743	0.615363	2.340778
H	-2.589832	1.722177	3.064690
C	1.754976	-0.719090	0.128757
C	2.806395	-1.612276	0.292052
C	2.516444	-2.952456	0.531471
C	1.196049	-3.391169	0.604237
C	0.137960	-2.496424	0.440123
H	3.834339	-1.276707	0.235790
H	3.323848	-3.660932	0.661300
H	0.989338	-4.437223	0.787445
H	-0.887377	-2.837097	0.477912
C	1.754623	0.720048	-0.128790
C	2.805612	1.613727	-0.292147
C	2.515017	2.953765	-0.531580
C	1.194411	3.391850	-0.604303
C	0.136754	2.496608	-0.440126
H	3.833717	1.278646	-0.235929
H	3.322080	3.662621	-0.661460
H	0.987195	4.437801	-0.787527

H	-0.888744	2.836799	-0.477898
C	-1.399104	-0.176953	-1.244377
O	-2.287864	-1.284034	-1.042169
H	-1.979838	0.734755	-1.424787
H	-0.751765	-0.364516	-2.111711
C	-3.158402	-1.497643	-2.156270
H	-3.793160	-2.344301	-1.910681
H	-2.589009	-1.723513	-3.064453
H	-3.783509	-0.617275	-2.340632

M06.ML01

Ti	0.106260	0.075909	1.358304
Cl	1.133586	1.567304	2.706094
Cl	1.341355	-1.440237	0.264848
Cl	-1.982732	0.526320	0.633321
Cl	-0.539004	-1.280414	3.012075
O	0.694616	1.377238	-0.178039
C	0.653257	2.523474	-0.673859
O	1.316906	2.790073	-1.787036
C	-0.108331	3.645793	-0.092831
C	2.096867	1.697533	-2.413911
C	2.765624	2.286624	-3.622724
H	2.801513	1.324129	-1.670988
H	1.402534	0.892941	-2.655873
H	3.353729	1.518717	-4.124857
H	2.030761	2.670285	-4.328529
H	3.433538	3.099602	-3.342794
H	-1.164317	3.373747	-0.044969
H	0.222309	3.808043	0.934408
H	0.018298	4.550538	-0.676379

M06.ML01-cis

Ti	-0.000001	0.000001	1.241230
Cl	0.659400	1.583804	2.722704
Cl	2.142898	-0.868601	0.912600
Cl	-2.142900	0.868603	0.912596
Cl	-0.659405	-1.583802	2.722703
O	0.537448	1.262237	-0.348059
C	0.596056	2.440405	-0.753104
O	1.297092	2.729122	-1.845872
C	-0.063081	3.588104	-0.103571
C	2.038252	1.632590	-2.500612
C	2.828623	2.254897	-3.617016
H	2.662589	1.152523	-1.746972
H	1.309753	0.900619	-2.851134
H	3.397750	1.485111	-4.138110
H	2.173610	2.744301	-4.336298
H	3.529057	2.993799	-3.231249
H	-1.118170	3.356714	0.048590
H	0.363981	3.725600	0.892057
H	0.058673	4.491392	-0.690505
O	-0.537447	-1.262236	-0.348059
C	-0.596054	-2.440405	-0.753104
O	-1.297091	-2.729122	-1.845871
C	-2.038253	-1.632592	-2.500611
C	-2.828623	-2.254900	-3.617014
H	-2.662592	-1.152526	-1.746971
H	-1.309756	-0.900619	-2.851132
H	-3.397752	-1.485115	-4.138108
H	-2.173609	-2.744303	-4.336297

