Electronic Supplementary Information for

Indenyl ring slippage in crown thioether complexes $[IndMo(CO)_2L]^+$ and C-S Activation of Trithiacyclononane: Experimental and Theoretical Studies

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Atomic coordinates for all the optimized structures

CO

O	-0.527879	-0.055476	0.201039
C	0.527879	0.055476	-0.201039

C_2H_4

C	-0.387825	-0.335916	0.417911
C	0.378310	0.318459	-0.447432
H	-0.078502	-1.282050	0.853800
H	-1.356880	0.046783	0.726666
H	1.347313	-0.064181	-0.756409
H	0.068884	1.264605	-0.883237

1 ≡ c

Mo	0.114575	-0.033415	0.094846
S	-0.815928	2.327604	-0.357964
S	-0.540897	0.536817	2.495950
S	2.130361	1.447802	0.849358
O	1.850666	-2.476876	0.963085
O	1.867410	-0.360996	-2.490691
C	1.181372	-1.593156	0.639691
C	1.189466	-0.234089	-1.570519
C	-1.615920	2.792435	1.216153
C	-0.959461	2.327370	2.504672
C	1.072840	0.523981	3.331257
C	2.187902	1.341179	2.680208
C	1.709371	3.220169	0.596635
C	0.646504	3.405445	-0.468736
C	-1.203703	-1.656389	-0.823651
C	-1.687362	-1.520288	0.504494
C	-2.805287	-0.561839	0.485365
C	-2.776890	0.073290	-0.781623
C	-1.635765	-0.496816	-1.517197
H	-1.733922	3.881499	1.230455
H	-2.617017	2.360235	1.117833
H	-1.659021	2.484339	3.331709
H	-0.053193	2.889918	2.731850
H	0.935029	0.845036	4.369152
H	1.334349	-0.537588	3.355749
H	3.153465	0.897012	2.936845
H	2.208858	2.368831	3.051252
H	1.394516	3.647872	1.550196
H	2.628925	3.728776	0.292195
H	1.047333	3.185238	-1.463676
H	0.309142	4.447277	-0.484032
H	-0.643163	-2.485690	-1.234181
H	-1.544545	-2.263866	1.280555
H	-1.429889	-0.294955	-2.562339
C	-3.778863	-0.243477	1.417922
C	-4.749373	0.709265	1.064539
H	-3.817168	-0.739292	2.383504
H	-5.540371	0.951032	1.768078
C	-4.725862	1.328513	-0.182042
C	-3.726578	1.023411	-1.121109
H	-5.497343	2.047932	-0.438772
H	-3.718602	1.504338	-2.094624

h

Mo	0.171960	-0.193721	-0.003259
S	-0.083871	1.883042	-1.251840
S	-0.250900	-0.489623	2.374786
S	2.081342	1.141694	1.027268
O	2.053949	-2.683756	0.680866
O	2.146865	-0.598298	-2.459416
C	1.370902	-1.801379	0.449899
C	1.411000	-0.441027	-1.599287
C	-1.977474	4.102476	1.691406
C	-1.975817	3.365548	2.800733
C	0.953011	0.501160	3.321436
C	1.367365	1.751212	2.581809
C	2.280699	2.627937	0.001865
C	0.951332	3.162451	-0.459896
C	-1.186195	-1.720269	-1.086095
C	-1.622226	-1.841100	0.253622
C	-2.686450	-0.855860	0.486339
C	-2.682406	0.019288	-0.622562
C	-1.629690	-0.451333	-1.538024
H	-1.717115	5.157863	1.704017
H	-2.274267	3.678947	0.734839
H	-2.270916	2.318951	2.783707
H	-1.713564	3.789124	3.767161
H	0.431664	0.760467	4.249557
H	1.815852	-0.115583	3.592259
H	2.144002	2.303009	3.121681
H	0.506360	2.394759	2.376589
H	2.849770	3.357278	0.588589
H	2.904643	2.310376	-0.838913
H	1.106051	3.942205	-1.213038
H	0.379499	3.593958	0.367771
H	-0.627805	-2.453149	-1.653640
H	-1.427137	-2.698911	0.888267
H	-1.481341	-0.078452	-2.545913
C	-3.574316	-0.679189	1.536204
C	-4.479557	0.383911	1.452874
H	-3.581292	-1.350724	2.388956
H	-5.202892	0.533362	2.248385
C	-4.473602	1.252771	0.359630
C	-3.565156	1.086922	-0.690258
H	-5.191021	2.066458	0.321922
H	-3.565296	1.765089	-1.537910

TS_{1h}

Mo	0.238646	0.026308	0.061267
S	-0.163537	2.244710	-0.734889
S	-0.561656	0.213356	2.302188
S	2.258541	1.143715	1.085003
O	1.898865	-2.614516	0.863867
O	2.046813	-0.409955	-2.529020
C	1.279122	-1.700513	0.583537
C	1.355407	-0.260537	-1.628237
C	-1.772104	3.357769	1.325718
C	-1.957320	2.547432	2.397199
C	0.789695	0.901498	3.319127
C	1.611609	1.939863	2.589319
C	2.549818	2.540893	-0.037590
C	1.285498	3.302658	-0.366715
C	-1.197294	-1.393527	-1.057763
C	-1.629324	-1.665942	0.261909
C	-2.758898	-0.781969	0.568818
C	-2.805930	0.191265	-0.456375
C	-1.688154	-0.100595	-1.376076
H	-1.046190	4.166021	1.346764
H	-2.471812	3.352962	0.498268
H	-2.811619	1.881030	2.445844
H	-1.405935	2.710449	3.319404
H	0.329172	1.334826	4.212446
H	1.409375	0.065012	3.661449
H	2.459599	2.281375	3.190939
H	0.987833	2.789984	2.303711
H	3.309128	3.187715	0.414488
H	2.988787	2.085936	-0.930130
H	1.456477	3.926403	-1.249365
H	1.008371	3.977381	0.448708
H	-0.654557	-2.067080	-1.707406
H	-1.397148	-2.570591	0.813635
H	-1.567788	0.365498	-2.347458
C	-3.700387	-0.805567	1.581701
C	-4.733202	0.146755	1.542113
H	-3.666090	-1.553727	2.367729
H	-5.504619	0.131428	2.305516
C	-4.788305	1.094919	0.527047
C	-3.813391	1.135099	-0.486981
H	-5.604228	1.811026	0.507857
H	-3.877309	1.869116	-1.285175

i

Mo	-0.510027	-0.000855	-0.370475
S	-0.061510	2.432725	-0.849738
S	-0.996659	0.870604	1.847506
S	1.909760	0.072552	0.347916
O	0.064131	-2.621934	1.326946
O	1.509138	-0.809756	-2.698953
C	-0.117260	-1.674960	0.718966
C	0.843104	-0.504836	-1.817246
C	-1.119482	3.271768	0.377339
C	-1.039364	2.698723	1.772282
C	1.774672	3.531593	4.399425
C	1.450959	2.258551	4.618387
C	2.085899	1.801513	0.849587

