1. Binding energies for the mononuclear and binuclear rhenium complexes complexes at the HF, DFT(B3LYP), DFT(BP86), RIMP2 and SOS-MP2 levels of theory

Calculations were performed using QCHEM (1,2). All optimizations were performed first at the HF level, followed by a higher-level (DFT(B3LYP), DFT(BP86), RIMP2, or SOS-MP2) optimization. The 6-31G* basis set (3) was used for all non-metal atoms and the LANL2DZ basis set and effective core potential (ECP) (4) were used for rhenium and manganese. In addition, the RIMP2-VDZ auxiliary basis set (5) was used on all atoms in the RIMP2 and SOS-MP2 calculations. Each transition metal complex-alkane interaction energy was found by optimizing three structures—the entire alkane-transition metal complex, the transition-metal complex alone, and the alkane alone—and then subtracting the latter two energies from the first. Favorable (negative) interaction energies were then reported as positive binding energies. The standard counterpoise method (6) was then used to correct the binding energies for basis set superposition error (BSSE) (Figure 8, Figure 10). However, the BSSE-uncorrected binding energies are also reported (Figure 9, Figure 11), since some experts recommend that the BSSE correction not be performed (7). Frequency calculations were performed on the HF-, DFT(B3LYP)-, and DFT(BP86)-optimized structures to ensure that they represented true minima; all structures calculated at the HF, BP86, and B3LYP levels had zero imaginary frequencies, or one imaginary frequency smaller than 36 cm^{-1} in magnitude. Frequency analyses are still in progress for the RIMP2 and SOS-MP2 structures. The binding energies reported here, unlike in the manuscript, were NOT corrected for zero-point vibrational frequencies (Figures 8-11).

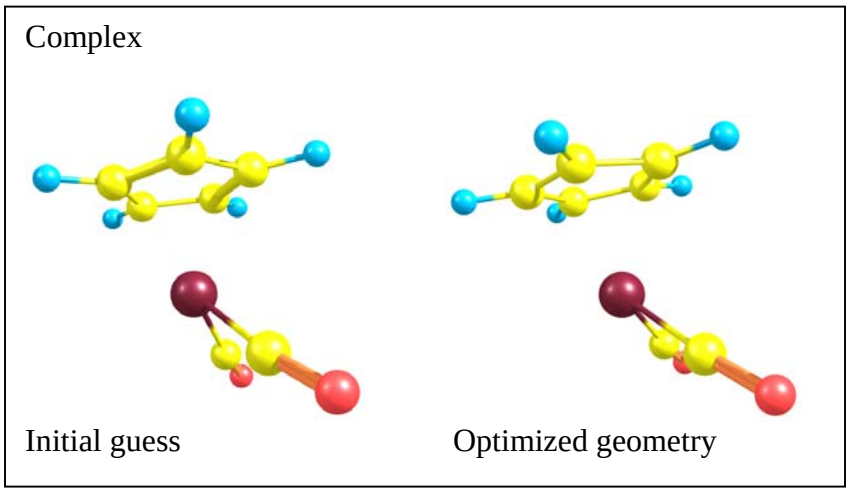
4. Snapshots and Cartesian coordinates of the optimized ([CpM(CO)$_2$](alkane)) and ([(CO)$_2$M(C$_5$H$_4$)C≡C(C$_5$H$_4$)M(CO)$_2$](alkane)) complexes (M = Mn or Re), at the DFT(B3LYP), DFT(BP86), and RIMP2 levels of theory.

4-1. Mononuclear rhenium complexes.

4-1a. Mononuclear Re, HF.

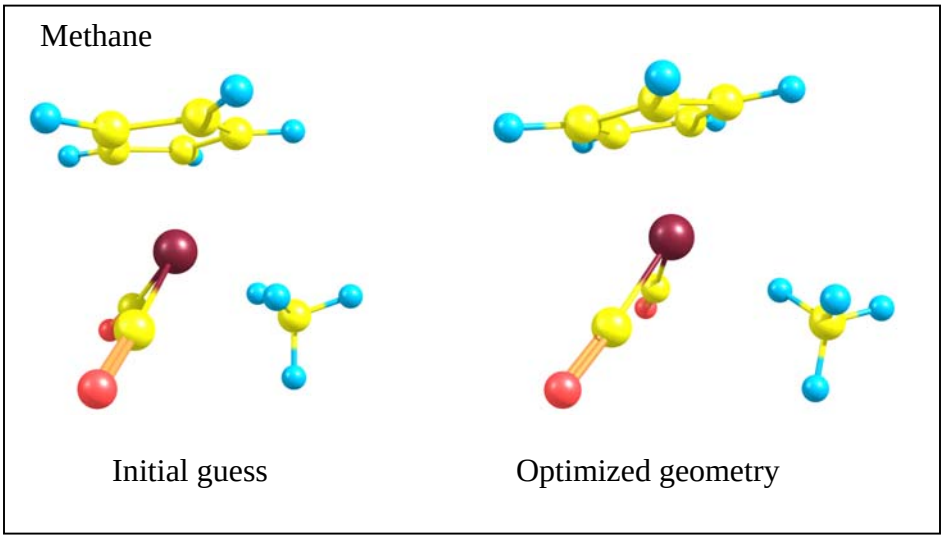
Complex only, optimized geometry:

C	3.605438	-0.860965	0.678797
C	3.923427	0.055197	-0.347927
C	3.300992	-0.395904	-1.555264
C	2.605470	-1.584618	-1.247764
C	2.782132	-1.889067	0.119236
H	3.965763	-0.821360	1.685977
H	4.566048	0.905662	-0.250418
H	3.395642	0.050637	-2.523123
H	2.023281	-2.159523	-1.941038
H	2.420456	-2.759001	0.626671
Re	1.676173	0.181311	0.039971
C	0.947931	0.278558	1.842373
O	0.610953	0.295916	2.922508
C	1.576885	2.107122	-0.225582
O	1.619230	3.225745	-0.391115



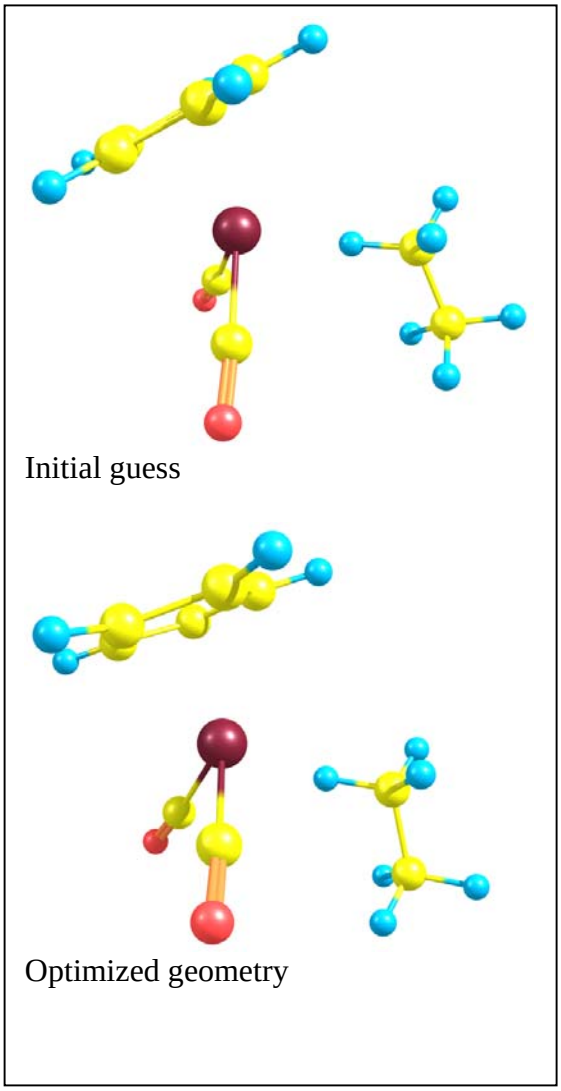
Methane, optimized geometry:

C	-1.955386	-1.176135	-0.320171
C	-1.640664	-0.438016	-1.505323
C	-1.719566	0.937634	-1.197992
C	-2.079131	1.067756	0.179623
C	-2.218628	-0.238445	0.699414
H	-2.033950	-2.240394	-0.238467
H	-1.439903	-0.853274	-2.471237
H	-1.583951	1.742124	-1.891116
H	-2.271755	1.981705	0.701831
H	-2.472385	-0.478357	1.713255
Re	0.033208	0.049106	-0.014932
C	1.190729	1.585549	-0.278207
O	1.799770	2.516603	-0.491587
C	1.334142	-1.167344	-0.790703
O	2.033425	-1.897872	-1.300627
C	1.148027	-0.762557	2.573603
H	2.211602	-0.900743	2.444765
H	0.930759	-0.442362	3.584975
H	0.823405	0.086395	1.942725
H	0.621769	-1.679371	2.359414



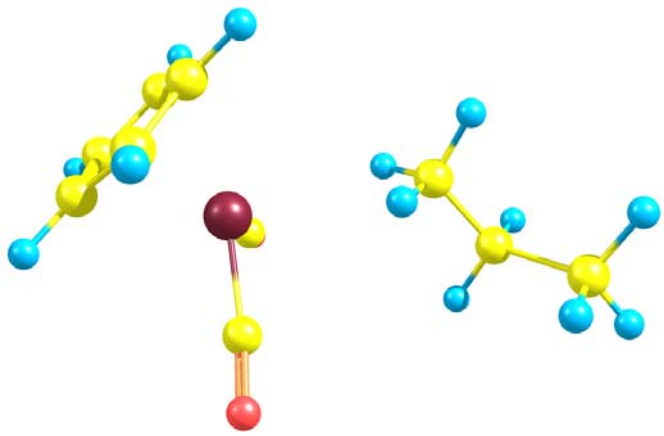
Ethane:

C	1.764567	-1.452154	0.803071
C	2.213127	-0.100680	0.946651
C	2.337273	0.458288	-0.343689
C	1.964167	-0.536755	-1.299876
C	1.616009	-1.699662	-0.576941
H	1.623902	-2.160524	1.592952
H	2.467754	0.384173	1.866377
H	2.697522	1.441341	-0.567122
H	2.004219	-0.440363	-2.364851
H	1.279838	-2.621507	-1.009269
Re	0.112125	0.040624	0.033903
C	-0.496311	1.677513	-0.812403
O	-0.761560	2.657634	-1.315124
C	-0.779830	0.477019	1.701452
O	-1.222088	0.730507	2.713349
C	-2.244637	-1.596279	-0.657008
H	-1.529257	-0.791782	-0.928725
H	-1.961278	-2.088524	0.261181
H	-2.153317	-2.310082	-1.467623
C	-3.646518	-1.001162	-0.575540
H	-4.380759	-1.783755	-0.414268
H	-3.725451	-0.294950	0.242944
H	-3.905821	-0.483104	-1.492297

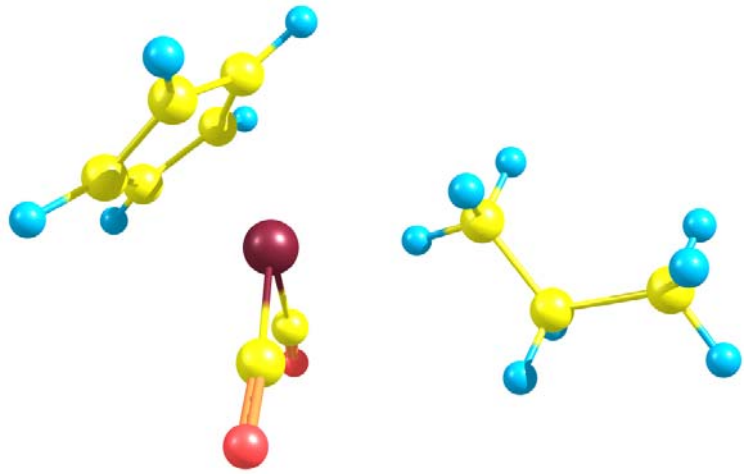


Propane:

C	-1.940721	-1.785645	-0.151116
C	-2.672195	-0.675603	-0.679270
C	-2.866171	0.257910	0.361507
C	-2.257931	-0.263550	1.546616
C	-1.696208	-1.514066	1.212264
H	-1.156820	-2.151260	1.885132
H	-1.683792	-2.682771	-0.675097
H	-3.054116	-0.590222	-1.675668
H	-3.420453	1.170792	0.288150
H	-2.277373	0.183246	2.518825
Re	-0.617259	0.161521	-0.089888
C	-0.324425	2.062522	0.164557
O	-0.248134	3.181636	0.324825
C	0.075485	0.212893	-1.901532
O	0.402752	0.215497	-2.986400
C	2.031729	-0.760636	0.792720
C	3.310239	-0.110487	0.268339
C	4.497840	-1.072033	0.298221
H	2.141718	-1.099254	1.817457
H	1.735110	-1.605368	0.187681
H	1.233159	0.008970	0.849230
H	3.146876	0.236042	-0.747287
H	3.537160	0.769210	0.863647
H	4.704088	-1.411148	1.309449
H	5.394969	-0.592929	-0.079782
H	4.307853	-1.949139	-0.313800



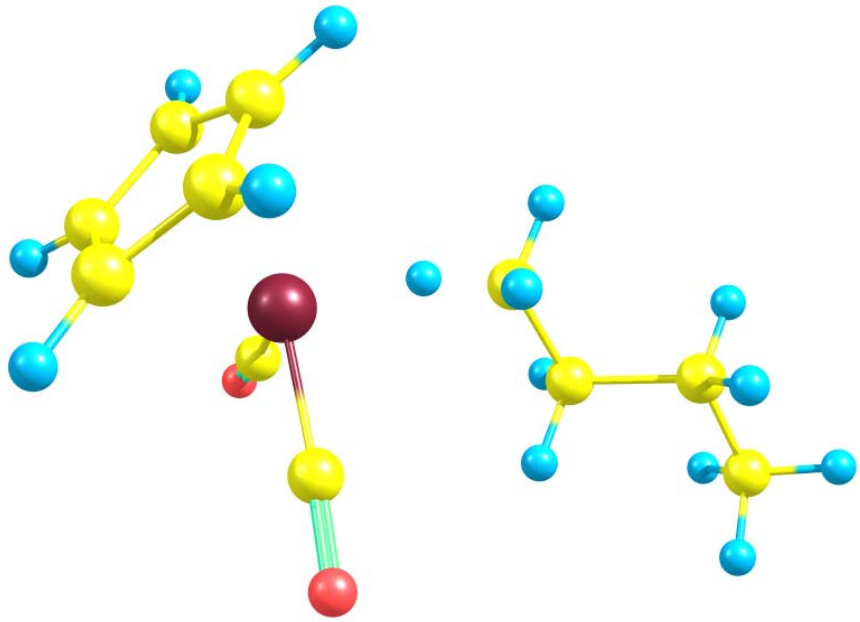
Initial guess



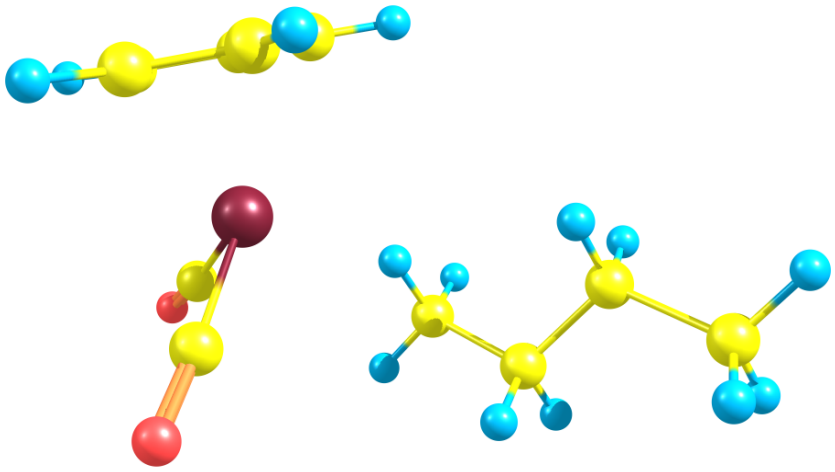
Optimized geometry

Butane:

C	-1.639343	-1.599299	1.292517
C	-2.536708	-1.133447	0.280221
C	-1.981673	-1.452320	-0.978069
C	-0.734314	-2.116438	-0.759926
C	-0.542279	-2.195904	0.637000
H	-1.798248	-1.555474	2.349919
H	-3.490257	-0.676148	0.446133
H	-2.442367	-1.275030	-1.927997
H	-0.097235	-2.532806	-1.512232
H	0.309120	-2.630315	1.122760
Re	-0.623244	0.102660	0.018482
C	-0.250799	1.070176	-1.622125
O	-0.089042	1.578986	-2.621584
C	-1.316992	1.685535	0.904221
O	-1.796684	2.566761	1.430118
C	2.058025	0.942791	1.067572
H	2.164158	0.698115	2.117781
H	1.662754	1.944349	0.986036
H	1.338059	0.201617	0.661557
C	3.370639	0.786135	0.303742
H	4.092020	1.490772	0.711773
H	3.217252	1.068094	-0.734352
C	3.945001	-0.629062	0.371812
H	3.219881	-1.329077	-0.038133
H	4.088882	-0.909499	1.413307
C	5.267463	-0.770356	-0.380423
H	5.648667	-1.784577	-0.316592
H	5.147515	-0.527124	-1.432124
H	6.023806	-0.106368	0.028173



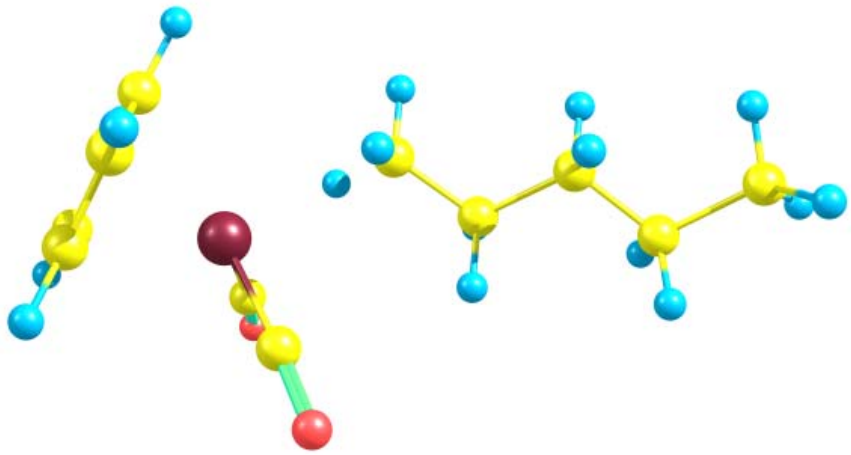
Initial guess



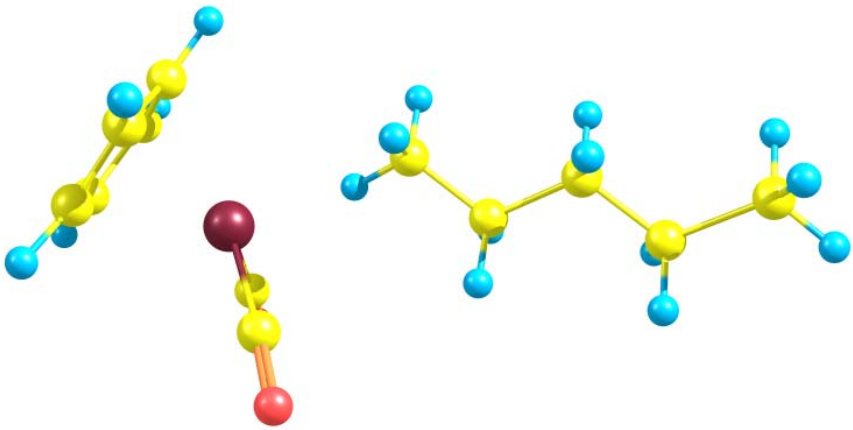
Optimized geometry

Pentane:

C	-1.938592	-1.796114	-0.176938
C	-2.692667	-0.690794	-0.683350
C	-2.896468	0.222318	0.373618
C	-2.270904	-0.306096	1.546248
C	-1.689280	-1.541432	1.188353
H	-1.134030	-2.179318	1.847529
H	-1.668539	-2.679855	-0.716859
H	-3.083667	-0.597157	-1.675451
H	-3.467215	1.126298	0.318093
H	-2.292541	0.124522	2.525667
Re	-0.649548	0.173885	-0.093853
C	-0.395690	2.078432	0.174198
O	-0.341707	3.197638	0.342843
C	0.038007	0.253077	-1.906477
O	0.362806	0.269659	-2.991979
C	2.011089	-0.709704	0.781422
C	3.282859	-0.073179	0.225022
C	4.476280	-1.029757	0.263770
H	2.132050	-1.021023	1.813427
H	1.707224	-1.569789	0.202262
H	1.213466	0.061751	0.826691
H	3.106220	0.247074	-0.797814
H	3.515518	0.823028	0.794360
H	4.648548	-1.350786	1.289909
H	4.235433	-1.928826	-0.301269
C	5.759527	-0.411657	-0.294154
H	6.000583	0.486708	0.269844
H	5.587862	-0.091817	-1.319390
C	6.948710	-1.370578	-0.253785
H	7.842663	-0.904247	-0.655720
H	7.167241	-1.682281	0.763739
H	6.751290	-2.265023	-0.837825



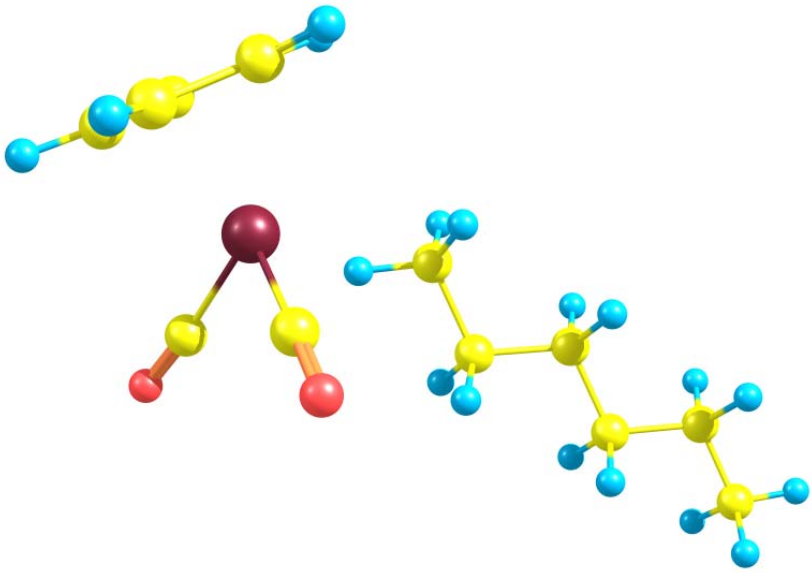
Initial guess



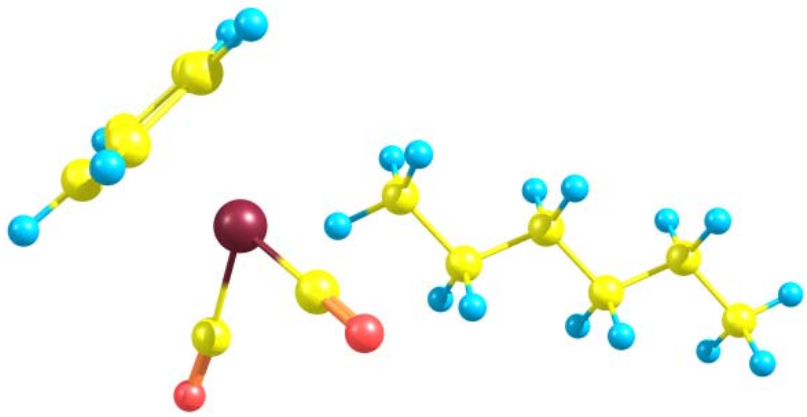
Optimized geometry

Hexane:

C	-2.983478	-1.052347	1.236409
C	-3.596846	-0.196987	0.267498
C	-3.255208	-0.672340	-1.016908
C	-2.425083	-1.826272	-0.858584
C	-2.269831	-2.041910	0.527932
H	-3.093607	-0.988594	2.298956
H	-4.247918	0.626414	0.477388
H	-3.602392	-0.269347	-1.945913
H	-2.046698	-2.447780	-1.643414
H	-1.689918	-2.826318	0.973026
Re	-1.334859	0.080326	-0.009013
C	-1.266927	1.777480	0.928876
O	-1.322405	2.764082	1.483386
C	-0.582066	0.848333	-1.624317
O	-0.214804	1.274383	-2.608006
C	1.366373	-0.850462	0.682550
H	1.464650	-1.526902	1.524708
H	0.488983	-0.221639	0.943519
H	1.189710	-1.439431	-0.205879
C	2.588521	0.052658	0.530590
H	2.690177	0.672174	1.417892
H	2.432283	0.730458	-0.303772
C	3.876721	-0.743088	0.310341
H	4.026437	-1.424969	1.145860
H	3.767498	-1.365287	-0.576383
C	5.111274	0.146730	0.155639
H	5.219256	0.769304	1.042134
H	4.960473	0.828797	-0.679096
C	6.402038	-0.643756	-0.065550
H	6.554054	-1.325817	0.768344
H	6.296172	-1.264838	-0.952432
C	7.630886	0.251770	-0.218006
H	8.529478	-0.337120	-0.373546
H	7.523940	0.922759	-1.065538
H	7.783861	0.861389	0.668044



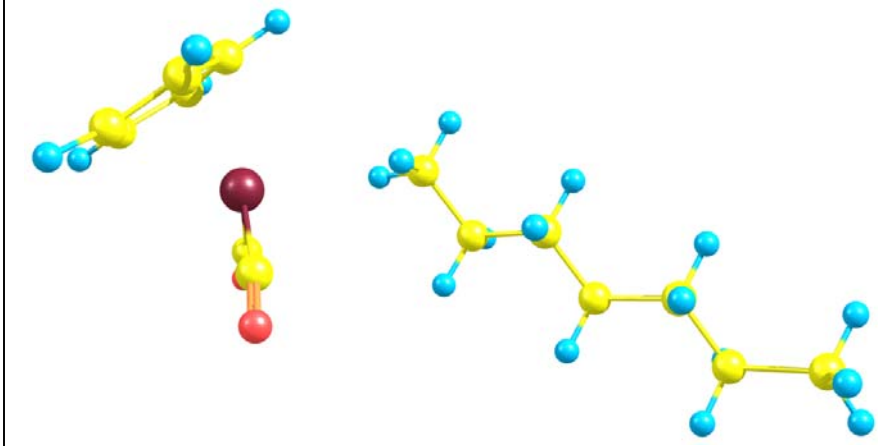
Initial guess



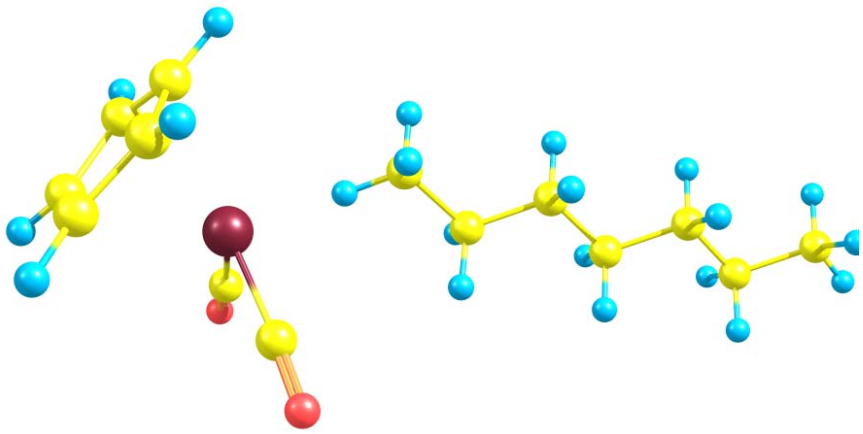
Optimized geometry

Heptane:

C	-4.690601	-0.126727	0.257823
C	-4.318609	-0.947366	-0.828711
C	-3.460871	-1.979585	-0.334290
C	-3.319814	-1.775091	1.055497
C	-4.068799	-0.642586	1.438463
H	-4.195223	-0.273382	2.434918
H	-2.725845	-2.377306	1.714474
H	-3.055469	-2.792531	-0.900119
H	-4.662641	-0.844233	-1.837174
H	-5.365503	0.703002	0.213224
Re	-2.432620	0.123108	-0.074694
C	-2.420312	2.021095	0.327614
O	-2.508412	3.124564	0.569577
C	-1.679182	0.410304	-1.839350
O	-1.310344	0.543065	-2.902594
C	0.271434	-0.503680	0.889347
C	1.484645	0.313382	0.450427
C	2.781806	-0.496030	0.509229
C	4.008464	0.303828	0.066865
C	5.307448	-0.501555	0.129573
C	6.535533	0.295203	-0.314466
C	7.829554	-0.515085	-0.246697
H	-0.614357	0.164692	0.933146
H	0.103778	-1.351881	0.241384
H	0.374639	-0.867858	1.905845
H	1.574649	1.192373	1.083426
H	1.326563	0.675505	-0.561429
H	2.682495	-1.379976	-0.118558
H	2.934474	-0.857921	1.524688
H	4.103881	1.189982	0.691835
H	3.855474	0.662534	-0.949255
H	5.211567	-1.389098	-0.493806
H	5.460842	-0.859340	1.146506
H	6.632793	1.182743	0.307149
H	6.385266	0.650611	-1.331589
H	8.681450	0.076181	-0.567942
H	8.026481	-0.855616	0.766024
H	7.776648	-1.392626	-0.884971