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  H     -3.529055    -2.993804    -3.231248
  C      0.063084    -3.588102    -0.103571
  H      1.118173    -3.356711     0.048589
  H     -0.363977    -3.725598     0.892058
  H     -0.058669    -4.491390    -0.690503
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M06.ML02
  Cl    -1.994709    -2.494695    -1.300057
  Ti    -0.018742    -2.426537    -0.187893
  Cl    -0.049185    -4.618178     0.269791
  Cl     2.023534    -2.505739    -1.157923
  Cl    -0.070763    -1.755663     1.951393
  H     -0.309410     0.831035     1.349762
  C     -0.392079     1.799826     0.875254
  C     -0.313208     1.896334    -0.517641
  C     -0.121245     0.679957    -1.297088
  O     -0.013041    -0.454909    -0.773858
  O     -0.060554     0.849829    -2.610510
  C      0.145824    -0.315992    -3.496538
  C     -0.574517     2.945562     1.633380
  C     -0.678045     4.184590     1.008504
  C     -0.599828     4.282500    -0.378694
  C     -0.418078     3.143060    -1.144572
  H     -0.356502     3.206814    -2.220667
  H     -0.681024     5.247162    -0.859177
  H     -0.820190     5.076792     1.602906
  H     -0.635978     2.872743     2.709720
  C      0.193933     0.217441    -4.900120
  H      1.073704    -0.802262    -3.195530
  H     -0.682572    -1.006000    -3.335309
  H      0.345929    -0.607014    -5.596470
  H     -0.737664     0.716860    -5.161473
  H      1.014247     0.922878    -5.023095
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M06.ML03
  Ti     0.029795    -1.737921     0.000000
  Cl    -2.163361    -0.945416     0.000003
  Cl    -0.236708    -3.122643     1.751400
  Cl    -0.236714    -3.122645    -1.751398
  Cl     2.361140    -1.819093    -0.000004
  O      0.374678    -0.121275     1.299703
  C      0.350074     1.088702     1.558415
  O      0.823442     1.517716     2.729343
  C     -0.196540     2.166113     0.706584
  C      1.337840     0.489418     3.658838
  C     -0.196541     2.166113    -0.706586
  C      0.350071     1.088701    -1.558418
  O      0.374674    -0.121276    -1.299706
  O      0.823438     1.517714    -2.729347
  C      1.337835     0.489416    -3.658842
  C     -0.741399     3.260997     1.379901
  C     -1.308982     4.323359     0.692938
  C     -1.308984     4.323358    -0.692940
  C     -0.741401     3.260996    -1.379903
  H     -0.721603     3.264903    -2.458566
  H     -1.743950     5.146179    -1.241903
  H     -1.743948     5.146180     1.241901
  H     -0.721598     3.264905     2.458564
  C      1.899552     1.197917    -4.869467
  H      2.102727    -0.089141    -3.133155
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H	0.512586	-0.180507	-3.906172
C	2.320037	0.138203	-5.887267
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C	3.079142	2.089058	-4.494878
C	1.899553	1.197919	4.869465
H	0.512594	-0.180509	3.906165
H	2.102736	-0.089135	3.133152
C	2.320040	0.138205	5.887264
C	3.079140	2.089065	4.494881
H	1.104341	1.812488	5.304321
H	3.479482	2.588494	5.378259
H	3.881594	1.487015	4.058888
H	2.794852	2.851793	3.770419
H	2.720503	0.610872	6.784380
H	1.484051	-0.497651	6.182997
H	3.102089	-0.502763	5.471560
H	2.720504	0.610871	-6.784381
H	3.102083	-0.502769	-5.471563
H	1.484046	-0.497648	-6.183004
H	3.479488	2.588487	-5.378255
H	2.794856	2.851785	-3.770416
H	3.881593	1.487003	-4.058885