C	1.634582	2.741443	-0.249568
C	-1.709559	-0.358547	-2.322436
C	-1.792707	-1.517264	-1.494128
C	-2.695424	-1.201873	-0.400156
C	-3.108658	0.166214	-0.552560
C	-2.412981	0.695382	-1.686161
H	-0.859188	4.335857	0.350695
H	-2.124485	3.167328	-0.041101
H	-1.928106	3.015125	2.329613
H	-0.171824	3.086531	2.314850
H	2.766315	3.819688	4.059554
H	1.074026	4.340756	4.590257
H	0.470110	1.971091	4.987339
H	2.162479	1.451561	4.462965
H	1.553421	1.961900	1.788668
H	3.157419	1.947873	1.031715
H	2.261273	2.632583	-1.139209
H	1.669363	3.791070	0.062905
H	-1.220328	-0.293011	-3.285158
H	-1.426808	-2.503041	-1.751806
H	-2.529087	1.692002	-2.094392
C	-3.201630	-1.982379	0.667859
C	-4.068407	-1.383155	1.545574
H	-2.920585	-3.025067	0.775905
H	-4.477924	-1.958345	2.369934
C	-4.473017	-0.027786	1.390419
C	-4.016704	0.746892	0.353524
H	-5.180147	0.387355	2.101796
H	-4.349820	1.772013	0.227554

TS_{1i}

Mo	-0.131281	0.399755	0.070215
S	0.270844	2.586659	-1.131798
S	-1.126681	1.771361	1.766835
S	2.022331	0.766149	1.015926
O	-0.092593	-1.820132	2.297708
O	1.873650	-1.107658	-1.922131
C	-0.122592	-1.038049	1.459455
C	1.148582	-0.584307	-1.207836
C	-0.793907	3.768359	-0.236890
C	-0.999972	3.526091	1.248855
C	0.577546	1.615051	3.769928
C	1.806714	1.083522	3.462553
C	2.308598	2.553753	0.776567
C	1.967268	3.007112	-0.626282
C	-1.520763	-0.247610	-1.661023
C	-1.506275	-1.347001	-0.737293
C	-2.696082	-1.197991	0.122275
C	-3.256196	0.075884	-0.144202
C	-2.441861	0.697215	-1.173158
H	-0.399093	4.772540	-0.425346
H	-1.744435	3.694490	-0.771990
H	-1.934966	4.008090	1.552822
H	-0.205984	3.991876	1.837907
H	0.449264	2.684207	3.908827
H	-0.207359	0.985031	4.172277
H	1.999572	0.028475	3.628702
H	2.684610	1.722225	3.415345
H	1.719492	3.093423	1.520272
H	3.370371	2.734491	0.975310
H	2.604540	2.518662	-1.369810
H	2.095643	4.088985	-0.737671
H	-1.000790	-0.185547	-2.608327
H	-1.030550	-2.299429	-0.941848
H	-2.657269	1.646448	-1.650774
C	-3.259089	-2.034882	1.074715
C	-4.399022	-1.588399	1.748029
H	-2.840849	-3.014380	1.285842
H	-4.871073	-2.233915	2.482182
C	-4.949054	-0.328976	1.488837
C	-4.377415	0.522857	0.544724
H	-5.838318	-0.015566	2.026389
H	-4.809595	1.499017	0.346277

j

Mo	0.503954	-0.657367	0.081666
S	0.955216	1.777132	-0.396118
S	0.022345	0.217944	2.302528
S	2.924383	-0.585671	0.798654
O	1.078336	-3.281622	1.774910
O	2.517015	-1.468738	-2.250790
C	0.896640	-2.333813	1.168752
C	1.851297	-1.163450	-1.369457
C	-0.112887	2.614290	0.823660
C	-0.030409	2.046214	2.220926
C	3.090194	1.138698	1.317053
C	2.645669	2.086505	0.220792
C	-0.701032	-1.013000	-1.866698
C	-0.783498	-2.171883	-1.038439
C	-1.681450	-1.855153	0.058968
C	-2.093294	-0.486262	-0.091840
C	-1.400587	0.041944	-1.227829
H	0.138034	3.680466	0.793573
H	-1.116685	2.499328	0.405603
H	-0.916536	2.363138	2.781540
H	0.837051	2.448501	2.751983
H	2.535709	1.280391	2.245875
H	4.157180	1.289832	1.518906
H	3.281328	1.983014	-0.663039
H	2.676667	3.134815	0.538026
H	-0.215522	-0.948118	-2.831384
H	-0.420081	-3.158218	-1.297590
H	-1.517055	1.038449	-1.636341
C	-2.185240	-2.635288	1.128597
C	-3.048691	-2.035249	2.008925
H	-1.905349	-3.678407	1.235434
H	-3.456210	-2.609945	2.834600
C	-3.452661	-0.679448	1.854812
C	-2.998560	0.095049	0.816808
H	-4.157518	-0.263855	2.568180
H	-3.332255	1.120078	0.691453

6+CO

Mo	0.278693	-0.173912	0.550038
S	0.618311	2.228534	-0.002961
S	-0.373294	0.609731	2.659388
S	2.587593	-0.235062	0.606370
O	0.828390	-2.814668	2.227570
O	2.873567	-4.936571	-2.064726
C	0.618730	-1.877834	1.613720
C	2.050339	-4.216230	-1.774179
C	0.015014	3.133238	1.465146
C	0.127550	2.373111	2.761921
C	3.247668	1.473486	0.635255
C	2.421120	2.469896	-0.137267
C	-0.426790	-0.399269	-1.585245
C	-0.407122	-1.689650	-0.997696
C	-1.538180	-1.775309	-0.082140
C	-2.185613	-0.493102	-0.062830
C	-1.461055	0.362686	-0.943376
H	0.532241	4.097665	1.499432
H	-1.032747	3.327380	1.216823
H	-0.512790	2.842999	3.515474
H	1.151079	2.385451	3.146935
H	3.332964	1.741618	1.691885
H	4.261413	1.427896	0.224657
H	2.601825	2.376470	-1.212026
H	2.644056	3.503378	0.147486
H	0.218989	-0.048334	-2.379156
H	0.242208	-2.509712	-1.282941
H	-1.736115	1.378765	-1.193901
C	-2.068892	-2.848583	0.676333
C	-3.192500	-2.612190	1.427640
H	-1.610774	-3.831693	0.640310
H	-3.632109	-3.424114	1.998836
C	-3.810084	-1.330772	1.475830
C	-3.320676	-0.273355	0.754343
H	-4.695410	-1.200711	2.089915
H	-3.801101	0.699069	0.779835

TS_{j6}

Mo	0.526996	-0.599591	0.194671
S	0.950703	1.828380	-0.374529
S	-0.027849	0.243959	2.279416
S	2.863612	-0.541582	0.670275
O	1.060764	-3.313634	1.732575
O	3.120189	-2.086576	-2.516023
C	0.878104	-2.335992	1.171309
C	2.201185	-1.771082	-1.933963
C	-0.129946	2.680889	0.826784
C	-0.158427	2.077603	2.212261
C	3.129603	1.158179	1.245106
C	2.642495	2.162501	0.221425
C	-0.673041	-0.886849	-1.750512
C	-0.755269	-2.070663	-0.966665
C	-1.712369	-1.814310	0.105694
C	-2.145535	-0.454228	-0.012770
C	-1.427285	0.124404	-1.106752