Initial guess

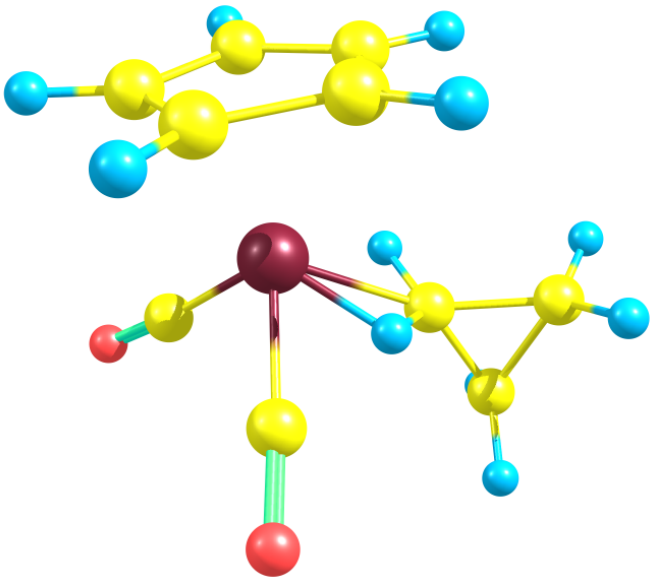


Optimized geometry

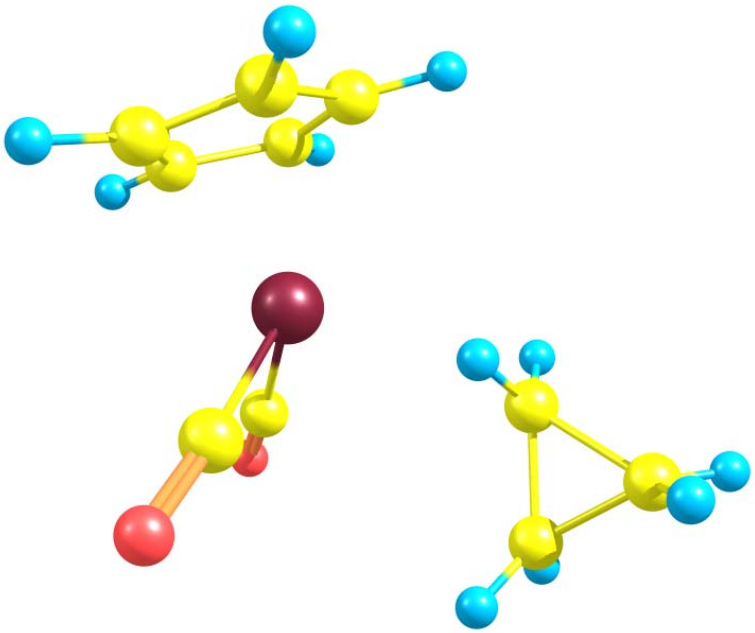
Cyclopropane:

C	-1.296421	-0.097736	-1.703984
C	-2.147881	0.615769	-0.832746
C	-2.344712	-0.178369	0.341954
C	-1.603297	-1.364932	0.175468
C	-0.950150	-1.334787	-1.078229
H	-1.000847	0.215326	-2.684188
H	-2.614801	1.555639	-1.043428
H	-2.979975	0.061105	1.169399
H	-1.534991	-2.160127	0.891548
H	-0.364394	-2.121101	-1.506755
Re	-0.085901	0.469055	0.161331
C	1.518394	0.924353	-0.825573
O	2.411174	1.178319	-1.476451
C	-0.151408	2.216517	1.010693
O	-0.263236	3.244727	1.471281
C	1.318164	-0.331701	2.542384
C	2.452202	0.578491	2.893897
C	2.601815	-0.892742	3.090505
H	0.448917	-0.348015	3.169654
H	2.999776	1.039834	2.092488
H	2.330992	1.202167	3.761394
H	3.243975	-1.431305	2.417060
H	2.581567	-1.283349	4.092267
H	1.155234	-0.602228	1.490174

Initial guess

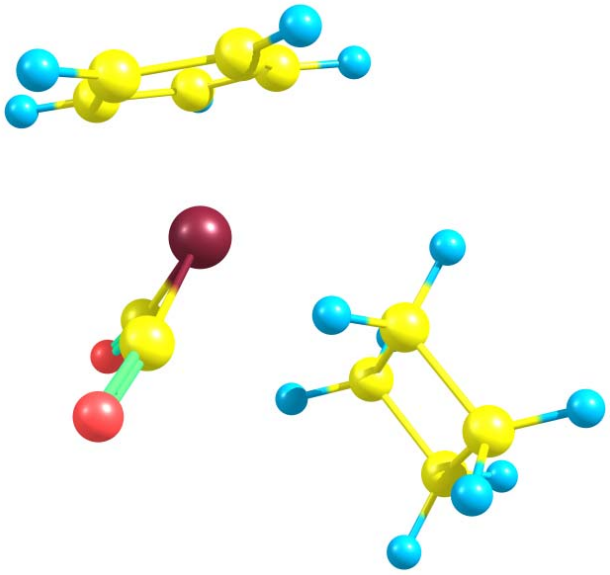


Optimized geometry

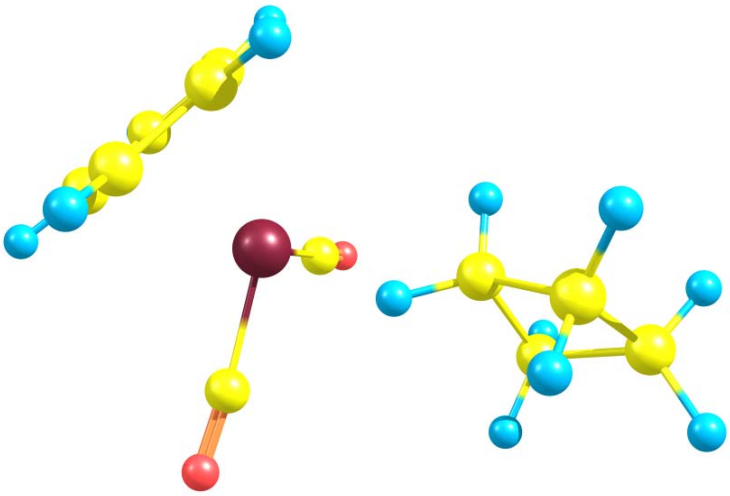


Cyclobutane:

C	-0.944192	0.328630	-1.698462
C	-2.021271	0.490684	-0.800522
C	-2.214775	-0.748973	-0.112038
C	-1.246945	-1.652468	-0.595955
C	-0.455220	-1.008555	-1.573492
H	-0.588981	1.066141	-2.388424
H	-2.624816	1.368831	-0.698280
H	-2.986667	-0.966199	0.596860
H	-1.122567	-2.664929	-0.265639
H	0.320767	-1.457874	-2.157461
Re	-0.114010	0.168219	0.437196
C	1.503542	1.168490	0.053837
O	2.414853	1.768337	-0.252988
C	-0.613314	1.379604	1.869320
O	-0.976546	2.103274	2.661892
C	2.338587	-2.284626	4.052697
C	1.907575	-0.858525	3.639891
C	1.038835	-1.492097	2.537934
C	1.860999	-2.792947	2.672747
H	3.381072	-2.437077	4.304342
H	2.732779	-0.292179	3.224004
H	1.402922	-0.247015	4.377437
H	1.126457	-1.036944	1.528123
H	0.010580	-1.622098	2.837227
H	2.672081	-2.832940	1.954827
H	1.317887	-3.729740	2.638044
H	1.726937	-2.673755	4.859100



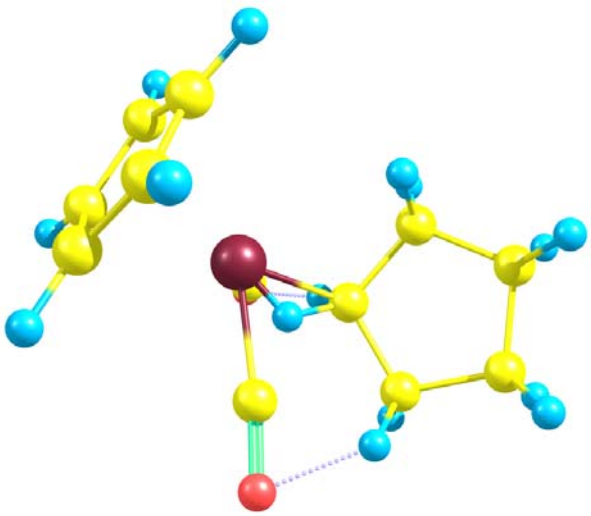
Initial guess



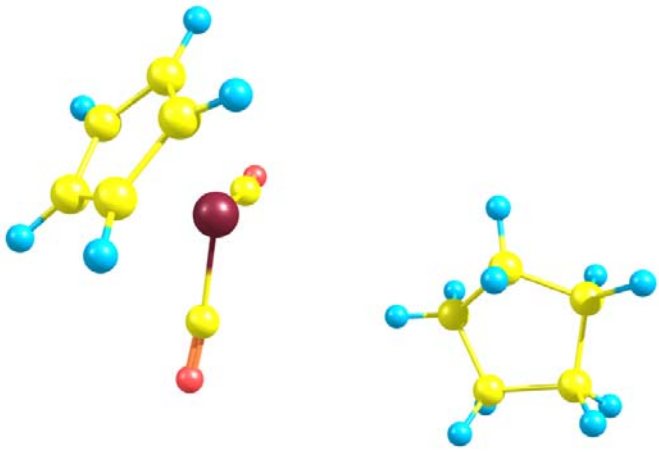
Optimized geometry

Cyclopentane:

C	-1.723569	0.265457	-2.453903
C	-2.747220	0.688201	-1.577373
C	-3.025144	-0.384247	-0.670241
C	-2.161084	-1.447809	-1.002259
C	-1.353572	-1.069554	-2.097951
H	-1.331342	0.829276	-3.274936
H	-3.265327	1.623649	-1.624838
H	-3.785767	-0.397324	0.082465
H	-2.115419	-2.391117	-0.494244
H	-0.646313	-1.689869	-2.607776
Re	-0.839012	0.417425	-0.353531
C	0.857068	1.159463	-0.954679
O	1.804302	1.594334	-1.395679
C	-1.194979	1.918077	0.833858
O	-1.485013	2.809946	1.467062
C	3.841174	-1.873437	4.123431
C	2.433237	-2.143873	4.680734
C	1.502947	-1.591949	3.597221
C	2.193461	-0.286621	3.183841
C	3.705671	-0.602043	3.243987
H	4.162643	-2.714247	3.516337
H	2.262061	-3.192205	4.901607
H	2.281232	-1.589995	5.604112
H	1.469045	-2.282216	2.756162
H	0.483873	-1.444635	3.940933
H	1.944509	0.493253	3.897977
H	1.884176	0.070281	2.206357
H	4.263617	0.232706	3.653400
H	4.101012	-0.782242	2.249950
H	4.578208	-1.754519	4.909816



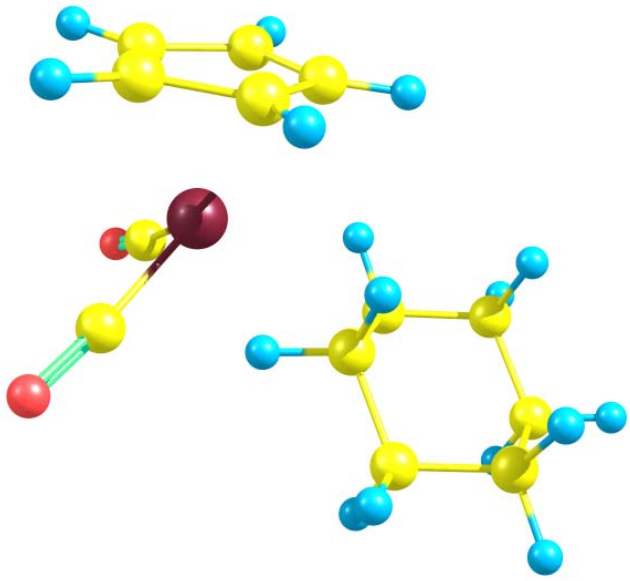
Initial guess



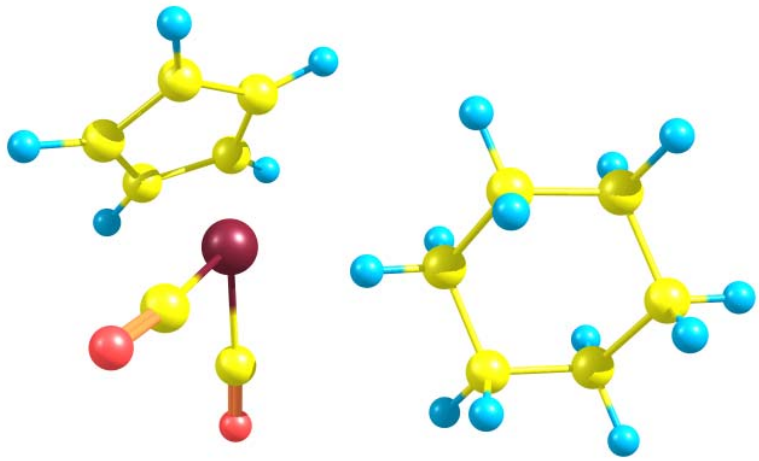
Optimized geometry

Cyclohexane:

C	0.674863	0.755414	-2.187590
C	-0.580807	0.735163	-1.543295
C	-0.889621	-0.622035	-1.213283
C	0.187156	-1.416296	-1.661374
C	1.158365	-0.588508	-2.264034
H	1.154457	1.620817	-2.596330
H	-1.214773	1.582342	-1.381121
H	-1.795861	-0.975561	-0.766973
H	0.261330	-2.480241	-1.551444
H	2.058943	-0.912377	-2.742866
Re	1.008036	0.095757	-0.013614
C	2.670382	1.072130	0.194801
O	3.628258	1.676706	0.231250
C	0.184161	1.010723	1.485050
O	-0.357596	1.572903	2.306495
C	2.608158	-3.287932	1.303651
C	2.408668	-4.563779	2.128564
C	2.556754	-4.290519	3.628344
C	1.611835	-3.176722	4.089173
C	1.807583	-1.896070	3.270520
C	1.661785	-2.179932	1.773711
H	3.635666	-2.946296	1.407610
H	1.416365	-4.967443	1.932761
H	3.119784	-5.321495	1.812195
H	2.367207	-5.198775	4.193351
H	3.584478	-4.000568	3.840417
H	0.581423	-3.513783	3.987456
H	1.765878	-2.965526	5.143292
H	2.799207	-1.491602	3.461837
H	1.094406	-1.139192	3.579449
H	0.636878	-2.446479	1.547184
H	1.946326	-1.258164	1.220084
H	2.451841	-3.491152	0.248588



Initial guess

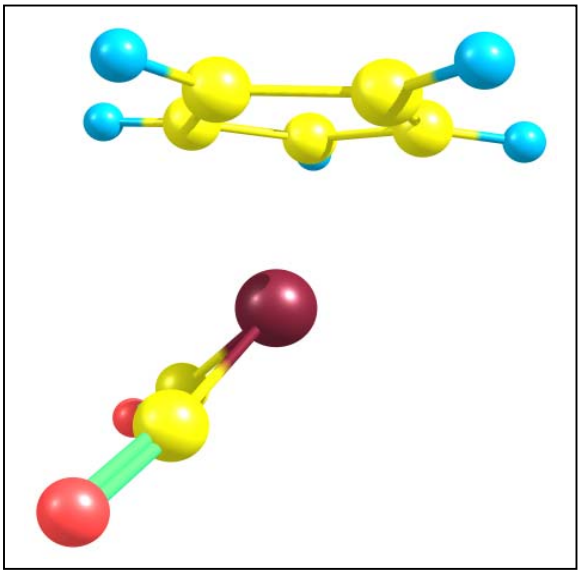


Optimized geometry

4-1b. Mononuclear Re, DFT(B3LYP).