M06.ML04

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Ti	-0.092026	-1.764742	0.000000
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Cl	2.237097	-1.900504	-0.000001
O	0.290386	-0.156575	1.298518
C	0.296353	1.053170	1.559643
O	0.773661	1.465841	2.735291
C	-0.214424	2.147138	0.706782
C	1.259603	0.416922	3.662013
C	-0.214424	2.147138	-0.706782
C	0.296353	1.053170	-1.559643
O	0.290385	-0.156575	-1.298518
O	0.773661	1.465841	-2.735291
C	1.259603	0.416921	-3.662013
C	-0.723880	3.259090	1.379791
C	-1.257721	4.338868	0.692899
C	-1.257721	4.338868	-0.692899
C	-0.723880	3.259090	-1.379791
H	-0.703085	3.262633	-2.458401
H	-1.665932	5.175190	-1.241965
H	-1.665932	5.175190	1.241965
H	-0.703085	3.262633	2.458401
C	1.780073	1.125955	-4.879514
H	2.023661	-0.158301	-3.138225
H	0.424409	-0.250583	-3.875129
H	2.159640	0.393170	-5.591289
H	0.993815	1.699359	-5.368418
H	2.593268	1.802283	-4.620620
C	1.780073	1.125955	4.879514
H	0.424408	-0.250583	3.875129
H	2.023661	-0.158301	3.138225
H	2.159641	0.393171	5.591289
H	2.593269	1.802284	4.620619
H	0.993816	1.699360	5.368419

M06.ML05

Cl	-2.010735	-2.423641	-1.400821
Ti	-0.045628	-2.397285	-0.271010
Cl	-0.084359	-4.598577	0.125669
Cl	2.000311	-2.449990	-1.232623
Cl	-0.112686	-1.782205	1.884532
H	-0.332007	0.820276	1.357680
C	-0.393664	1.805497	0.914460
C	-0.297994	1.943528	-0.474095
C	-0.118206	0.747388	-1.290499
O	-0.029577	-0.402047	-0.799253
O	-0.048855	0.958859	-2.596099
C	0.144644	-0.179695	-3.520444
C	-0.565743	2.929288	1.707905
C	-0.641426	4.186101	1.123844
C	-0.545266	4.328062	-0.262307
C	-0.374049	3.206601	-1.063792
H	-0.300344	3.315091	-2.134502
C	-0.630539	5.690650	-0.827870
H	-0.775128	5.075388	1.724456
H	-0.640481	2.824083	2.780358
C	0.198497	0.400180	-4.905229
H	1.067277	-0.685176	-3.235462
H	-0.691270	-0.865440	-3.381186
H	0.341644	-0.401838	-5.629093
H	-0.727610	0.918303	-5.148980
H	1.026138	1.100760	-5.004356
O	-0.517898	5.707185	-2.177839
O	-0.785962	6.707872	-0.156307
C	-0.589042	7.012255	-2.833989
C	-0.430365	6.769570	-4.310571
H	-1.546820	7.470570	-2.584793
H	0.199349	7.645840	-2.425970
H	-0.476473	7.715507	-4.850341
H	0.528230	6.299278	-4.525967
H	-1.222736	6.122907	-4.685301

M06.ML06

Cl	-2.018460	-2.458989	-1.366096
Ti	-0.045721	-2.450070	-0.248708
Cl	-0.090575	-4.653478	0.131865
Cl	1.995773	-2.500901	-1.219949
Cl	-0.097821	-1.844443	1.906914
H	-0.297021	0.775452	1.393314
C	-0.369000	1.758877	0.948757
C	-0.294062	1.897971	-0.439861
C	-0.119507	0.700719	-1.259665
O	-0.025463	-0.448279	-0.771067
O	-0.060320	0.915006	-2.565722
C	0.129258	-0.222754	-3.492425
C	-0.533881	2.881073	1.741301
C	-0.623975	4.143777	1.155780
C	-0.549423	4.282232	-0.231299
C	-0.385316	3.163324	-1.028338
H	-0.326955	3.259238	-2.101995
H	-0.620964	5.264939	-0.671657
C	-0.798889	5.309737	2.051773
H	-0.594940	2.799191	2.817059
C	0.180592	0.357887	-4.876893
H	1.051863	-0.729734	-3.210050