H	0.171248	3.733290	0.847124
H	-1.115023	2.635821	0.354870
H	-1.095324	2.354554	2.705869
H	0.654080	2.468963	2.831280
H	2.622326	1.266539	2.208408
H	4.207024	1.274706	1.403750
H	3.260626	2.125826	-0.679591
H	2.658507	3.190125	0.599996
H	-0.130903	-0.762556	-2.676643
H	-0.375722	-3.043211	-1.252000
H	-1.555723	1.130379	-1.487921
C	-2.225581	-2.636054	1.132576
C	-3.118498	-2.079693	2.017935
H	-1.930684	-3.677545	1.212880
H	-3.534807	-2.690123	2.813063
C	-3.530991	-0.726192	1.907799
C	-3.064112	0.089121	0.902712
H	-4.250753	-0.340877	2.623361
H	-3.404121	1.115821	0.808929

[(η^5-Cp)Mo(CO)$_2$(κ^2-tt)]$^+$

Mo	-0.106965	2.780702	3.396528
S	2.305173	1.909267	3.442764
S	0.081387	0.409542	2.429140
S	0.968985	-0.138170	5.350711
O	-2.477790	1.487962	4.976673
O	0.550643	3.518358	6.364207
C	-1.595870	1.950334	4.401054
C	0.313893	3.229903	5.276175
C	1.836253	0.758503	2.118023
C	0.329643	-0.792110	3.805070
C	2.477309	0.652740	4.780896
C	0.156801	4.993317	2.839716
C	-1.228421	4.704675	3.046734
C	-1.641786	3.798060	2.021034
C	-0.522926	3.561425	1.170098
H	-0.526168	2.940868	0.281954
H	1.569879	4.333958	1.234942
C	0.579122	4.293029	1.671493
H	2.458450	-0.143381	2.087328
H	1.916049	1.283828	1.164640
H	-0.657571	-1.204919	4.029110
H	0.948686	-1.597990	3.397389
H	3.225505	-0.065429	4.429750
H	2.894081	1.180960	5.642505
H	0.759370	5.681049	3.418502
H	-1.863946	5.142150	3.805335
H	-2.644012	3.419003	1.869812

[(η^3-Cp)Mo(CO)$_2$(κ^3-tt)]$^+$

Mo	0.805628	-0.174007	-0.313612
S	-1.133148	1.221696	-1.256974
S	-1.371148	-1.525612	-0.469221
S	-0.902332	-0.931334	-3.477106
O	1.985084	-2.741081	-1.658455
O	2.304565	0.973446	-2.807060
C	1.539814	-1.796979	-1.175559
C	1.738305	0.544493	-1.902245
C	-2.265068	0.054909	-0.447036
C	-1.704854	-1.947849	-2.233138
C	-1.471048	0.702057	-2.991637
C	1.927187	1.340754	1.000318
C	2.598529	0.078676	1.028323
C	1.733586	-0.859989	1.673913
C	0.552421	-0.166426	2.068859
H	-0.281925	-0.597246	2.609335
H	-0.056136	1.966725	1.824642
C	0.671458	1.181593	1.656684
H	-3.249691	0.003043	-0.925599
H	-2.385802	0.364074	0.592639
H	-1.332578	-2.965475	-2.377820
H	-2.794390	-1.967509	-2.340200
H	-2.546086	0.839456	-3.147352
H	-0.943492	1.415276	-3.630548
H	2.330613	2.269987	0.619722
H	3.604590	-0.116019	0.680892
H	1.964288	-1.894233	1.893542

[(η^5-Ind)Mo(CO)$_2$(κ^2-tt)]$^+$

Mo	-0.553771	2.782761	3.604261
S	1.884422	1.883423	3.705813
S	-0.340438	0.373971	2.643322
S	0.493281	-0.153343	5.580720
O	-2.980039	1.504270	5.089438
O	0.045116	3.516416	6.574560
C	-2.077764	1.968261	4.545684
C	-0.174483	3.232047	5.480818
C	1.408100	0.763795	2.360312
C	-0.109243	-0.820169	4.024749
C	2.021145	0.621684	5.039002
C	-0.279512	4.982609	3.117108
C	-1.672796	4.715076	3.258558
C	-2.064416	3.792433	2.244030
C	-0.941564	3.613205	1.353130
C	-0.781070	2.866550	0.161830
C	0.440644	2.905107	-0.477608
C	1.533183	3.632997	0.056791
C	1.422139	4.334917	1.239120
C	0.168865	4.353301	1.896072
H	2.043629	-0.126832	2.295537
H	1.472076	1.326449	1.425082
H	-1.096478	-1.241797	4.231354
H	0.526847	-1.622710	3.637155
H	2.764293	-0.107534	4.700069
H	2.429843	1.140463	5.910096
H	0.297289	5.671549	3.720453
H	-2.321649	5.132310	4.017691
H	-3.068824	3.427006	2.073998
H	-1.617134	2.315392	-0.257666
H	0.570111	2.374558	-1.416125
H	2.474342	3.642987	-0.484692
H	2.259846	4.898460	1.638336

[(η^3-Ind)Mo(CO)$_2$(κ^3-tt)]$^+$

Mo	1.088320	-0.393277	-0.991989
S	-1.025516	1.298389	-1.269574
S	-1.287498	-1.586310	-0.407529
S	-0.474098	-0.910026	-3.196672
O	2.886596	-2.831734	-1.705491
O	3.220534	0.932154	-2.831536
C	2.220070	-1.938654	-1.413471
C	2.433938	0.464523	-2.131650
C	-2.038627	0.071568	-0.384993
C	-1.534844	-1.965017	-2.167936
C	-1.291904	0.693613	-2.962860
C	1.853891	1.188998	0.551988
C	2.574440	-0.026772	0.678877
C	1.663861	-0.982351	1.199200
C	0.548029	-0.255612	1.815261
C	-0.475665	-0.656798	2.668446
C	-1.366820	0.317302	3.134401
C	-1.249157	1.652620	2.738571
C	-0.236555	2.061156	1.862160
C	0.667297	1.103643	1.411381
H	-3.062057	0.048247	-0.773139
H	-2.069213	0.387466	0.661822
H	-1.205278	-2.994767	-2.328478
H	-2.586367	-1.888938	-2.460722
H	-2.354279	0.647730	-3.220511
H	-0.802524	1.398383	-3.640102
H	2.276126	2.118321	0.187711
H	3.609679	-0.196562	0.413217
H	1.913807	-2.013940	1.418343
H	-0.560186	-1.687903	2.998693
H	-2.152015	0.033504	3.828321
H	-1.944429	2.388662	3.130324
H	-0.138823	3.104461	1.576937

[(η^5-Cp)Mo(CO)$_2$(κ^2-ttcd)]$^+$ (1)

Mo	0.443229	0.165432	1.445832
S	1.667569	0.083495	-0.806201
S	-0.715571	-1.797020	0.331928
S	-0.177754	3.183681	-2.183926
O	-2.492746	0.947896	2.140839
O	0.498291	3.275374	1.129471
C	-1.418290	0.659675	1.838722
C	0.460897	2.128325	1.148460
C	1.661011	-1.724748	-1.063166
C	0.267934	-2.321963	-1.119390
C	-2.444499	-1.778746	-0.305028
C	-2.815918	-1.029273	-1.593114
C	0.980420	1.966212	-2.871263
C	0.856086	0.525945	-2.397843
C	1.021720	0.526771	3.603075
C	0.559825	-0.823295	3.516115
C	1.507591	-1.557246	2.742421