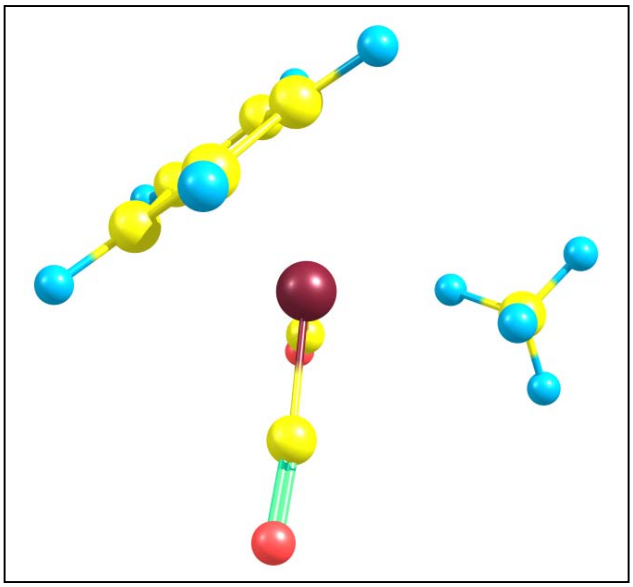
Complex:

C	3.545177	-0.922036	0.714706
C	3.874920	0.076494	-0.267969
C	3.329393	-0.360196	-1.532427
C	2.628290	-1.567854	-1.298451
C	2.770469	-1.944863	0.075168
H	3.860299	-0.916213	1.749294
H	4.501083	0.942098	-0.104083
H	3.416554	0.155919	-2.478296
H	2.057162	-2.111465	-2.041349
H	2.390725	-2.845675	0.535963
Re	1.680782	0.127930	0.066840
C	1.096397	0.371261	1.865996
O	0.849101	0.492911	3.000042
C	1.501764	1.995185	-0.305573
O	1.517706	3.136216	-0.546557



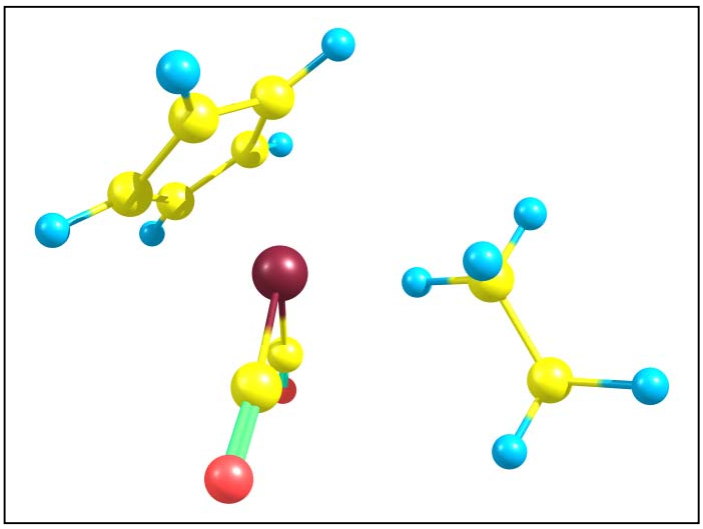
Methane:

C	-1.956586	-1.204733	-0.342735
C	-1.583204	-0.404854	-1.483201
C	-1.668079	0.973678	-1.098084
C	-2.077372	1.032334	0.277645
C	-2.227193	-0.315445	0.728916
H	-2.025916	-2.283304	-0.313674
H	-1.363068	-0.774531	-2.475258
H	-1.503924	1.821926	-1.748702
H	-2.261940	1.926335	0.856278
H	-2.490179	-0.609683	1.738099
Re	0.029314	0.011358	0.030413
C	1.215934	1.459095	-0.323029
O	1.871713	2.382762	-0.607494
C	1.281481	-1.216226	-0.718300
O	1.978226	-1.990180	-1.246009
C	1.096396	-0.655456	2.474104
H	2.184561	-0.725517	2.480208
H	0.713057	-0.389905	3.462551
H	0.835011	0.255794	1.851355
H	0.663283	-1.601447	2.156160



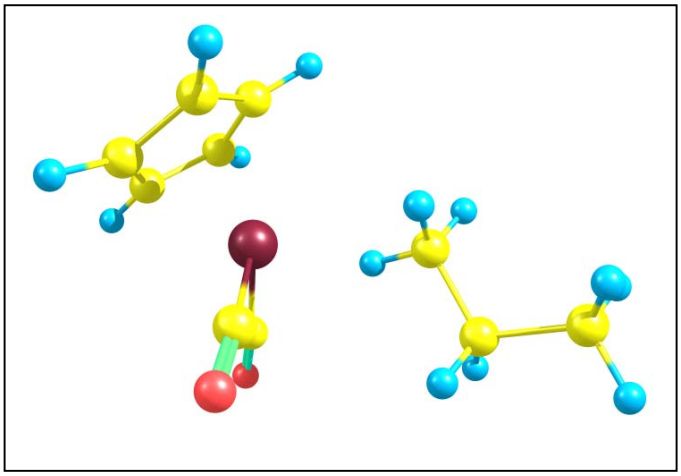
Ethane:

C	1.775377	-1.451113	0.831477
C	2.159648	-0.063884	0.919634
C	2.240524	0.453051	-0.415766
C	1.899847	-0.602146	-1.328882
C	1.595299	-1.755606	-0.542399
H	1.646396	-2.132741	1.660873
H	2.416131	0.470411	1.823758
H	2.548212	1.453998	-0.686468
H	1.893553	-0.541142	-2.407748
H	1.267345	-2.710675	-0.934153
Re	0.081490	-0.018625	0.042859
C	-0.533399	1.623348	-0.699642
O	-0.806471	2.657368	-1.169639
C	-0.799931	0.359423	1.689722
O	-1.257457	0.582975	2.741017
C	-2.154332	-1.529026	-0.650446
H	-1.452090	-0.702543	-1.004973
H	-1.870268	-1.980000	0.300236
H	-2.033552	-2.284019	-1.434602
C	-3.564412	-0.940841	-0.608518
H	-4.301774	-1.732233	-0.432200
H	-3.659030	-0.204259	0.195046
H	-3.817430	-0.445903	-1.552042



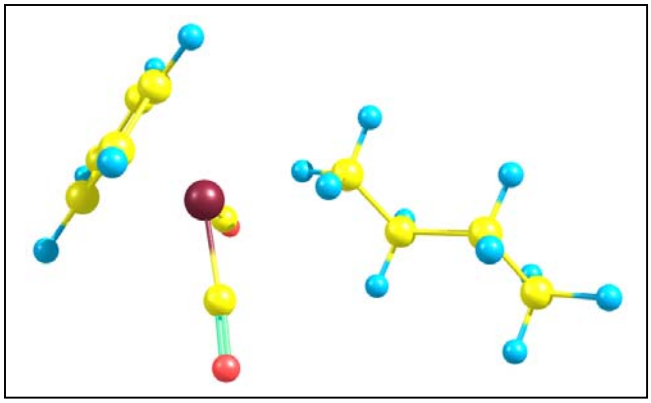
Propane:

C	-1.874858	-1.818281	-0.139196
C	-2.538488	-0.680395	-0.719872
C	-2.776850	0.273259	0.323196
C	-2.263871	-0.272909	1.553250
C	-1.694065	-1.539613	1.245795
H	-1.191624	-2.186521	1.955418
H	-1.586186	-2.724910	-0.652267
H	-2.857841	-0.585848	-1.748570
H	-3.308330	1.208584	0.215369
H	-2.311139	0.190618	2.528680
Re	-0.553423	0.125995	-0.017783
C	-0.269610	1.993927	0.222593
O	-0.193776	3.148888	0.379625
C	0.203428	0.221562	-1.762248
O	0.601293	0.252907	-2.860395
C	1.942374	-0.746300	0.805566
C	3.192126	-0.104221	0.196203
C	4.396230	-1.050989	0.231395
H	2.111944	-1.108225	1.826687
H	1.586978	-1.584692	0.205521
H	1.160544	0.065395	0.984930
H	2.977613	0.184961	-0.838988
H	3.428234	0.821412	0.736161
H	4.671828	-1.309300	1.261222
H	5.270331	-0.592725	-0.243590
H	4.180519	-1.986449	-0.299920

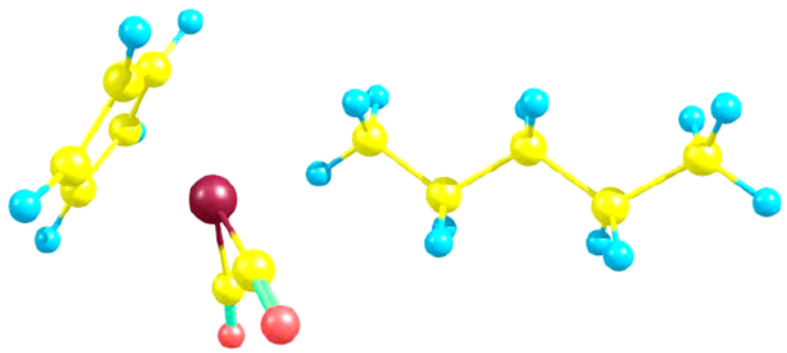


Butane:

C	-1.879376	-1.823389	-0.118818
C	-2.544606	-0.692704	-0.711234
C	-2.781552	0.273010	0.321130
C	-2.266416	-0.259189	1.556555
C	-1.696285	-1.528805	1.262601
H	-1.192135	-2.167228	1.978665
H	-1.590554	-2.735362	-0.622225
H	-2.866169	-0.610895	-1.740353
H	-3.314609	1.206326	0.203911
H	-2.313018	0.214783	2.527007
Re	-0.558665	0.122259	-0.021809
C	-0.269762	1.991537	0.201926
O	-0.189886	3.147426	0.350150
C	0.193480	0.200099	-1.768990
O	0.589407	0.218431	-2.868205
C	1.937682	-0.746434	0.797776
C	3.186521	-0.098787	0.194315
C	4.395084	-1.044305	0.195913
H	2.105865	-1.116341	1.816180
H	1.581788	-1.579656	0.191052
H	1.156487	0.064993	0.982250
H	2.969333	0.213902	-0.834386
H	3.433150	0.815290	0.751203
H	4.613218	-1.357094	1.226986
H	4.139948	-1.961291	-0.354354
C	5.643686	-0.405939	-0.421777
H	5.938307	0.495441	0.128805
H	6.492734	-1.098624	-0.409307
H	5.463811	-0.114828	-1.463680



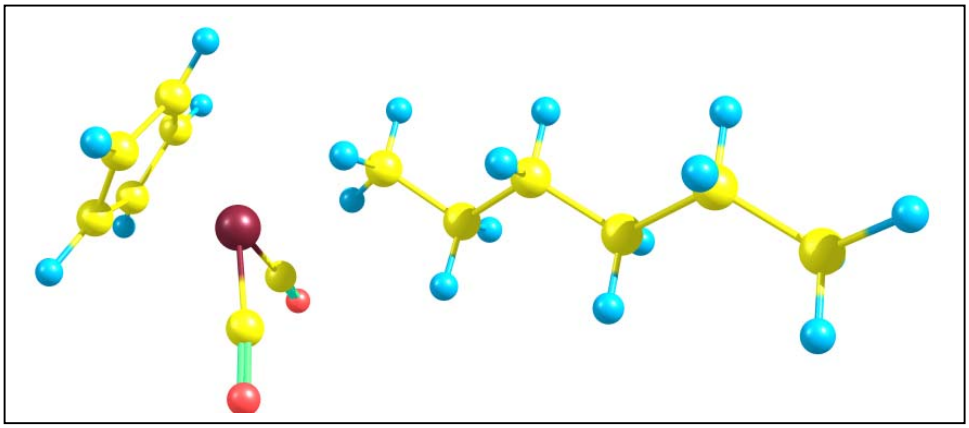
Pentane:



C	-1.869114	-1.819592	-0.177335
C	-2.526283	-0.676591	-0.755281
C	-2.783149	0.264587	0.294609
C	-2.288650	-0.294686	1.526541
C	-1.711694	-1.556673	1.213861
H	-1.219614	-2.210845	1.924027
H	-1.570739	-2.720012	-0.695812
H	-2.826623	-0.569046	-1.788357
H	-3.313657	1.200652	0.188783
H	-2.350047	0.159293	2.505578
Re	-0.554986	0.126325	-0.012375
C	-0.282119	1.992033	0.256111
O	-0.214290	3.145532	0.427046
C	0.228583	0.248603	-1.743048
O	0.645853	0.297129	-2.833435
C	1.932698	-0.750469	0.827074
C	3.179073	-0.098007	0.223613
C	4.401048	-1.024867	0.261124
H	2.099963	-1.112878	1.848371
H	1.582428	-1.589245	0.224790
H	1.144604	0.055503	1.007518
H	2.968835	0.188557	-0.813899
H	3.404981	0.831897	0.762588
H	4.624049	-1.297641	1.303523
H	4.164001	-1.966361	-0.256443
C	5.648036	-0.399197	-0.378445
H	5.867848	0.554780	0.120548
H	5.428314	-0.151381	-1.426315
C	6.876412	-1.311354	-0.311908
H	7.741257	-0.856524	-0.807497
H	7.159022	-1.520562	0.727225
H	6.680490	-2.274006	-0.800648