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  H      1.009417     1.056778    -4.978127
  O     -0.867957     6.483010     1.379020
  O     -0.874143     5.233303     3.275263
  C     -1.040590     7.696049     2.178342
  C     -1.078194     8.853250     1.217403
  H     -1.961290     7.598722     2.754884
  H     -0.211705     7.762898     2.884004
  H     -1.206676     9.787126     1.764795
  H     -0.151886     8.915460     0.647786
  H     -1.906296     8.750485     0.517378
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M06.ML07
  Cl    -1.562444    -0.857739    -1.006977
  Ti     0.456488    -1.520220    -0.036314
  Cl    -0.456186    -2.871336     1.506875
  Cl     0.992935    -3.024248    -1.614424
  Cl     2.575542    -1.425465     0.942611
  O      0.118703     0.162593     1.238990
  C      0.736832     1.176539     1.608094
  O      0.943717     1.433854     2.887418
  C      1.317346     2.186668     0.676577
  C      0.544701     0.391917     3.868475
  C      0.582795     2.297330    -0.657830
  C      0.891298     1.195611    -1.614762
  O      1.221934     0.046982    -1.271756
  O      0.771226     1.529994    -2.887409
  C      0.896526     0.444731    -3.894327
  H      1.339560     3.149794     1.183376
  H      0.806607     3.246403    -1.141576
  C      0.613298     1.065402    -5.231820
  H      1.902890     0.035413    -3.811785
  H      0.185189    -0.334253    -3.619341
  H      0.691709     0.304957    -6.008572
  H     -0.392464     1.481037    -5.263148
  H      1.324582     1.858716    -5.456996
  C      0.992013     0.878691     5.216588
  H     -0.534651     0.264998     3.790907
  H      1.023218    -0.539064     3.563738
  H      0.721593     0.144777     5.975529
  H      2.072045     1.013277     5.243249
  H      0.517260     1.825060     5.471551
  H     -0.501990     2.273909    -0.504652
  H      2.361503     1.893465     0.520074
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M06.ML08
  Ti    -0.114667    -1.613001     0.351195
  Cl    -2.357764    -1.057230     0.643577
  Cl     0.023089    -2.966913     2.127950
  Cl    -0.480872    -3.114030    -1.289382
  Cl     2.197979    -1.476486    -0.015596
  O      0.283667     0.072954     1.601959
  C      0.219923     1.315117     1.558079
  O      1.009853     2.049343     2.336979
  C     -0.702172     2.088642     0.658155
  C      2.009641     1.350247     3.174612
  C     -0.053227     2.361747    -0.722255
  C      0.042973     1.098144    -1.523504
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H	-1.551086	1.418088	0.481128
C	1.300434	3.132462	-0.674135
C	1.061440	0.568083	-4.965753
H	1.286469	-0.543728	-3.106613
H	-0.375731	-0.470039	-3.698486
H	1.258718	-0.282537	-5.617696
H	0.325760	1.208111	-5.450643
H	1.987794	1.130477	-4.850162
C	3.007482	2.390996	3.598244
H	1.475048	0.897468	4.009137
H	2.450442	0.551280	2.577574
H	3.775654	1.932958	4.220846
H	3.492765	2.831748	2.727247
H	2.531283	3.186677	4.169162
H	-0.761322	2.990091	-1.269799
C	-1.265192	3.341629	1.362514
C	1.433409	4.096979	-1.850706
H	1.265990	3.723631	0.247192
C	2.520425	2.213535	-0.603227
H	3.417664	2.804314	-0.412857
H	2.451000	1.453647	0.176662
H	2.672987	1.686889	-1.549500
H	2.362440	4.663915	-1.770130
H	1.448755	3.554560	-2.797308
H	0.605900	4.809354	-1.879652
C	-2.143429	4.170748	0.428444
C	-2.091837	2.890517	2.569314
H	-0.436119	3.960958	1.714403
H	-2.661734	4.943171	0.998040
H	-1.573671	4.675708	-0.353745
H	-2.905219	3.544842	-0.046055
H	-2.483911	3.752472	3.110200
H	-2.938896	2.282569	2.239450
H	-1.509530	2.294932	3.274339