C	2.528748	-0.671788	2.332093
C	2.228623	0.622029	2.845624
H	1.448963	-2.614346	2.514636
H	3.400454	-0.925925	1.741176
S	-3.683901	0.555072	-1.411406
C	-2.297547	1.711999	-1.197398
C	-1.773752	2.345412	-2.482790
H	2.205572	-1.943376	-1.988115
H	2.238841	-2.140042	-0.233969
H	0.327402	-3.414363	-1.103659
H	-0.252816	-2.027487	-2.033172
H	-2.673029	-2.843877	-0.414534
H	-3.030397	-1.411381	0.542279
H	-3.531437	-1.660507	-2.130302
H	-1.968031	-0.915987	-2.275877
H	0.855225	1.946213	-3.960034
H	1.982349	2.363069	-2.680750
H	1.373068	-0.116031	-3.120762
H	-0.189782	0.218518	-2.358736
H	0.569312	1.320643	4.182882
H	-0.305019	-1.236328	4.018456
H	2.846845	1.503816	2.736777
H	-2.653295	2.492511	-0.518296
H	-1.494820	1.191583	-0.668639
H	-2.472418	3.097248	-2.858519
H	-1.649803	1.612536	-3.287564

$[(\eta^5\text{-Cp})Mo(CO)_2(\kappa^2\text{-ttcd})]^+$ (2)

Mo	1.152715	-0.567865	-0.060014
S	-0.840941	0.386626	1.183164
S	0.079477	3.378690	0.266327
S	-3.697606	-1.491902	-0.018760
O	0.449817	-3.269854	-1.414453
O	1.018779	-2.440594	2.452852
C	0.650914	-2.256359	-0.896161
C	1.071221	-1.749360	1.534821
C	-0.413333	1.635735	2.443727
C	-0.690816	3.026114	1.882386
C	-1.233550	2.927149	-0.924281
C	-0.768036	2.080448	-2.106810
C	-2.344481	-1.908374	1.118934
C	-1.857405	-0.836006	2.085084
C	3.358164	-1.071387	-0.238259
C	2.978832	-0.395231	-1.431413
C	2.678532	0.960294	-1.080863
C	2.851211	1.120049	0.309362
C	3.253309	-0.134920	0.841363
H	-1.030451	1.449171	3.329367
H	0.634796	1.509032	2.723737
H	-0.291144	3.778566	2.569560
H	-1.766096	3.210182	1.802248
H	-2.054646	2.465323	-0.377038
H	-1.613108	3.860822	-1.353535
H	-1.540222	2.108088	-2.884919
H	-2.782910	-2.718164	1.712338
H	-1.505539	-2.349311	0.573358
H	-1.269451	-1.288821	2.889698
H	-2.699646	-0.287576	2.516859
H	3.710643	-2.091897	-0.166329
H	2.986259	-0.808889	-2.431011
H	3.509361	-0.330341	1.875099
H	2.386946	1.743313	-1.769160
H	2.692340	2.034153	0.863503
H	0.124391	2.528814	-2.554302
S	-0.339749	0.300215	-1.986496
C	-1.959325	-0.550461	-2.129751
H	-1.705962	-1.613500	-2.101071
H	-2.278063	-0.335046	-3.154726
C	-3.086800	-0.200943	-1.144819
H	-3.989994	0.010339	-1.727144
H	-2.870958	0.705167	-0.583012

$[(\eta^3\text{-Cp})Mo(CO)_2(\kappa^3\text{-ttcd})]^+$

Mo	-0.932101	-0.141691	-0.065707
S	-0.703702	2.271692	0.792120
S	0.984537	-0.427687	1.688513
S	0.565426	0.811577	-1.966818
O	-0.776748	-2.941692	-1.457882
O	-2.972145	0.393409	-2.357957
C	-0.850488	-1.927286	-0.914170
C	-2.253912	0.196590	-1.474937
C	0.314836	2.160865	2.309017
C	1.510583	1.232038	2.224370
C	2.553010	-1.385719	1.706641
C	3.792273	-0.814536	1.017462
C	0.327970	2.607383	-1.769569
C	0.459536	3.114042	-0.347767
C	-2.202861	-0.427991	1.706678
C	-3.211661	0.029712	0.800531
C	-3.942046	-1.152850	0.296166
C	-3.230976	-2.245631	0.634956
C	-2.030452	-1.798625	1.376507
H	-4.833904	-1.106775	-0.315185
H	-3.431947	-3.273904	0.362349
S	4.143919	-1.351614	-0.680215
C	2.606408	-0.918535	-1.525564
C	2.318281	0.577283	-1.526004
H	0.639567	3.173761	2.566488
H	-0.382469	1.839344	3.087525
H	1.964624	1.142791	3.217220
H	2.269637	1.632714	1.546317
H	2.760847	-1.528783	2.771665
H	2.281998	-2.364435	1.299288
H	4.667252	-1.176796	1.568020
H	3.836958	0.275963	1.096755
H	1.044586	3.118674	-2.420767
H	-0.671103	2.799190	-2.173306
H	0.234166	4.184447	-0.316526
H	1.477283	2.975010	0.026102
H	-1.823021	0.079586	2.583995
H	-3.616596	1.036609	0.803378
H	-1.354764	-2.467938	1.897771
H	2.720671	-1.291943	-2.547270
H	1.779382	-1.476322	-1.075750
H	2.937856	1.099711	-2.260410
H	2.491216	1.011685	-0.540047

$[(\eta^5\text{-Ind})Mo(CO)_2(\kappa^2\text{-ttcd})]^+$ (1)

Mo	0.261396	0.476131	1.523038
S	1.486806	0.366530	-0.759030
S	-0.939164	-1.484521	0.398941
S	-0.320235	3.483526	-2.121029
O	-2.655845	1.322347	2.158543
O	0.435899	3.570804	1.181431
C	-1.580381	1.008629	1.881239
C	0.361403	2.425384	1.224649
C	1.437558	-1.442447	-0.985565
C	0.035391	-2.016188	-1.052665
C	-2.668737	-1.445354	-0.232774
C	-3.030206	-0.691960	-1.521799
C	0.816860	2.253588	-2.821890
C	0.678204	0.814610	-2.348584
C	0.753404	0.873748	3.696043
C	0.265161	-0.461061	3.597266
C	1.293821	-1.260350	2.968253
C	2.356255	-0.374037	2.576359
C	1.973127	0.961829	2.964541
C	1.404690	-2.647515	2.726096
C	2.568901	-3.122376	2.158954
C	3.617301	-2.248936	1.777969
C	3.516969	-0.884018	1.953839
S	-3.865793	0.909925	-1.341374
C	-2.456617	2.039897	-1.129735
C	-1.929767	2.670026	-2.415194
H	1.991612	-1.689238	-1.897836
H	1.995779	-1.852074	-0.138967
H	0.083064	-3.109032	-1.041294
H	-0.480937	-1.711504	-1.965565
H	-2.916431	-2.506192	-0.341111
H	-3.247932	-1.065766	0.613754
H	-3.759988	-1.309621	-2.055470
H	-2.182354	-0.596121	-2.207144
H	0.682927	2.239035	-3.909637
H	1.824740	2.637960	-2.637159
H	1.184254	0.165570	-3.073119
H	-0.371606	0.520292	-2.307618
H	0.271855	1.687545	4.222975
H	-0.623548	-0.845240	4.081252
H	2.597821	1.842111	2.881570
H	0.608139	-3.322824	3.021446
H	2.693516	-4.190361	2.007280
H	4.520234	-2.668062	1.344191
H	4.325386	-0.219049	1.666398
H	-2.793025	2.822779	-0.443709
H	-1.659676	1.502343	-0.609482
H	-2.619271	3.433371	-2.784672
H	-1.820480	1.937964	-3.222754