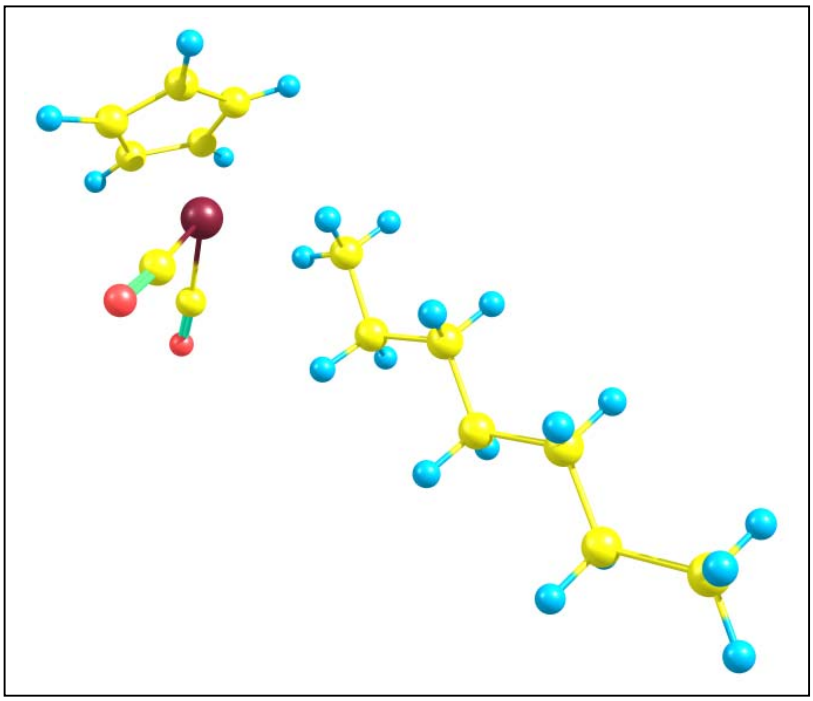
Hexane:

C	-2.843918	-1.228954	1.196240
C	-3.488026	-0.347960	0.258047
C	-3.081532	-0.726938	-1.062644
C	-2.184796	-1.847942	-0.945533
C	-2.032159	-2.123857	0.441283
H	-2.972553	-1.226461	2.269464
H	-4.202696	0.426700	0.499962
H	-3.442718	-0.290625	-1.983121
H	-1.715977	-2.379221	-1.762040
H	-1.383459	-2.884127	0.860209
Re	-1.290279	0.099690	0.030904
C	-1.423561	1.761959	0.949673
O	-1.609205	2.768137	1.513952
C	-0.564527	0.973950	-1.498972
O	-0.191848	1.479185	-2.484199
C	1.270247	-0.608500	0.788115
H	1.335765	-1.219955	1.694649
H	0.430054	0.121491	1.028160
H	1.069570	-1.270747	-0.055215
C	2.535282	0.221418	0.550799
H	2.693681	0.902206	1.397675
H	2.392794	0.853329	-0.334384
C	3.774105	-0.664425	0.360540
H	3.898778	-1.312081	1.241212
H	3.607998	-1.338672	-0.492883
C	5.061616	0.136257	0.131987
H	5.233267	0.803171	0.989839
H	4.932402	0.791740	-0.741670
C	6.296437	-0.749561	-0.078254
H	6.420580	-1.409628	0.792114
H	6.122380	-1.411321	-0.938701
C	7.581660	0.053251	-0.301509
H	8.442427	-0.606046	-0.460668
H	7.493392	0.704387	-1.179976
H	7.805563	0.692002	0.561676

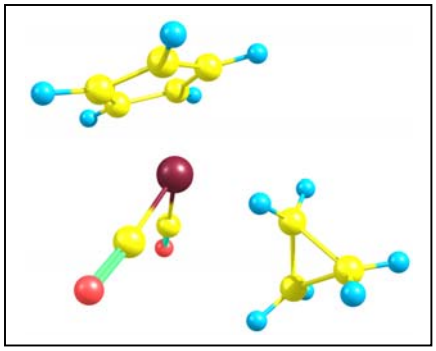


Heptane:

C	-4.556018	-0.019141	0.130065
C	-4.178846	-1.005235	-0.839216
C	-3.448717	-2.042369	-0.161205
C	-3.371867	-1.673518	1.214190
C	-4.069989	-0.452464	1.416239
H	-4.206531	0.060093	2.358114
H	-2.853472	-2.231767	1.984478
H	-3.049268	-2.943556	-0.605051
H	-4.441314	-0.995849	-1.887961
H	-5.157315	0.858674	-0.061199
Re	-2.314453	0.016558	-0.079521
C	-2.204325	1.907189	0.131077
O	-2.252828	3.065698	0.271237
C	-1.495705	0.143894	-1.795032
O	-1.057298	0.188837	-2.877078
C	0.202352	-0.572285	0.886877
C	1.419785	0.306851	0.586987
C	2.710528	-0.515160	0.474318
C	3.951697	0.344056	0.200953
C	5.234298	-0.480533	0.037293
C	6.480665	0.373213	-0.228354
C	7.753780	-0.461252	-0.399967
H	-0.693711	0.120507	1.043146
H	0.058088	-1.333142	0.118646
H	0.278347	-1.078527	1.855665
H	1.528908	1.064794	1.374269
H	1.249339	0.853054	-0.348908
H	2.596461	-1.255372	-0.331152
H	2.862959	-1.090467	1.399849
H	4.081877	1.064836	1.021421
H	3.785295	0.942565	-0.706708
H	5.103610	-1.194971	-0.788993
H	5.395937	-1.087916	0.940695
H	6.615285	1.084673	0.598616
H	6.315722	0.981730	-1.128930
H	8.624888	0.172257	-0.601985
H	7.968945	-1.046521	0.502731
H	7.654171	-1.166737	-1.234216



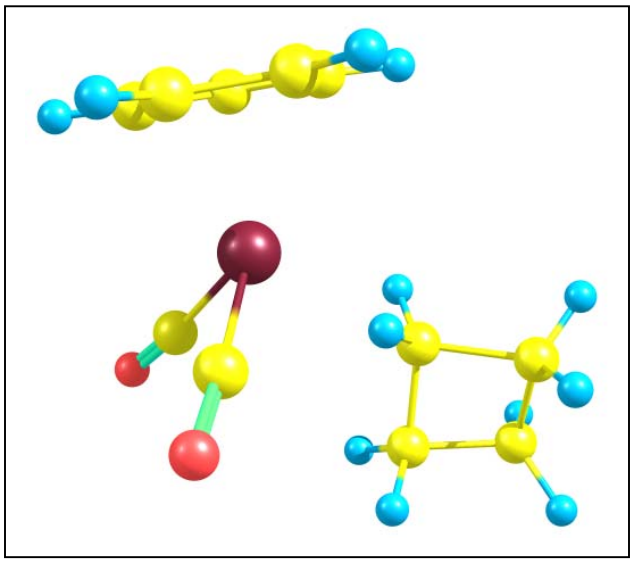
Cyclopropane:



C	-1.208097	-0.159747	-1.645258
C	-2.039001	0.660237	-0.814272
C	-2.334059	-0.085957	0.384243
C	-1.652722	-1.326446	0.291510
C	-0.969168	-1.398814	-0.962388
H	-0.859075	0.095634	-2.636530
H	-2.443983	1.627218	-1.077938
H	-2.952322	0.245534	1.206968
H	-1.645949	-2.097386	1.052905
H	-0.412105	-2.244201	-1.340796
Re	-0.040591	0.422932	0.205573
C	1.514971	0.891379	-0.783834
O	2.416434	1.165912	-1.475527
C	-0.053768	2.135067	1.044689
O	-0.138167	3.190593	1.535349
C	1.269674	-0.379498	2.390636
C	2.254006	0.627481	2.924639
C	2.632032	-0.822245	2.918954
H	0.397839	-0.631726	2.980251
H	2.741840	1.287312	2.214527
H	2.003679	1.098187	3.870979
H	3.369341	-1.155366	2.194123
H	2.641300	-1.371577	3.856076
H	1.232086	-0.619611	1.285266

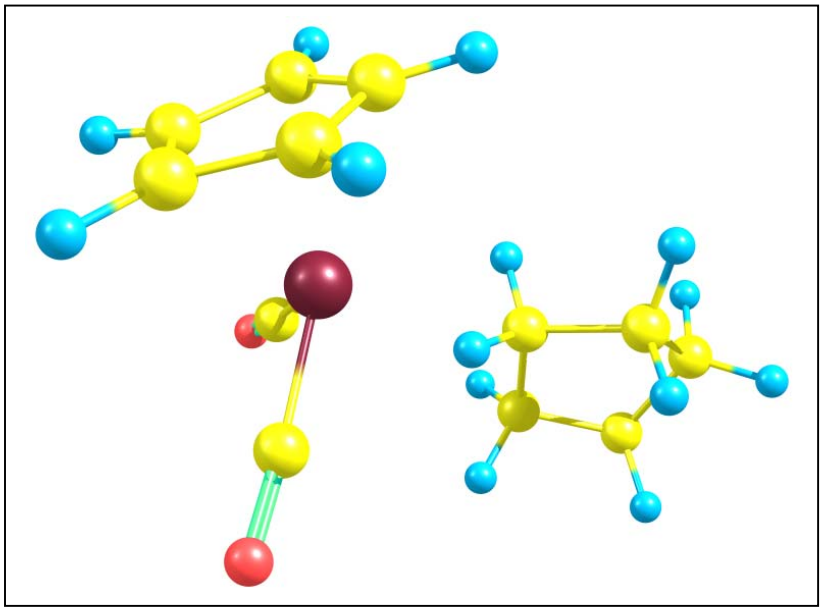
Cyclobutane:

C	-0.878447	0.279417	-1.645283
C	-1.950754	0.535156	-0.729829
C	-2.243383	-0.694745	-0.037566
C	-1.329728	-1.674326	-0.509004
C	-0.497023	-1.099714	-1.516462
H	-0.462519	0.992318	-2.344465
H	-2.493789	1.465375	-0.634345
H	-3.014056	-0.842007	0.706202
H	-1.266179	-2.695150	-0.151589
H	0.260492	-1.612127	-2.092506
Re	-0.085479	0.104048	0.466622
C	1.499628	1.080573	0.073219
O	2.435572	1.694810	-0.261980
C	-0.510936	1.323935	1.866446
O	-0.853237	2.095384	2.674012
C	2.284767	-2.244390	4.014997
C	1.739140	-0.838147	3.639010
C	1.032165	-1.492296	2.432082
C	1.977219	-2.720496	2.566899
H	3.324420	-2.306761	4.349757
H	2.538517	-0.162084	3.320441
H	1.105505	-0.316901	4.361666
H	1.207648	-0.987554	1.421374
H	-0.007155	-1.748116	2.633205
H	2.853004	-2.635258	1.915638
H	1.532946	-3.711355	2.432519
H	1.648232	-2.746319	4.751158



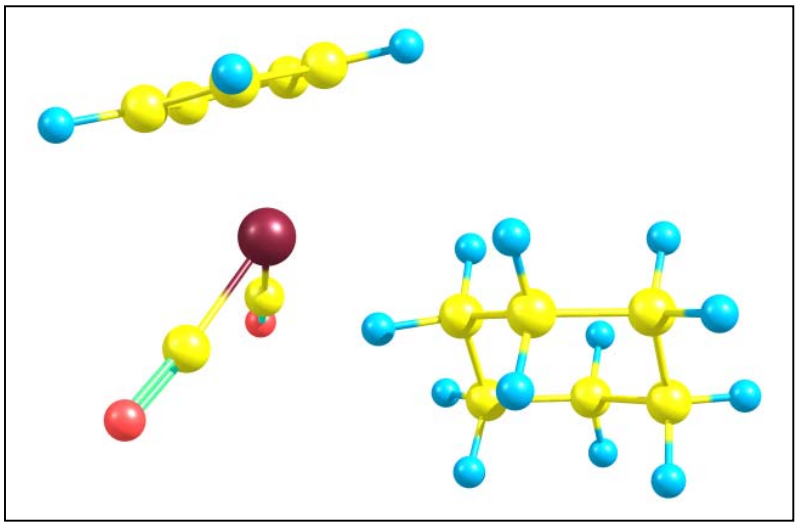
Cyclopentane:

C	-1.372027	0.174483	-1.695744
C	-2.096042	0.913483	-0.703909
C	-2.394180	0.019377	0.384978
C	-1.828626	-1.245185	0.061499
C	-1.219806	-1.176977	-1.225250
H	-1.054026	0.554061	-2.657117
H	-2.411716	1.944221	-0.790395
H	-2.949437	0.262226	1.280139
H	-1.843277	-2.119566	0.701208
H	-0.745560	-1.991691	-1.753794
Re	-0.077470	0.362260	0.142125
C	1.509769	0.696199	-0.855839
O	2.425668	0.900059	-1.551968
C	0.132684	2.007803	1.077047
O	0.169848	3.044486	1.614123
C	3.145358	-1.051226	3.836913
C	2.282599	-2.330422	3.875889
C	1.586141	-2.344946	2.505681
C	1.209033	-0.861768	2.311883
C	2.357812	-0.040850	2.950684
H	4.115644	-1.273355	3.377561
H	2.869014	-3.235948	4.065150
H	1.528541	-2.258350	4.671546
H	2.294968	-2.659909	1.729264
H	0.719852	-3.012982	2.457719
H	0.256815	-0.650131	2.799699
H	1.176575	-0.693065	1.182888
H	1.955883	0.793476	3.532947
H	3.000858	0.394670	2.179844
H	3.349580	-0.656268	4.837069



Cyclohexane:

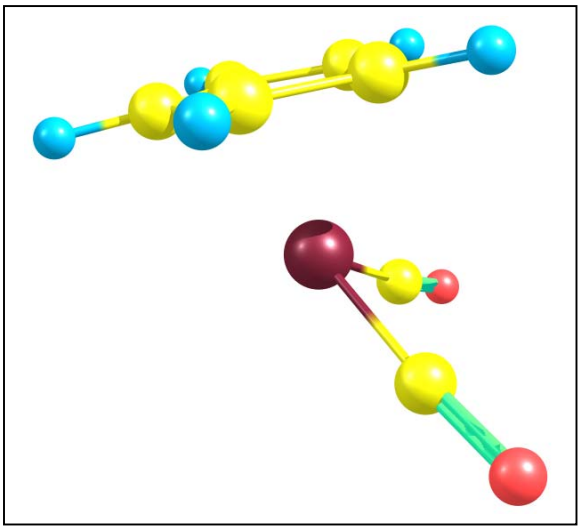
C	0.744092	0.615267	-2.134867
C	-0.528563	0.680781	-1.480860
C	-0.915518	-0.661937	-1.130199
C	0.132612	-1.526779	-1.546475
C	1.152266	-0.763025	-2.187106
H	1.276159	1.453266	-2.564035
H	-1.119641	1.574187	-1.335917
H	-1.837315	-0.955898	-0.647696
H	0.157243	-2.599242	-1.397671
H	2.049174	-1.149037	-2.650287
Re	1.019624	0.024012	0.027488
C	2.632084	1.019596	0.198638
O	3.610293	1.658462	0.204721
C	0.222761	0.964258	1.478934
O	-0.338969	1.565716	2.308317
C	2.651943	-3.142254	1.265999
C	2.417031	-4.468242	2.009343
C	2.509466	-4.284196	3.532332
C	1.558749	-3.183224	4.028097
C	1.786626	-1.852271	3.291089
C	1.685882	-2.061031	1.772103
H	3.685753	-2.807814	1.432226
H	1.421152	-4.857050	1.749882
H	3.142969	-5.218036	1.670940
H	2.286938	-5.230264	4.041827
H	3.543034	-4.022242	3.801766
H	0.518442	-3.505478	3.872204
H	1.678502	-3.033423	5.108143
H	2.782740	-1.459306	3.537259
H	1.058907	-1.101229	3.616894
H	0.657367	-2.323564	1.511358
H	2.021449	-1.079030	1.295219
H	2.538285	-3.279464	0.184192



4-1c. Mononuclear Re, DFT(BP86).