M06.ML09

Cl	0.700730	1.507233	-2.209753
Ti	-0.000250	1.826659	-0.000364
Cl	1.653624	3.258709	0.520498
Cl	-1.654576	3.258058	-0.521581
Cl	-0.701121	1.507555	2.209104
O	1.282766	0.194779	0.373040
C	1.547005	-1.016185	0.304332
O	2.788371	-1.419200	0.054565
C	0.564638	-2.124760	0.530689
C	3.807005	-0.363308	-0.170304
C	-0.563915	-2.125060	-0.530454
C	-1.546630	-1.016737	-0.304367
O	-1.282778	0.194294	-0.373375
O	-2.787870	-1.420085	-0.054505
C	-3.806843	-0.364465	0.170094
H	1.116500	-3.060405	0.411683
H	-1.115487	-3.060849	-0.411225
C	-5.087107	-1.068413	0.518159
H	-3.437836	0.284714	0.965100
H	-3.873857	0.224148	-0.745320
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  H     -5.405057    -1.727721    -0.288184
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  H      3.437782     0.285557    -0.965467
  H      3.873837     0.225552     0.744963
  H      5.872707    -0.330678    -0.688498
  H      5.405659    -1.725938     0.288298
  H      4.974113    -1.659106    -1.425082
  C     -0.044409    -2.079076    -1.991112
  C      0.045117    -2.078590     1.991337
  C     -0.781194    -3.324807     2.297910
  C      1.213770    -1.966968     2.968800
  H     -0.577739    -1.184394     2.111030
  C     -1.213096    -1.968018    -2.968600
  H      0.578188    -1.184727    -2.111008
  C      0.782258    -3.325127    -2.297402
  H      0.850081    -2.006951     3.995641
  H      1.918234    -2.792072     2.825889
  H      1.753712    -1.024071     2.856902
  H     -1.095625    -3.312390     3.342249
  H     -1.680868    -3.397773     1.686455
  H     -0.182846    -4.227834     2.142530
  H     -0.849397    -2.008135    -3.995432
  H     -1.917321    -2.793293    -2.825495
  H     -1.753311    -1.025251    -2.856921
  H      1.096701    -3.312849    -3.341739
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  H      0.184161    -4.228288    -2.141835
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M06.ML10
  Ti     0.015496     0.114365     1.012328
  Cl     2.225726    -0.177421     0.755347
  Cl    -1.425397    -0.710341    -0.528038
  Cl    -0.265882    -1.582494     2.443958
  Cl    -0.698106     1.711834     2.412354
  O      0.242964     1.685205    -0.422619
  C     -0.717362     2.799313    -0.590406
  C     -0.328225     3.442327    -1.906845
  C      0.186736     2.253670    -2.719695
  C      0.973433     1.464735    -1.693595
  H     -1.718449     2.364045    -0.621756
  H     -0.621307     3.439474     0.280560
  H      0.465605     4.175670    -1.756753
  H     -1.173137     3.941925    -2.376043
  H      0.802822     2.548800    -3.566412
  H     -0.649828     1.657147    -3.088461
  H      0.998960     0.395038    -1.884394
  H      1.987239     1.835018    -1.544834
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M06.ML10-cis
  Ti     0.000001     0.000000     0.940192
  Cl     2.319638    -0.010036     0.689667
  Cl    -2.319637     0.010037     0.689672
  Cl     0.002416    -1.728649     2.405322
  Cl    -0.002411     1.728650     2.405321
  O     -0.004528     1.387049    -0.691596
  O      0.004527    -1.387050    -0.691595
  C     -0.955961     2.514987    -0.814987
  C     -0.346370     3.410112    -1.876593
  C      0.388375     2.413209    -2.775909
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C	1.000984	1.463514	-1.766837
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C	-0.388374	-2.413209	-2.775909
C	-1.000984	-1.463513	-1.766837
H	-1.914971	2.091476	-1.114128
H	-1.052160	2.965825	0.169539
H	0.363615	4.108066	-1.430365
H	-1.104992	3.983013	-2.405875
H	1.143121	2.881387	-3.404547
H	-0.320974	1.888654	-3.420826
H	1.174223	0.450835	-2.125135
H	1.923094	1.847488	-1.331737
H	1.914970	-2.091478	-1.114126
H	1.052157	-2.965828	0.169540
H	1.104990	-3.983014	-2.405875
H	-0.363618	-4.108066	-1.430366
H	0.320976	-1.888653	-3.420826
H	-1.143121	-2.881385	-3.404549
H	-1.174221	-0.450834	-2.125135
H	-1.923095	-1.847486	-1.331739