$[(\eta^5\text{-Ind})Mo(CO)_2(\kappa^2\text{-ttcd})]^+$ (2)

Mo	1.142434	-0.689779	0.013711
S	-0.940752	0.130176	1.246026
S	-0.203228	3.081074	0.329544
S	-3.627544	-1.950119	-0.044029
O	0.427800	-3.450342	-1.151210
O	1.147109	-2.360821	2.655365
C	0.636423	-2.406624	-0.692614
C	1.170868	-1.734493	1.688865
C	-0.662834	1.402996	2.524987
C	-1.012086	2.763356	1.933831
C	-1.500046	2.628765	-0.874849
C	-0.959257	1.856369	-2.074158
C	-2.290267	-2.270614	1.143867
C	-1.893600	-1.166155	2.114573
C	3.291773	-1.342166	-0.355292
C	2.861753	-0.611273	-1.489179
C	2.859448	0.799620	-1.135942
C	3.141190	0.896568	0.266217
C	3.314936	-0.451275	0.759202
H	-1.299335	1.168241	3.384870
H	0.381261	1.358623	2.843793
H	-0.676805	3.554578	2.611298
H	-2.093245	2.878634	1.815607
H	-2.293582	2.092865	-0.355023
H	-1.932375	3.554448	-1.270365
H	-1.716863	1.838176	-2.866355
H	-2.707242	-3.093779	1.734821
H	-1.413644	-2.679178	0.636782
H	-1.295735	-1.582731	2.931687
H	-2.779662	-0.676311	2.529111
H	3.528568	-2.398048	-0.328275
H	2.759317	-1.009695	-2.490463
H	3.649679	-0.706686	1.757093
C	2.716789	1.968635	-1.907857
C	3.275116	2.152729	0.884822
H	-0.092024	2.379444	-2.486936
S	-0.386205	0.118345	-1.958141
C	-1.927892	-0.864178	-2.124262
H	-1.590227	-1.903347	-2.095219
H	-2.257235	-0.674030	-3.150627
C	-3.086905	-0.607649	-1.145963
H	-3.996804	-0.444952	-1.733366
H	-2.935279	0.299611	-0.566273
C	3.171598	3.281468	0.097324
C	2.896312	3.188582	-1.284069
H	3.510413	2.225709	1.942440
H	3.312166	4.262026	0.540898
H	2.838974	4.101737	-1.868961
H	2.538780	1.904588	-2.977344

$[(\eta^3\text{-Ind})Mo(CO)_2(\kappa^3\text{-ttcd})]^+$

Mo	-0.255557	1.163958	0.499426
S	-2.578184	1.482450	1.574214
S	-0.194403	3.724683	1.065683
S	-1.648968	1.419602	-1.660217
O	2.311212	0.962865	-1.273126
O	-0.630336	-1.803146	-0.360383
C	1.379466	1.040701	-0.597877
C	-0.481712	-0.713941	-0.005789
C	-2.525789	3.123168	2.384477
C	-1.865389	4.229969	1.583609
C	0.439212	5.209716	0.187838
C	-0.418561	5.875152	-0.888362
C	-3.338078	1.075024	-1.071666
C	-3.735559	1.812415	0.190699
C	0.443646	1.032568	2.578604
C	0.091515	-0.339318	2.361369
C	1.333436	-1.089368	2.087803
C	2.334599	-0.133013	1.815575
C	1.703460	1.196691	1.935232
C	1.605774	-2.442920	2.033238
C	2.916791	-2.838776	1.724336
C	3.903257	-1.897162	1.458126
C	3.619348	-0.522322	1.489498
S	-0.128990	5.407485	-2.618833
C	-0.328725	3.612627	-2.553650
C	-1.729297	3.175154	-2.144108
H	-3.553181	3.401847	2.638428
H	-1.998208	2.947954	3.326246
H	-1.773841	5.120448	2.214939
H	-2.473246	4.499741	0.714796
H	0.635986	5.926809	0.990972
H	1.410329	4.898040	-0.208743
H	-0.172195	6.942577	-0.886473
H	-1.484721	5.828473	-0.645633
H	-4.035516	1.310175	-1.882419
H	-3.361855	-0.009642	-0.927058
H	-4.731045	1.487633	0.508444
H	-3.773772	2.891164	0.020134
H	-0.037853	1.739152	3.242525
H	-0.813463	-0.795566	2.750440
H	2.258336	2.129104	1.934078
H	0.838042	-3.184474	2.233185
H	3.161765	-3.895759	1.694224
H	4.910025	-2.227616	1.222424
H	4.395909	0.205782	1.274702
H	-0.091270	3.257256	-3.560499
H	0.426837	3.190797	-1.883997
H	-2.434122	3.278899	-2.973938
H	-2.090924	3.757231	-1.294842

$[(\eta^5\text{-Cp})Mo(CO)_2(\kappa^2\text{-ttcn})]^+$

Mo	1.224727	7.074913	4.396680
S	-0.566933	5.583045	3.443637
S	1.294525	7.754109	1.952437
S	1.861939	4.348476	0.691478
O	4.323094	7.097964	4.014841
O	2.079226	4.415555	5.792440
C	3.174922	7.066934	4.122117
C	1.763800	5.380383	5.245562
C	-1.206872	6.541496	2.037034
C	-0.159317	7.050918	1.076759
C	2.667577	7.082243	0.946636
C	3.079390	5.631221	1.131223
C	1.351959	3.695428	2.310485
C	-0.078981	3.950063	2.757032
C	1.470393	8.218859	6.337486
C	1.452366	9.190149	5.288722
C	0.142964	9.200574	4.725242
C	-0.635504	8.231534	5.397558
C	0.180783	7.608499	6.386204
H	-1.946822	5.927367	1.512745
H	-1.745127	7.362808	2.519660
H	-0.573797	7.848929	0.453244
H	0.210040	6.241840	0.443920
H	2.387906	7.294988	-0.090018
H	3.517882	7.730401	1.184390
H	3.418261	5.443586	2.151737
H	3.944329	5.464874	0.479639
H	1.460389	2.607546	2.239731
H	2.066925	4.031301	3.064936
H	-0.314717	3.264127	3.578186
H	-0.797634	3.744740	1.957345
H	2.295522	8.020608	7.008849
H	2.262752	9.854972	5.019519
H	-0.192535	9.842511	3.920318
H	-1.676868	8.002650	5.206707
H	-0.144906	6.857349	7.093992

$[(\eta^3\text{-Cp})Mo(CO)_2(\kappa^3\text{-ttcn})]^+$

Mo	-0.510299	-0.019343	0.035790
S	0.978105	-1.996925	-0.483955
S	1.046140	1.175924	-1.561946
S	1.410509	0.553675	1.654792
O	-1.853428	2.616382	1.046218
O	-1.859252	-1.187365	2.610226
C	-1.387139	1.639325	0.643918
C	-1.390693	-0.786878	1.636052
C	2.072617	-1.413716	-1.829520
C	2.477033	0.049755	-1.808909
C	1.754220	2.446520	-0.469662
C	2.303077	1.956559	0.869524
C	2.642934	-0.810453	1.496609
C	2.053633	-2.111041	0.982791
C	-1.733502	-0.708422	-1.656113
C	-2.341536	-1.464737	-0.606777
C	-3.584975	-0.761203	-0.207432
C	-3.562040	0.466148	-0.759700
C	-2.305103	0.588290	-1.531701
H	2.962105	-2.052268	-1.849882
H	1.501197	-1.642824	-2.734892
H	2.934435	0.308504	-2.768940
H	3.211333	0.253169	-1.029093
H	2.535264	2.987050	-1.014793