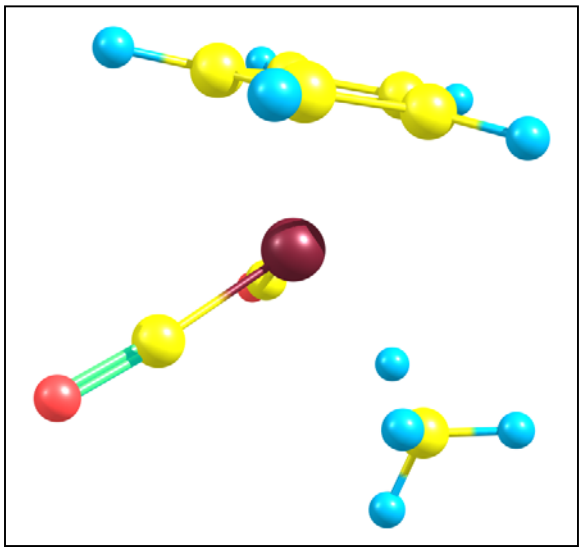
Complex:

C	3.538441	-0.921959	0.727355
C	3.869488	0.089747	-0.261597
C	3.333000	-0.355475	-1.538447
C	2.623657	-1.568982	-1.303410
C	2.768452	-1.954911	0.078194
H	3.848974	-0.913619	1.772607
H	4.493918	0.966529	-0.091894
H	3.413119	0.170630	-2.489569
H	2.044046	-2.112393	-2.053000
H	2.379723	-2.861349	0.541311
Re	1.695099	0.114523	0.061206
C	1.114178	0.368500	1.855963
O	0.871637	0.499522	3.005017
C	1.505355	1.976785	-0.313376
O	1.520736	3.132162	-0.557058



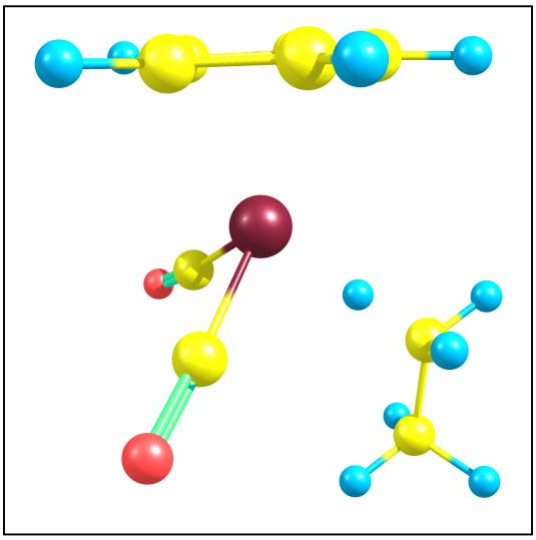
Methane:

C	-1.931396	-1.223334	-0.321101
C	-1.562537	-0.412645	-1.467219
C	-1.651264	0.975139	-1.072306
C	-2.062838	1.027785	0.312652
C	-2.195121	-0.332020	0.764211
H	-1.984111	-2.311695	-0.291557
H	-1.339421	-0.780183	-2.469119
H	-1.490446	1.833416	-1.725480
H	-2.239856	1.925678	0.904016
H	-2.444709	-0.633241	1.784231
Re	0.031780	0.008778	0.042990
C	1.212070	1.452151	-0.335450
O	1.865677	2.387761	-0.644374
C	1.282101	-1.211020	-0.713249
O	1.983909	-1.992474	-1.255005
C	1.037772	-0.640513	2.426101
H	2.126378	-0.763177	2.516170
H	0.582059	-0.349653	3.385021
H	0.901758	0.309836	1.784376
H	0.589713	-1.578588	2.074336



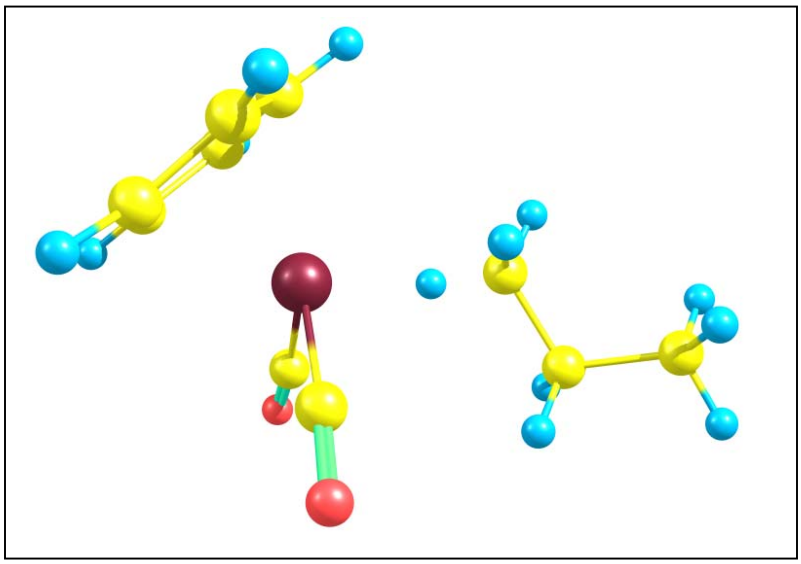
Ethane:

C	1.737921	-1.464776	0.841394
C	2.131910	-0.070218	0.926231
C	2.219875	0.443893	-0.422504
C	1.877360	-0.620940	-1.338203
C	1.551614	-1.773782	-0.540734
H	1.588288	-2.144270	1.680587
H	2.386492	0.473185	1.836067
H	2.532695	1.451553	-0.698157
H	1.862659	-0.560695	-2.425896
H	1.212985	-2.734527	-0.933685
Re	0.076169	-0.024594	0.033976
C	-0.511000	1.628289	-0.699339
O	-0.763786	2.682010	-1.172778
C	-0.808554	0.359347	1.674240
O	-1.272702	0.586001	2.737934
C	-2.099652	-1.487506	-0.659217
H	-1.451813	-0.597886	-1.035693
H	-1.781782	-1.940764	0.290868
H	-1.947976	-2.230019	-1.461554
C	-3.538844	-0.964754	-0.589002
H	-4.240183	-1.799778	-0.412398
H	-3.655541	-0.239526	0.233026
H	-3.832457	-0.464426	-1.528020

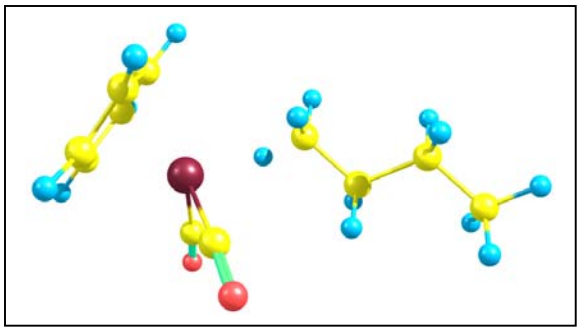


Propane:

C	-1.845406	-1.831008	-0.136439
C	-2.502356	-0.683449	-0.728602
C	-2.746525	0.281225	0.319000
C	-2.244164	-0.269339	1.562543
C	-1.666207	-1.543603	1.257405
H	-1.162880	-2.193198	1.977867
H	-1.549862	-2.746097	-0.649602
H	-2.813088	-0.587246	-1.769033
H	-3.277692	1.226105	0.204182
H	-2.287871	0.204787	2.542904
Re	-0.537758	0.109194	-0.003024
C	-0.253222	1.974858	0.232810
O	-0.177803	3.144376	0.389268
C	0.217774	0.220198	-1.743962
O	0.614424	0.264525	-2.857611
C	1.902701	-0.745156	0.788781
C	3.158929	-0.099616	0.185621
C	4.365639	-1.049876	0.230893
H	2.068922	-1.135206	1.809953
H	1.530958	-1.572344	0.166803
H	1.130253	0.093683	1.016713
H	2.946759	0.189856	-0.859188
H	3.392342	0.835691	0.728381
H	4.644415	-1.300574	1.270994
H	5.247051	-0.593667	-0.252596
H	4.148048	-1.997991	-0.295282



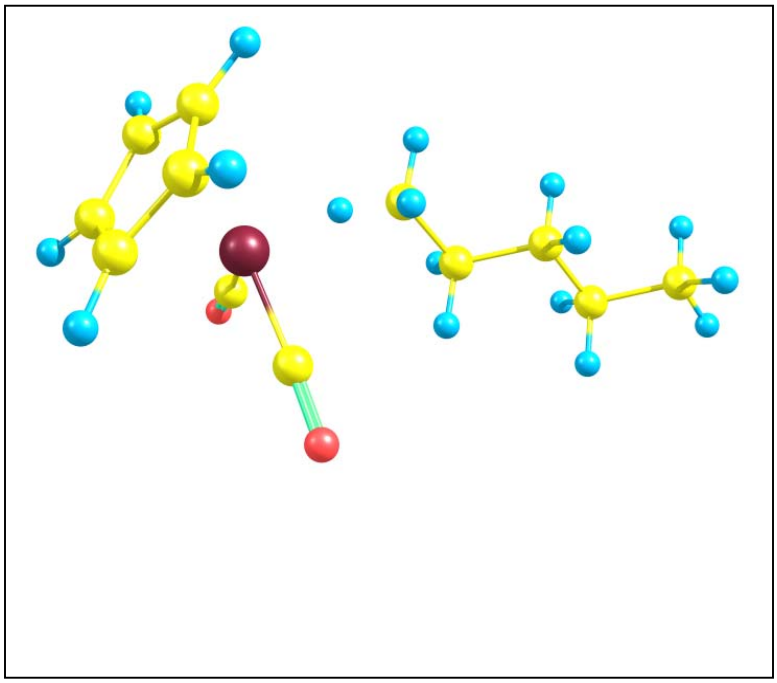
Butane:



C	-1.849078	-1.835422	-0.118220
C	-2.505651	-0.693810	-0.721919
C	-2.748821	0.282082	0.315611
C	-2.246255	-0.256113	1.564614
C	-1.668826	-1.533548	1.272389
H	-1.165519	-2.175785	1.999415
H	-1.553188	-2.755407	-0.622333
H	-2.817069	-0.609159	-1.763163
H	-3.280334	1.225641	0.191598
H	-2.290214	0.227366	2.540405
Re	-0.540361	0.105095	-0.005621
C	-0.250088	1.971702	0.214772
O	-0.170363	3.141985	0.363284
C	0.212970	0.198651	-1.748322
O	0.610080	0.230412	-2.862281
C	1.901261	-0.744645	0.785708
C	3.156055	-0.095688	0.185692
C	4.367227	-1.045592	0.193671
H	2.066352	-1.138234	1.805646
H	1.529172	-1.569106	0.160533
H	1.129035	0.094217	1.01508
H	2.940475	0.217751	-0.852500
H	3.403454	0.827599	0.745069
H	4.584522	-1.358728	1.234560
H	4.110730	-1.971936	-0.358562
C	5.620134	-0.405441	-0.425267
H	5.914616	0.504971	0.127795
H	6.477183	-1.101900	-0.410074
H	5.439968	-0.114328	-1.476297

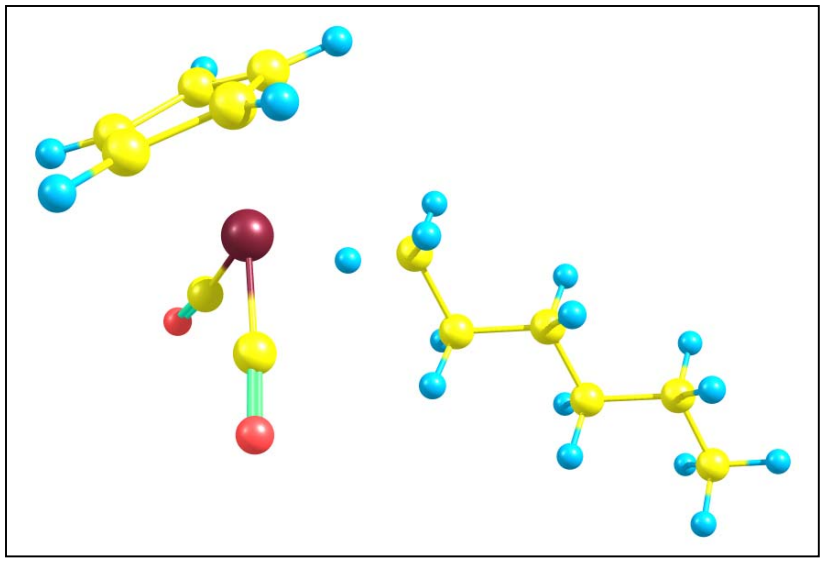
Pentane:

C	-1.832956	-1.834151	-0.172676
C	-2.486815	-0.683840	-0.762619
C	-2.751301	0.268819	0.290992
C	-2.265617	-0.292669	1.536539
C	-1.677533	-1.560893	1.227316
H	-1.183087	-2.216153	1.948714
H	-1.525463	-2.742721	-0.690473
H	-2.778472	-0.575767	-1.807311
H	-3.283635	1.213142	0.177563
H	-2.323331	0.173274	2.519984
Re	-0.537752	0.110899	0.001569
C	-0.267519	1.974553	0.267900
O	-0.202731	3.142594	0.439673
C	0.240367	0.253676	-1.726692
O	0.653878	0.319309	-2.833250
C	1.897553	-0.747167	0.805118
C	3.152312	-0.092203	0.211390
C	4.375725	-1.024511	0.256352
H	2.059409	-1.139757	1.825972
H	1.530512	-1.572831	0.178597
H	1.120181	0.087412	1.033349
H	2.947005	0.198845	-0.835185
H	3.378091	0.845054	0.756313
H	4.596918	-1.298331	1.308654
H	4.138116	-1.975066	-0.263943
C	5.629675	-0.399392	-0.382522
H	5.845718	0.566662	0.114863
H	5.412526	-0.156395	-1.441659
C	6.861384	-1.313240	-0.302147
H	7.734078	-0.864123	-0.808240
H	7.146260	-1.509331	0.748086
H	6.663033	-2.290740	-0.780097



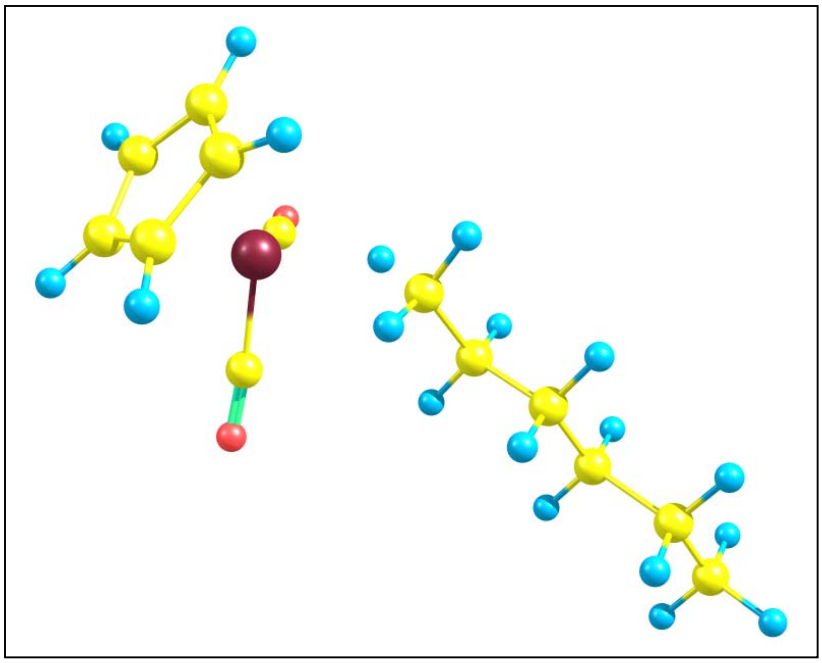
Hexane:

C	-2.813055	-1.240780	1.189974
C	-3.441689	-0.349241	0.236942
C	-3.012617	-0.730206	-1.088998
C	-2.119766	-1.864975	-0.958142
C	-1.983309	-2.139488	0.440354
H	-2.953076	-1.234468	2.270639
H	-4.161198	0.435867	0.470813
H	-3.361263	-0.287212	-2.021467
H	-1.631364	-2.396202	-1.774869
H	-1.332568	-2.904304	0.871397
Re	-1.253305	0.072804	0.038384
C	-1.411593	1.743805	0.931257
O	-1.619124	2.768141	1.485090
C	-0.502179	0.943274	-1.478294
O	-0.112291	1.454789	-2.470736
C	1.232218	-0.581929	0.815060
H	1.291930	-1.227554	1.708902
H	0.386196	0.161409	1.100391
H	1.043510	-1.223673	-0.059430
C	2.501069	0.257148	0.602741
H	2.666183	0.919616	1.474299
H	2.355881	0.917870	-0.271570
C	3.734467	-0.638268	0.383859
H	3.864664	-1.306006	1.260304
H	3.547702	-1.305428	-0.482961
C	5.032598	0.150792	0.145181
H	5.230051	0.810842	1.014625
H	4.898449	0.823986	-0.725734
C	6.251894	-0.756911	-0.097150
H	6.382405	-1.430591	0.773445
H	6.043849	-1.416760	-0.963378
C	7.550606	0.024416	-0.346778
H	8.399939	-0.655544	-0.536541
H	7.452222	0.691342	-1.223231
H	7.813309	0.655292	0.522356



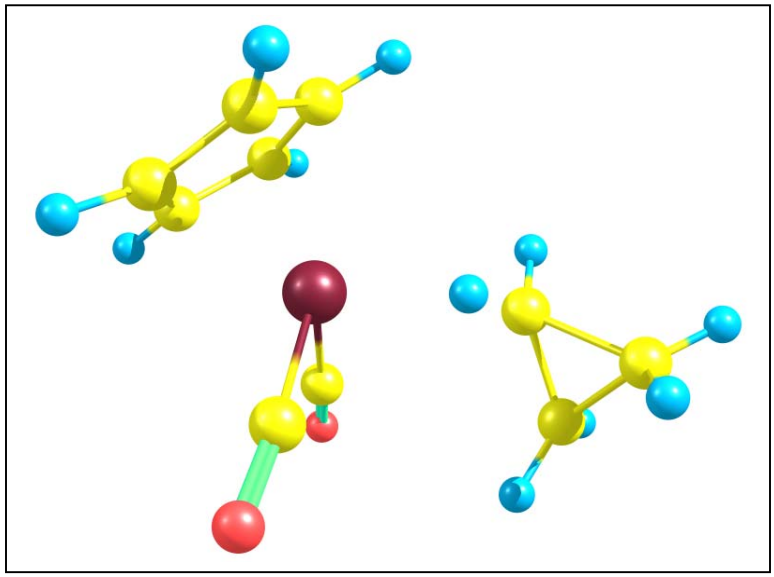
Heptane:

C	-4.489852	-0.357103	0.160611
C	-3.917692	-0.996200	-1.002251
C	-2.983193	-2.004648	-0.542649
C	-2.970346	-1.949383	0.888910
C	-3.910151	-0.965725	1.341057
H	-4.145318	-0.726098	2.378041
H	-2.330765	-2.552457	1.537725
H	-2.400520	-2.678598	-1.170544
H	-4.188412	-0.795124	-2.039239
H	-5.270036	0.404353	0.147691
Re	-2.314874	0.161594	0.045477
C	-2.611343	1.979677	0.523642
O	-2.891194	3.093282	0.805214
C	-1.505378	0.715325	-1.582153
O	-1.071107	1.000108	-2.645133
C	0.141605	-0.167012	1.079851
C	1.370685	0.553236	0.507560
C	2.637075	-0.315266	0.627102
C	3.892079	0.341422	0.025973
C	5.146422	-0.542392	0.141676
C	6.408984	0.090079	-0.470170
C	7.653221	-0.800762	-0.330035
H	-0.742234	0.588528	1.107751
H	-0.038914	-1.112500	0.545888
H	0.245885	-0.402823	2.154411
H	1.523830	1.517457	1.029721
H	1.183667	0.798037	-0.553991
H	2.458984	-1.287375	0.123063
H	2.822992	-0.554095	1.694582
H	4.076361	1.312959	0.527606
H	3.704799	0.578813	-1.040974
H	4.954142	-1.518317	-0.349393
H	5.335096	-0.772900	1.210606
H	6.593775	1.070232	0.011979
H	6.226059	0.306223	-1.541856
H	8.536369	-0.346320	-0.813037
H	7.903873	-0.973728	0.732902
H	7.486708	-1.789800	-0.796223



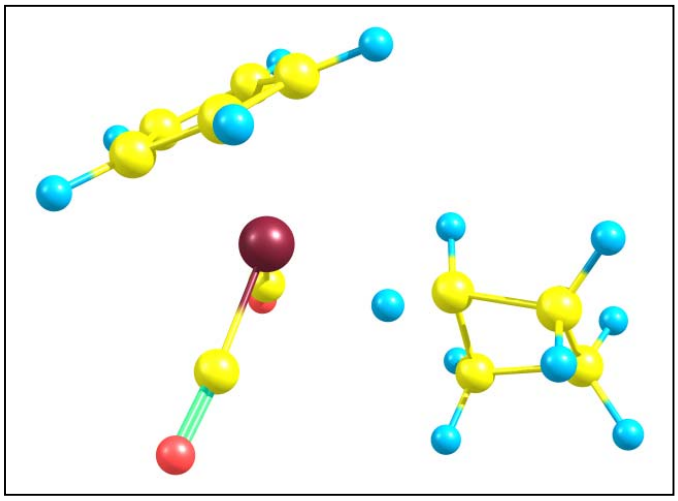
Cyclopropane:

C	-1.159114	-0.192745	-1.622706
C	-1.998106	0.668994	-0.823104
C	-2.328972	-0.047289	0.396419
C	-1.654826	-1.304259	0.352227
C	-0.947461	-1.422294	-0.898800
H	-0.781201	0.035470	-2.619819
H	-2.386237	1.642292	-1.122352
H	-2.950747	0.323215	1.211770
H	-1.673648	-2.060978	1.140035
H	-0.388256	-2.291241	-1.244739
Re	-0.036017	0.415386	0.233649
C	1.514206	0.921067	-0.741529
O	2.427199	1.225078	-1.430482
C	-0.068526	2.123144	1.075197
O	-0.174686	3.191381	1.568279
C	1.233982	-0.382684	2.337357
C	2.217212	0.622615	2.897742
C	2.622356	-0.823269	2.842530
H	0.372515	-0.683427	2.935101
H	2.684738	1.317053	2.193894
H	1.964132	1.063958	3.867197
H	3.362107	-1.124296	2.093249
H	2.642269	-1.410244	3.766636
H	1.231279	-0.652018	1.212393



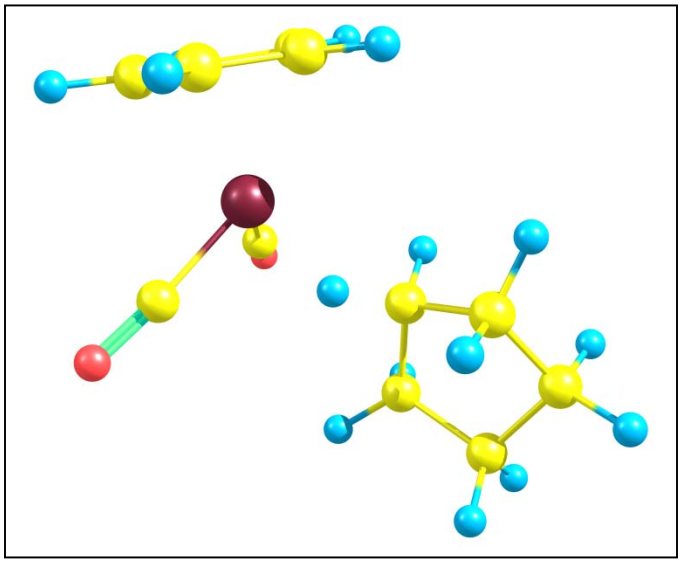
Cyclobutane:

C	-0.839294	0.251063	-1.629880
C	-1.927392	0.532517	-0.722558
C	-2.240778	-0.694285	-0.013519
C	-1.318679	-1.691753	-0.456113
C	-0.467634	-1.136791	-1.475538
H	-0.402683	0.958597	-2.335930
H	-2.468207	1.475896	-0.646440
H	-3.016764	-0.821273	0.741420
H	-1.263596	-2.714473	-0.076642
H	0.305724	-1.666495	-2.031126
Re	-0.088590	0.089199	0.485320
C	1.471806	1.102656	0.101410
O	2.404187	1.747370	-0.237166
C	-0.532471	1.286797	1.895726
O	-0.896091	2.054723	2.718018
C	2.258278	-2.246429	3.980853
C	1.750455	-0.819400	3.607925
C	1.025046	-1.457070	2.397535
C	1.951368	-2.709276	2.522623
H	3.301047	-2.339993	4.327984
H	2.574524	-0.160756	3.284856
H	1.126301	-0.275904	4.335549
H	1.242954	-0.955288	1.365616
H	-0.026211	-1.698304	2.604010
H	2.840184	-2.629404	1.873010
H	1.488634	-3.699479	2.372861
H	1.594453	-2.739177	4.712413



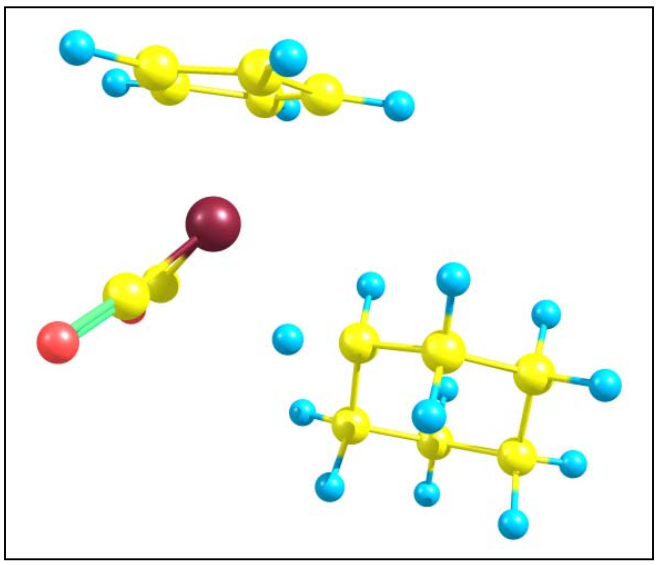
Cyclopentane:

C	-1.311817	0.188867	-1.689342
C	-2.090658	0.836050	-0.658556
C	-2.340307	-0.133334	0.389133
C	-1.683788	-1.349836	0.006995
C	-1.081093	-1.182338	-1.282303
H	-1.011766	0.636679	-2.636996
H	-2.477537	1.854913	-0.697243
H	-2.904358	0.034817	1.306329
H	-1.642648	-2.260665	0.608461
H	-0.539105	-1.941885	-1.845241
Re	-0.059302	0.350748	0.160191
C	1.534329	0.739561	-0.803072
O	2.469581	0.975429	-1.487434
C	0.100685	1.997212	1.100100
O	0.112539	3.043838	1.650320
C	3.172167	-1.089681	3.732658
C	2.161370	-2.242051	3.943161
C	1.379695	-2.286512	2.613563
C	1.175239	-0.781087	2.300147
C	2.417383	-0.034789	2.868584
H	4.054255	-1.468573	3.184630
H	2.645869	-3.203771	4.187484
H	1.469524	-1.997748	4.772417
H	1.995954	-2.767340	1.829688
H	0.427238	-2.841475	2.676128
H	0.246779	-0.424446	2.768616
H	1.189473	-0.710280	1.134584
H	2.093816	0.833739	3.466585
H	3.051904	0.358368	2.056948
H	3.539058	-0.670245	4.685304