M06.ML11

Ti	-1.185745	-1.978302	0.207062
Cl	-3.294434	-1.280875	0.825590
Cl	-1.058667	-3.699589	1.641861
Cl	-1.863774	-2.989269	-1.684754
Cl	1.091532	-2.040180	-0.375510
O	-0.512020	-0.609653	1.734788
C	-0.804460	0.782241	1.441685
O	-1.045658	0.004862	-0.774417
C	-0.398674	1.031744	0.014719
H	-1.875433	0.915311	1.581472
H	-0.254402	1.423911	2.129859
H	-0.738804	2.011803	-0.326591
H	0.684804	0.946684	-0.120425
C	-0.820211	0.165749	-2.200116
H	-1.101678	1.179409	-2.485252
H	0.229276	-0.027791	-2.428640
H	-1.451189	-0.556362	-2.704280
C	0.609523	-0.838540	2.628232
H	1.531701	-0.480328	2.168640
H	0.411508	-0.328065	3.569895
H	0.671204	-1.909434	2.787021

M06.ML12

Ti	-1.114437	-1.899140	0.179069
Cl	-2.501883	-0.048644	0.379844
Cl	-1.623328	-2.759736	2.200920
Cl	-2.555654	-3.109411	-1.064169
Cl	0.709359	-3.318071	-0.189951
O	0.377466	-0.625319	1.120475
C	0.647445	0.749510	0.710247
O	-0.415084	-0.921343	-1.633080
C	1.074684	0.805250	-0.741417
H	-0.268113	1.314692	0.882874
H	1.431172	1.137192	1.361630
H	1.434986	1.815560	-0.953705
H	1.910788	0.118169	-0.909761
C	-0.024336	-1.674404	-2.815239