H	0.923762	3.141356	-0.319167
H	2.265706	2.780219	1.587849
H	3.351537	1.657373	0.795119
H	3.459447	-0.465447	0.859623
H	3.054559	-0.975164	2.496747
H	1.403862	-2.571775	1.733618
H	2.856682	-2.824724	0.769997
H	-1.129877	-1.080432	-2.474937
H	-2.172311	-2.524834	-0.450553
H	-2.072054	1.420923	-2.187035
H	-4.320833	-1.164987	0.476235
H	-4.271848	1.270403	-0.616397

$[(\eta^5\text{-Ind})Mo(CO)_2(\kappa^2\text{-ttcn})]^+$
left fig 5

Mo	0.569236	10.097570	6.922980
S	-1.506722	10.501101	8.279185
S	1.469546	9.852425	9.262261
S	0.352715	13.145221	10.441486
O	3.147219	11.847933	6.613178
O	-0.549855	12.615855	5.423684
C	2.184937	11.228653	6.761235
C	-0.144272	11.706786	6.004365
C	-1.239281	9.524764	9.787765
C	0.086412	9.761110	10.469405
C	2.437120	11.239351	9.960315
C	1.963451	12.666717	9.738296
C	-0.721123	13.227613	8.974549
C	-1.846548	12.211857	8.860415
C	0.263147	7.802203	6.878984
C	-0.642317	8.362624	5.933246
C	0.127189	8.921200	4.857351
C	1.519870	8.756145	5.183011
C	1.596181	8.098805	6.460939
H	-2.069522	9.722177	10.474220
H	-1.341082	8.492943	9.439819
H	0.315608	8.939539	11.154722
H	0.076108	10.706623	11.014989
H	2.530370	11.007075	11.025869
H	3.433820	11.120823	9.521950
H	1.961385	12.923117	8.677542
H	2.704337	13.319632	10.212914
H	-1.199395	14.212443	9.009970
H	-0.090899	13.216361	8.082558
H	-2.568244	12.576572	8.121256
H	-2.390169	12.097071	9.803441
H	-0.007345	7.215167	7.747455
H	-1.722748	8.299280	5.967165
H	2.504505	7.779955	6.955736
C	-0.247853	9.521260	3.620005
C	0.742958	9.896369	2.755008
H	-1.296288	9.639269	3.365244
H	0.479692	10.328370	1.794538
C	2.123251	9.728344	3.075355
C	2.522680	9.186099	4.265341
H	2.868862	10.036858	2.349295
H	3.573332	9.049326	4.501091

center fig 5

Mo	0.188446	10.169383	6.925129
S	0.776963	9.671497	9.305986
S	2.476107	11.269781	7.098963
S	1.592891	13.417430	9.943270
O	-0.498815	12.867278	5.476088
O	-2.530302	10.966464	8.211049
C	-0.221566	11.898713	6.036422
C	-1.507524	10.685917	7.754595
C	2.594557	9.584437	9.301516
C	3.285876	10.767869	8.668747
C	2.525614	13.091301	7.254548
C	1.523696	13.788506	8.161019
C	0.125822	12.372122	10.201838
C	0.351206	10.918800	10.587040
C	-0.702745	8.096084	6.556070
C	-0.955942	8.942322	5.432764
C	0.302703	9.168220	4.766818
C	1.325888	8.461424	5.502053
C	0.698221	7.865001	6.644425
H	2.933810	9.441280	10.332972
H	2.798229	8.658889	8.754927
H	4.324136	10.517973	8.430022
H	3.257329	11.631954	9.335313
H	3.556077	13.323313	7.541538
H	2.393688	13.453914	6.229477
H	0.499979	13.627784	7.817671
H	1.715210	14.863583	8.071240
H	-0.422948	12.829146	11.032388
H	-0.516198	12.447748	9.321851
H	-0.580376	10.522806	11.006075
H	1.116393	10.815491	11.362892
H	-1.452229	7.684084	7.219634
H	-1.930316	9.239188	5.067059
H	1.181759	7.226434	7.373400
C	0.642247	9.875470	3.577785
C	1.943799	9.846084	3.152075
H	-0.125714	10.397161	3.014991
H	2.221604	10.358445	2.236389
C	2.946863	9.142773	3.876669
C	2.663554	8.468096	5.037735
H	3.961022	9.136183	3.488896
H	3.435351	7.922771	5.572136

right fig 5

Mo	0.482291	10.134791	6.921072
S	2.553924	11.591755	6.694094
S	-0.506955	12.217921	5.817453
S	0.675877	14.548285	8.410669
O	-2.067801	10.443698	8.674436
O	1.648024	9.716325	9.777004
C	-1.114925	10.361364	8.027105
C	1.219736	9.896135	8.720774
C	2.177031	12.582269	5.218560
C	0.856185	13.310817	5.255363
C	-1.445956	13.358711	6.895918
C	-0.916018	13.671042	8.286547
C	1.821445	13.253837	8.980488
C	2.918492	12.802781	8.027268
C	0.039306	7.915595	6.774925
C	-0.732736	8.577877	5.776102
C	0.171745	9.016960	4.738379
C	1.510019	8.711401	5.169220
C	1.419181	8.095688	6.472138
H	3.001534	13.285154	5.057880
H	2.210478	11.843614	4.411244
H	0.593636	13.663314	4.253421
H	0.895426	14.155114	5.946839
H	-1.578191	14.268513	6.302084
H	-2.433350	12.893549	6.986683
H	-0.860412	12.771663	8.902436
H	-1.654689	14.326024	8.761878
H	2.329952	13.675684	9.854227
H	1.237826	12.403322	9.339276
H	3.694551	12.293972	8.609497
H	3.400900	13.650965	7.531269
H	-0.356251	7.379968	7.628332
H	-1.813372	8.586987	5.714292
H	2.248459	7.680455	7.030297
C	-0.046910	9.628942	3.482767
C	1.042983	9.873408	2.676068
H	-1.054298	9.860273	3.151798
H	0.893773	10.303193	1.690185
C	2.360734	9.563004	3.096791
C	2.611094	9.010852	4.334910
H	3.188159	9.759548	2.421495
H	3.621597	8.771100	4.650354

$[(\eta^3\text{-Ind})Mo(CO)_2(\kappa^3\text{-ttcn})]^+$
b fig 6

Mo	0.274296	0.584260	0.098621
S	1.269436	2.890257	0.413109
S	2.073643	0.393561	-1.673518
S	2.262604	-0.097324	1.574074
O	-0.427669	-2.460700	0.047333
O	-1.383519	0.562406	2.751601
C	-0.191792	-1.330387	0.045708
C	-0.794846	0.589839	1.760528
C	2.481307	3.067149	-0.946417
C	3.209430	1.811435	-1.394052
C	3.055860	-0.993810	-1.024765
C	3.476031	-0.888558	0.439563
C	3.136411	1.464864	2.022009
C	2.270392	2.707526	1.924155
C	-1.011416	1.529093	-1.408558
C	-1.785654	1.782088	-0.231244
C	-2.873813	0.783263	-0.180798
C	-2.545504	-0.227718	-1.108912

C	-1.262452	0.160852	-1.728357
C	-4.021210	0.702771	0.582974
C	-4.862633	-0.406139	0.393578
C	-4.539110	-1.402041	-0.518912
C	-3.360975	-1.329545	-1.280122
H	3.201909	3.842972	-0.666584
H	1.881978	3.477763	-1.765428
H	3.721154	2.012564	-2.340366
H	3.966208	1.507327	-0.669670
H	3.941328	-1.129661	-1.654814
H	2.408159	-1.860107	-1.183291
H	3.648055	-1.894768	0.831714
H	4.417008	-0.344615	0.555343
H	4.025620	1.552569	1.394797
H	3.475610	1.347258	3.055447
H	1.521367	2.728536	2.722131
H	2.890875	3.602474	2.041489
H	-0.491882	2.254865	-2.022683
H	-1.839262	2.752559	0.251440
H	-0.830483	-0.344145	-2.586488
H	-4.279755	1.474563	1.301882
H	-5.779759	-0.483294	0.969082
H	-5.205827	-2.248755	-0.648279
H	-3.113219	-2.114393	-1.988678

c fig 6

Mo	0.165641	0.710073	-0.022368
S	-0.259737	-1.829760	0.162706
S	-0.706823	0.688697	2.372154
S	2.283151	-0.056439	1.300269
O	1.289103	3.609177	0.234815
O	2.193047	0.684485	-2.422407
C	0.844140	2.548491	0.130831
C	1.421390	0.672664	-1.570176
C	-1.186498	-1.998406	1.727387
C	-0.799579	-1.077902	2.872494
C	0.743120	1.268416	3.301212
C	2.065268	0.557222	3.015712
C	2.226300	-1.877593	1.550284
C	1.366650	-2.570109	0.510564
C	-1.268727	1.711285	-1.490058
C	-1.915878	1.825442	-0.231322
C	-2.828182	0.678686	-0.084052
C	-2.489806	-0.245328	-1.104506
C	-1.372766	0.345541	-1.859956
C	-3.862074	0.414202	0.799279
C	-4.576877	-0.785467	0.642975
C	-4.246156	-1.692109	-0.360394
C	-3.185646	-1.435219	-1.244822
H	-1.122125	-3.042898	2.051800
H	-2.222449	-1.818241	1.421173
H	-1.563085	-1.146277	3.653754
H	0.154535	-1.358566	3.320359
H	0.518224	1.220084	4.371864
H	0.806491	2.326769	3.033657
H	2.891464	1.246962	3.208251
H	2.214992	-0.301252	3.674833
H	1.874189	-2.086105	2.561859
H	3.255039	-2.242963	1.477843
H	1.858779	-2.566695	-0.467531
H	1.216062	-3.618838	0.787786
H	-0.811458	2.505206	-2.065364
H	-2.028351	2.758506	0.309189
H	-0.979771	-0.072236	-2.780051
H	-4.139676	1.126625	1.570658
H	-5.411330	-0.999106	1.304135
H	-4.824191	-2.604349	-0.471212
H	-2.938347	-2.142513	-2.030712

d fig 6

Mo	0.212764	0.641828	-0.033105
S	1.887746	0.053063	-1.827585
S	-0.011435	-1.908336	0.119184
S	2.123284	0.127603	1.505801
O	-1.308128	0.837202	2.703186
O	1.458941	3.513334	-0.023926
C	-0.777866	0.802185	1.678856
C	0.958241	2.474841	-0.016278
C	1.767805	-1.755521	-2.047353
C	1.423776	-2.573816	-0.813409
C	0.529470	-2.205312	1.831689
C	1.831567	-1.531108	2.253369
C	3.593816	-0.202253	0.438650
C	3.469956	0.339769	-0.973826
C	-1.166955	1.620157	-1.517020
C	-1.890137	1.846750	-0.303902
C	-2.885675	0.767184	-0.161184
C	-2.525663	-0.240995	-1.083514
C	-1.333865	0.242346	-1.807879
C	-3.974716	0.615901	0.677373
C	-4.728105	-0.562685	0.573245
C	-4.377053	-1.556136	-0.334400
C	-3.260686	-1.410265	-1.171570
H	2.703772	-2.111712	-2.490106
H	0.994119	-1.867584	-2.813029
H	1.167967	-3.591632	-1.123779
H	2.275486	-2.642664	-0.135152
H	0.601243	-3.285326	1.996803
H	-0.310432	-1.843084	2.430022
H	1.825430	-1.382128	3.336462
H	2.704946	-2.147987	2.027006
H	3.772979	-1.279044	0.435869
H	4.450259	0.270365	0.928293
H	3.557633	1.430548	-0.984636
H	4.281372	-0.054681	-1.594820
H	-0.675268	2.363879	-2.130276
H	-1.973736	2.817903	0.171958
H	-0.956977	-0.224662	-2.712464
H	-4.253558	1.389517	1.386628
H	-5.600601	-0.696602	1.204915
H	-4.980869	-2.455737	-0.403739
H	-3.001982	-2.190014	-1.882216

ttch – cluster 1

C	0.395717	-1.534704	0.400619
C	1.130985	1.110922	0.400118
C	-1.525916	0.423767	0.403159
S	1.715591	-0.476650	-0.251280
S	-0.445601	1.723318	-0.252550
S	-1.270625	-1.246638	-0.252789
H	-1.456812	0.404405	1.496697
H	0.378724	-1.470652	1.494517
H	1.084434	1.065611	1.494113
H	-2.546768	0.707339	0.138222
H	0.660157	-2.559314	0.130334
H	1.885715	1.852214	0.128640

ttch – cluster 2

C	-0.657950	1.189377	-0.699130
C	1.752811	0.000448	-0.000081
C	-0.657101	-1.189608	0.699255
S	0.786044	1.508689	0.343661
S	0.786924	-1.508273	-0.343655
S	-1.846912	-0.000561	-0.000034
H	-1.187503	-2.136873	0.816533
H	-0.325859	0.852900	-1.684117
H	2.391869	0.142230	-0.876000
H	-0.325094	-0.852658	1.684113
H	-1.188959	2.136343	-0.816091
H	2.392093	-0.140928	0.875743

ttcn – cluster 1

C	0.125326	2.325587	0.232428
C	1.904116	0.171898	0.724096
C	1.952423	-1.272406	0.230846
C	-0.801185	-1.730902	0.726697
C	-2.077844	-1.055114	0.231223
C	-1.100505	1.560332	0.725354
S	1.462134	1.383895	-0.559345
S	0.466314	-1.957921	-0.558864
S	-1.930153	0.574167	-0.559171
H	-1.810156	2.289722	1.131997
H	0.526435	2.916076	1.064734
H	2.892534	0.421240	1.126472
H	2.263117	-1.914925	1.063341
H	-1.075962	-2.708976	1.137748
H	-2.791593	-1.004485	1.062154
H	-0.835623	0.898223	1.554809
H	-0.170555	3.038899	-0.544121
H	1.202317	0.273239	1.557239
H	2.717517	-1.373619	-0.546202
H	-0.360433	-1.165607	1.553038
H	-2.544323	-1.668405	-0.546976