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  H      1.064007    -1.716877    -2.877438
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  C      1.367528    -1.151214     2.048079
  C     -0.050978     0.490565    -1.704190
  H      0.245286     0.700552    -2.732254
  H     -0.951320     1.058789    -1.471735
  H      1.435976    -0.476846     2.901170
  H      1.030207    -2.126910     2.374694
  H      2.329035    -1.244170     1.541112
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M06.ML13
  Ti    -0.657857    -2.197254     0.040884
  Cl    -2.577553    -1.066601     0.722789
  Cl    -0.439679    -3.412736     1.934413
  Cl    -1.775474    -3.756708    -1.154968
  Cl     1.448141    -2.751996    -0.788907
  O      0.385748    -0.555320     1.011998
  C      1.528215     0.200612     0.484947
  O     -0.735221    -0.865826    -1.676580
  C      1.172766     0.947009    -0.794914
  H      1.805306     0.909750     1.266875
  H      2.346544    -0.502115     0.336693
  H      1.849072     1.801009    -0.867565
  H      1.381315     0.311955    -1.656791
  C     -0.540462    -1.397727    -3.019929
  H      0.153722    -0.751537    -3.558529
  H     -0.119366    -2.390817    -2.931187
  H     -1.503332    -1.442414    -3.528499
  C      0.117335    -0.248069     2.411717
  C     -0.289027     1.415848    -0.817653
  H     -0.358583     2.431544    -1.211996
  H     -0.692267     1.447360     0.195300
  H     -0.010059     0.829856     2.518475
  H     -0.796106    -0.752747     2.698304
  H      0.948914    -0.602871     3.020287
  C     -1.175059     0.534419    -1.689180
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  H     -1.117219     0.857943    -2.729902
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M06.ML14
  Ti    -1.214898    -1.657676     0.423023
  Cl    -1.768688     0.598238     0.660822
  Cl    -1.563070    -2.168791     2.594843
  Cl    -3.265446    -2.192130    -0.365990
  Cl    -0.272336    -3.708143    -0.150614
  O      0.792569    -1.062656     0.906442
  C      1.423575     0.163527     0.420715
  O     -0.486382    -1.077170    -1.564321
  C      1.629568     0.134436    -1.094894
  H      0.781133     0.988169     0.724353
  H      2.382010     0.260207     0.931868
  C      2.357420     1.445691    -1.484492
  C      2.481791    -1.113365    -1.484614
  C     -1.214407    -1.563810    -2.727214
  H     -0.566783    -1.502702    -3.601180
  H     -1.476572    -2.598389    -2.535322
  H     -2.114980    -0.967247    -2.874020
  C      1.599200    -1.805994     1.863627
  C      0.281392     0.140274    -1.814560
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H	0.444703	0.211821	-2.891638
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H	1.120323	-2.763857	2.025827
H	2.594051	-1.960870	1.447190
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C	1.553797	2.746450	-1.391113
H	3.244478	1.543404	-0.848174
C	2.434165	4.001255	-1.431182
H	0.836626	2.814035	-2.218940
H	0.960368	2.773429	-0.470735
C	1.569260	5.247766	-1.264167
H	3.134774	3.946411	-0.587361
C	3.239798	4.088673	-2.725929
H	2.179622	6.152242	-1.243358
H	0.869656	5.336866	-2.100643
H	0.985476	5.209918	-0.342539
H	3.800699	5.023834	-2.771181
H	3.953893	3.270039	-2.828312
H	2.567161	4.062265	-3.589389
C	2.497565	-1.412931	-2.984630
C	3.931983	-1.023569	-0.996243
H	2.007051	-1.970554	-0.996511
H	3.204240	-2.219721	-3.185533
H	1.528157	-1.745125	-3.354382
H	2.818549	-0.549686	-3.574107
H	4.408479	-2.000490	-1.092771
H	4.511022	-0.319501	-1.598347
H	4.024935	-0.719368	0.048058

M06.ML15

Ti	-0.920642	-2.095145	0.272683
Cl	-2.299062	-0.220255	0.446770
Cl	-1.221104	-2.679080	2.431877
Cl	-2.519799	-3.342977	-0.716081
Cl	0.755767	-3.683124	-0.081635
O	0.710033	-0.775777	0.826566
C	0.792991	0.617402	0.401065
O	-0.311856	-1.301831	-1.652515
C	0.975925	0.739915	-1.109816
H	-0.115832	1.118570	0.733074
H	1.655893	1.069585	0.893120
C	1.036037	2.222236	-1.451401
C	2.341771	0.254950	-1.569454
C	-0.302150	-2.127233	-2.853605
H	0.574564	-1.868349	-3.446749
H	-0.240598	-3.161961	-2.537771
H	-1.221402	-1.957512	-3.413789
C	1.650294	-1.122443	1.884830
C	-0.163100	0.124687	-1.919686
H	0.059957	0.247509	-2.980985
H	-1.115329	0.603487	-1.693179
H	1.344533	-0.636099	2.810933
H	1.627379	-2.199603	2.001017
H	2.647589	-0.803376	1.583004
C	2.272384	2.541643	-2.032070
C	2.542009	3.846504	-2.424948
C	1.566196	4.820586	-2.231003
C	0.339592	4.499277	-1.653964
C	0.064567	3.190093	-1.257991

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H	1.762173	5.840736	-2.532169
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H	-0.891503	2.944860	-0.809688
C	2.883476	-1.020067	-1.518247
C	4.175313	-1.217725	-2.009881
C	4.907188	-0.158702	-2.541044
C	4.365368	1.122426	-2.592916
C	3.081115	1.325498	-2.105461
H	2.323820	-1.851115	-1.107274
H	4.610558	-2.207299	-1.976294
H	5.906326	-0.333598	-2.916638
H	4.938543	1.942358	-3.006545