ttcn – cluster 2

C	2.391767	0.584290	0.419496

C	0.528399	-1.637669	0.448654
C	-0.571916	-1.582159	-0.619152
C	-1.975058	0.470016	0.808922
C	-1.566067	1.680334	-0.023653
C	1.173471	1.463850	0.668127
S	2.154145	-1.124364	-0.201362
S	-2.231208	-1.127595	-0.016523
S	0.092787	1.676682	-0.783131
H	1.534548	2.444009	0.999414
H	2.963153	0.543227	1.353303
H	0.648680	-2.655628	0.828206
H	-0.721069	-2.572331	-1.061465
H	-2.961997	0.682190	1.237042
H	-1.674235	2.580814	0.593177
H	0.578259	1.058626	1.490040
H	3.040061	1.044995	-0.332703
H	0.293958	-1.022384	1.319818
H	-0.283785	-0.900298	-1.417715
H	-1.311778	0.340158	1.670851
H	-2.240945	1.789064	-0.878081

ttcd – cluster 1

C	-0.717411	1.932665	0.801782
C	1.932298	2.192407	0.020680
C	2.484732	0.940856	0.699666
C	2.208084	-1.861089	0.497031
C	0.717411	-1.932665	0.801782
C	-1.932298	-2.192407	0.020680
C	-2.484732	-0.940856	0.699666
C	-2.208084	1.861088	0.497031
S	0.279168	2.050978	-0.711601
S	2.776959	-0.428363	-0.466987
S	-0.279168	-2.050978	-0.711601
S	-2.776959	0.428363	-0.466987
H	-2.510405	2.725823	-0.102788
H	-0.412526	1.053630	1.381112
H	2.580564	2.484249	-0.812114
H	1.800113	0.597132	1.481179
H	2.510405	-2.725823	-0.102789
H	0.412526	-1.053630	1.381112
H	-2.580564	-2.484249	-0.812114
H	-1.800114	-0.597132	1.481179
H	-2.768668	1.913796	1.436933
H	-0.536175	2.815608	1.428352
H	1.948615	3.023296	0.737166
H	3.429113	1.198973	1.192614
H	2.768668	-1.913796	1.436932
H	0.536175	-2.815607	1.428353
H	-1.948615	-3.023296	0.737167
H	-3.429113	-1.198973	1.192614

ttcd – cluster 2

C	-1.393483	-1.960163	0.179107
C	-2.890996	0.365840	0.821989
C	-1.613719	1.183036	0.946040
C	0.341328	2.874083	-0.060877
C	1.494847	2.072090	0.532662
C	2.963347	-0.304359	0.450655
C	1.989077	-1.334613	1.015719
C	-0.205579	-1.706567	-0.741429
S	-2.877216	-1.032038	-0.344971
S	-1.102324	1.928129	-0.629915
S	2.255530	0.937449	-0.673586
S	1.325212	-2.527244	-0.189364
H	-0.009619	-0.640278	-0.877294
H	-1.166023	-1.700431	1.218653
H	-3.715171	0.997018	0.474869
H	-0.809822	0.544553	1.329124
H	0.677860	3.420392	-0.948282
H	1.152221	1.495615	1.397911
H	3.731403	-0.813009	-0.139028
H	1.156829	-0.855203	1.543364
H	-0.412846	-2.114327	-1.735270
H	-1.660032	-3.020720	0.176337
H	-3.160877	-0.003035	1.817960
H	-1.781977	1.977657	1.683873
H	0.021372	3.625253	0.671267
H	2.253590	2.775092	0.895712
H	3.477057	0.212848	1.270689
H	2.517864	-1.938255	1.762292

ttcd – cluster 3

C	1.744372	-2.521570	0.094019
C	2.183083	0.287808	0.371001
C	2.051954	1.561700	-0.454576
C	-0.463568	2.147592	0.664525
C	-1.123507	1.676902	-0.621167
C	-2.661767	-0.736448	-0.836402
C	-2.376045	-1.724015	0.289197
C	0.240093	-2.648952	-0.147589
S	2.588905	-1.127969	-0.715108
S	1.177856	2.901373	0.411965
S	-2.804990	1.011486	-0.344641
S	-0.719864	-1.635240	1.028440
H	-0.058315	-3.695632	-0.013491
H	2.237213	-3.399898	-0.335517
H	1.233347	0.053247	0.853922
H	1.553791	1.352443	-1.405739
H	-0.405251	1.323884	1.381160
H	-0.539754	0.880488	-1.089243
H	-3.635518	-0.985530	-1.274082
H	-2.538463	-2.750329	-0.063449
H	0.008299	-2.353556	-1.175502
H	1.978349	-2.530759	1.164190
H	2.946164	0.405797	1.145277
H	3.033610	1.978167	-0.700332
H	-1.055377	2.941283	1.130804
H	-1.197605	2.502726	-1.334696
H	-1.926627	-0.820320	-1.643517
H	-3.072056	-1.554529	1.115676

ttcd – cluster 4

C	-2.568040	-0.085617	1.036286
C	-1.024180	1.621558	-0.660643
C	-0.144277	2.250652	0.409431
C	2.224751	1.017249	-0.533617
C	2.472253	0.145701	0.690620
C	1.306395	-2.101183	-0.539697
C	0.057632	-2.006959	0.328848
C	-2.700720	-1.484014	0.439964
S	-2.735841	1.316998	-0.110048
S	1.545038	2.660629	-0.143961
S	2.837624	-1.598645	0.306981
S	-1.420932	-2.013199	-0.737508
H	-3.632883	-1.555896	-0.128329
H	-1.643477	0.020965	1.612073
H	-0.618200	0.682024	-1.043038
H	-0.093859	1.623354	1.305473
H	1.561540	0.527729	-1.250742
H	1.631524	0.192319	1.389227
H	1.183810	-1.511768	-1.453937
H	0.063589	-1.069257	0.891273
H	-2.759570	-2.216749	1.254461
H	-3.381324	0.048464	1.758594
H	-1.123079	2.303197	-1.510846
H	-0.566179	3.209187	0.725678
H	3.164082	1.208517	-1.059899
H	3.347065	0.503030	1.241171
H	1.483842	-3.132995	-0.856031
H	0.025998	-2.828967	1.050308

ttcd – cluster 5

C	2.734369	-1.086726	-0.439251
C	0.463423	-2.355477	0.795799
C	-0.687323	-1.472053	1.251263
C	-2.116033	-0.474296	-1.035736
C	-2.621221	0.930943	-0.731416
C	-0.190210	2.305376	-0.707567
C	1.066397	2.630813	0.090347
C	2.684144	0.433420	-0.541848
S	1.193198	-1.973148	-0.836975
S	-2.244118	-1.674807	0.325960
S	-1.589906	1.922557	0.391036
S	1.861250	1.204332	0.888657
H	2.148906	0.718016	-1.452983
H	3.085087	-1.407923	0.547438
H	0.135328	-3.397085	0.731471
H	-0.406639	-0.417050	1.261327
H	-1.087022	-0.474028	-1.404975
H	-3.599601	0.882710	-0.244469
H	-0.006513	1.447200	-1.363159
H	0.840033	3.330773	0.901260
H	3.706459	0.822248	-0.616695
H	3.468511	-1.455194	-1.163947
H	1.273252	-2.311859	1.533266
H	-0.947560	-1.750657	2.279389
H	-2.735648	-0.899792	-1.833907

H	-2.752879	1.488491	-1.667352
H	-0.449629	3.162128	-1.340733
H	1.799835	3.127069	-0.554334