Cyclohexane:

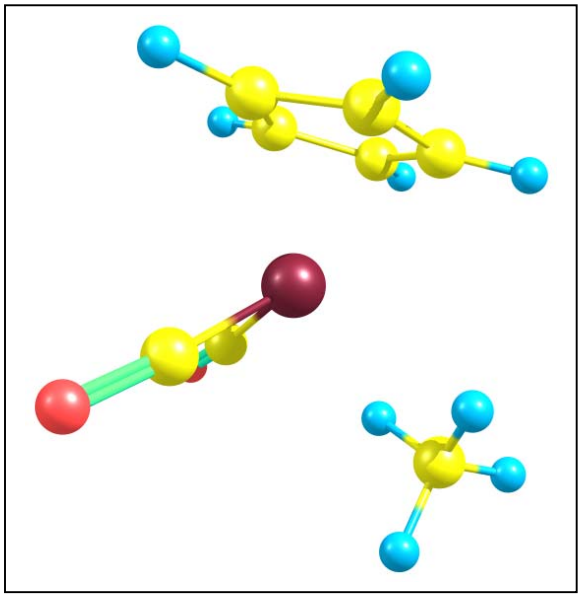
C	0.711664	0.551156	-2.100247
C	-0.549137	0.598736	-1.399132
C	-0.892457	-0.753408	-1.004882
C	0.173478	-1.606602	-1.440292
C	1.152187	-0.828319	-2.143439
H	1.210140	1.399096	-2.570389
H	-1.156276	1.490171	-1.242935
H	-1.795155	-1.060766	-0.476675
H	0.239989	-2.680901	-1.253768
H	2.055179	-1.199838	-2.626923
Re	1.061989	0.005692	0.046235
C	2.677013	1.004534	0.140812
O	3.666106	1.651791	0.101260
C	0.306439	1.016538	1.467540
O	-0.246578	1.673156	2.281418
C	2.689032	-3.062908	1.250277
C	2.408612	-4.415841	1.936066
C	2.442835	-4.288664	3.470868
C	1.480906	-3.192892	3.968567
C	1.753363	-1.833630	3.292493
C	1.711850	-1.987584	1.759156
H	3.727142	-2.742531	1.471348
H	1.409814	-4.784452	1.622618
H	3.142806	-5.169258	1.594009
H	2.186508	-5.257871	3.938836
H	3.475990	-4.050205	3.795491
H	0.436808	-3.501662	3.754100
H	1.553535	-3.085428	5.067099
H	2.751679	-1.459332	3.594817
H	1.015642	-1.079468	3.618158
H	0.680930	-2.232644	1.450404
H	2.101240	-0.968270	1.349520
H	2.618265	-3.156887	0.151449



4-1d. Mononuclear Re, SOS-MP2.

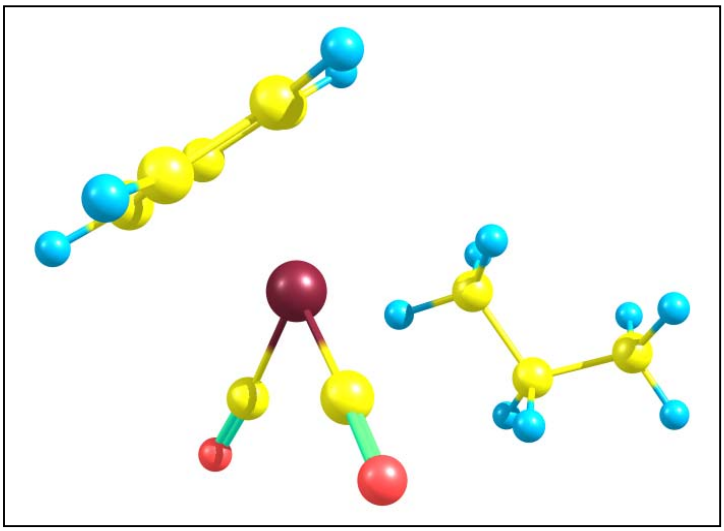
Methane:

C	-1.902915	-1.215819	-.242486
C	-1.551871	-.479469	-1.431269
C	-1.647280	.918851	-1.130419
C	-2.051733	1.054996	.245157
C	-2.182475	-.261245	.776710
H	-1.972401	-2.293208	-.151633
H	-1.348523	-.903839	-2.407031
H	-1.519786	1.727958	-1.839565
H	-2.252445	1.981981	.768403
H	-2.455392	-.497295	1.800840
Re	.051269	.044322	.039668
C	1.166181	1.536293	-.285967
O	1.793915	2.494494	-.560467
C	1.347462	-1.068120	-.771238
O	2.100556	-1.769245	-1.343556
C	1.015918	-.747073	2.432654
H	2.042615	-1.109247	2.383751
H	.781177	-.367275	3.430478
H	.970581	.196589	1.805806
H	.326665	-1.551647	2.179408



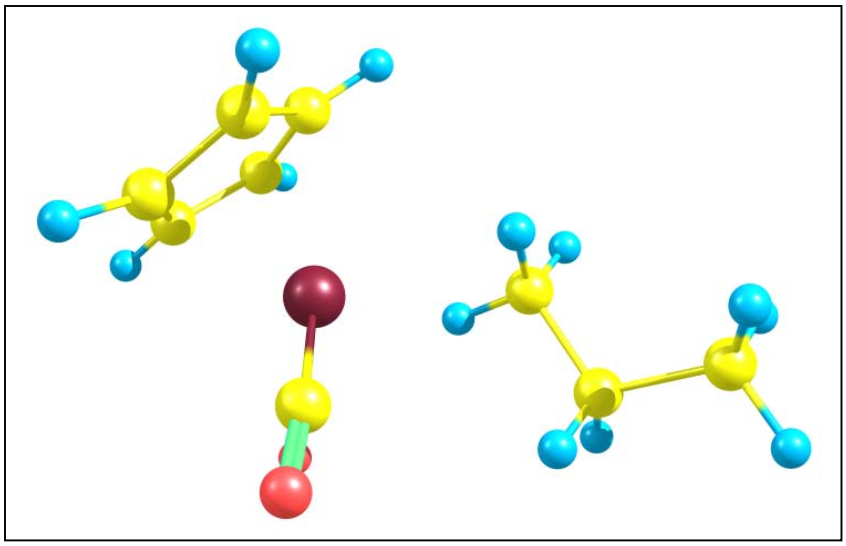
Ethane:

C	-1.750931	-1.818941	-.172473
C	-2.452963	-.691894	-.733198
C	-2.731929	.229728	.328547
C	-2.202613	-.320447	1.550121
C	-1.586637	-1.562533	1.219261
H	-1.074896	-2.213490	1.921594
H	-1.437042	-2.709240	-.704141
H	-2.794102	-.598723	-1.757253
H	-3.314730	1.138748	.239508
H	-2.283140	.113786	2.539262
Re	-.514645	.163344	-.002809
C	-.331438	2.032253	.208139
O	-.318433	3.203807	.331612
C	.221517	.313085	-1.735762
O	.606285	.390635	-2.847022
C	1.900901	-.653313	.870425
C	3.155303	-.128553	.169234
C	4.296963	-1.147985	.220260
H	2.087621	-.914040	1.919387
H	1.505182	-1.539843	.369915
H	1.175041	.219489	.987118
H	2.908542	.108377	-.871066
H	3.470187	.810488	.641796
H	4.573319	-1.381154	1.255470
H	5.188098	-.763138	-.287380
H	4.007919	-2.084317	-.271765

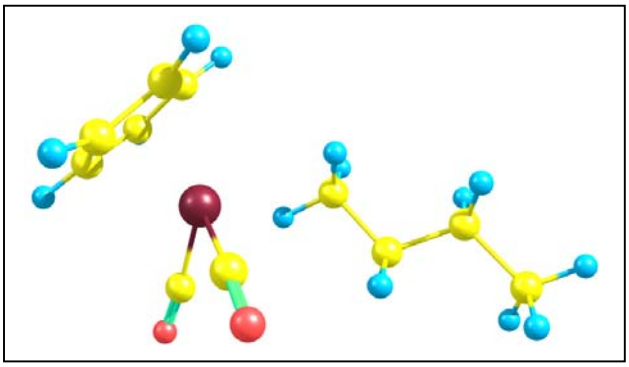


Propane:

C	-1.750931	-1.818941	-.172473
C	-2.452963	-.691894	-.733198
C	-2.731929	.229728	.328547
C	-2.202613	-.320447	1.550121
C	-1.586637	-1.562533	1.219261
H	-1.074896	-2.213490	1.921594
H	-1.437042	-2.709240	-.704141
H	-2.794102	-.598723	-1.757253
H	-3.314730	1.138748	.239508
H	-2.283140	.113786	2.539262
Re	-.514645	.163344	-.002809
C	-.331438	2.032253	.208139
O	-.318433	3.203807	.331612
C	.221517	.313085	-1.735762
O	.606285	.390635	-2.847022
C	1.900901	-.653313	.870425
C	3.155303	-.128553	.169234
C	4.296963	-1.147985	.220260
H	2.087621	-.914040	1.919387
H	1.505182	-1.539843	.369915
H	1.175041	.219489	.987118
H	2.908542	.108377	-.871066
H	3.470187	.810488	.641796
H	4.573319	-1.381154	1.255470
H	5.188098	-.763138	-.287380
H	4.007919	-2.084317	-.271765



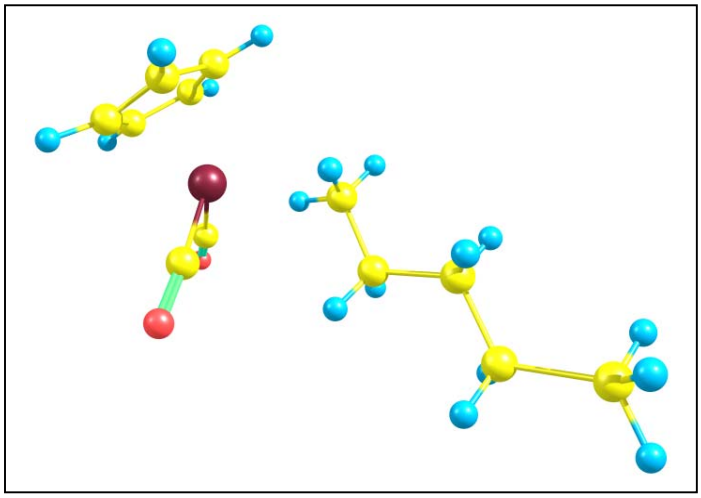
Butane:



C	-1.721698	-1.829769	-.182235
C	-2.436698	-.711485	-.744144
C	-2.735571	.202931	.318430
C	-2.205629	-.342948	1.541673
C	-1.569694	-1.575036	1.211187
H	-1.052646	-2.220365	1.914825
H	-1.391347	-2.713726	-.714521
H	-2.773143	-.620517	-1.769946
H	-3.331315	1.103423	.228402
H	-2.298490	.087227	2.531507
Re	-.515524	.169991	.000318
C	-.360446	2.040626	.217614
O	-.364814	3.211931	.344357
C	.229701	.335697	-1.727126
O	.621588	.422622	-2.835284
C	1.904283	-.615103	.884330
C	3.151907	-.072810	.185147
C	4.313485	-1.071354	.230704
H	2.091950	-.874019	1.933541
H	1.520857	-1.506314	.382637
H	1.166471	.247909	1.001454
H	2.904882	.161900	-.856669
H	3.456424	.870628	.658331
H	4.551628	-1.307896	1.277392
H	3.997687	-2.013965	-.238353
C	5.565954	-.542324	-.474624
H	5.917479	.383674	-.004941
H	6.382398	-1.271951	-.433931
H	5.357791	-.326350	-1.528787

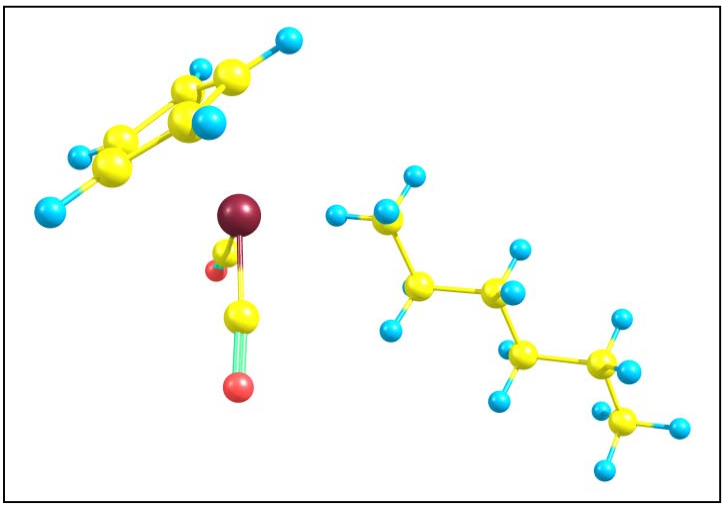
Pentane:

C	3.142821	-.924488	.795877
C	3.564321	-.076526	-.280197
C	3.010912	-.596705	-1.504044
C	2.240270	-1.746251	-1.161402
C	2.329004	-1.977142	.241255
H	3.460970	-.841512	1.828159
H	4.248962	.758933	-.195353
H	3.174714	-.206576	-2.501230
H	1.676300	-2.353107	-1.863222
H	1.892863	-2.806134	.785690
Re	1.345530	.132419	-.024980
C	.570129	.413558	1.674105
O	.156275	.566000	2.767105
C	1.396719	2.003648	-.282131
O	1.529047	3.164909	-.430800
C	-1.119377	-.404433	-.968028
C	-2.314355	.307047	-.331267
C	-3.584514	-.548379	-.386450
C	-4.793850	.142227	.253529
C	-6.060920	-.716773	.202101
H	-.859590	-1.315031	-.423825
H	-.281050	.361057	-1.089331
H	-1.304352	-.678574	-2.013858
H	-2.073289	.548079	.710426
H	-2.487973	1.262214	-.845180
H	-3.817948	-.794148	-1.433231
H	-3.400769	-1.505184	.124853
H	-4.975771	1.097955	-.257114
H	-4.556937	.388351	1.297596
H	-6.909767	-.201340	.665220
H	-5.913063	-1.664778	.732687
H	-6.333985	-.951029	-.833680



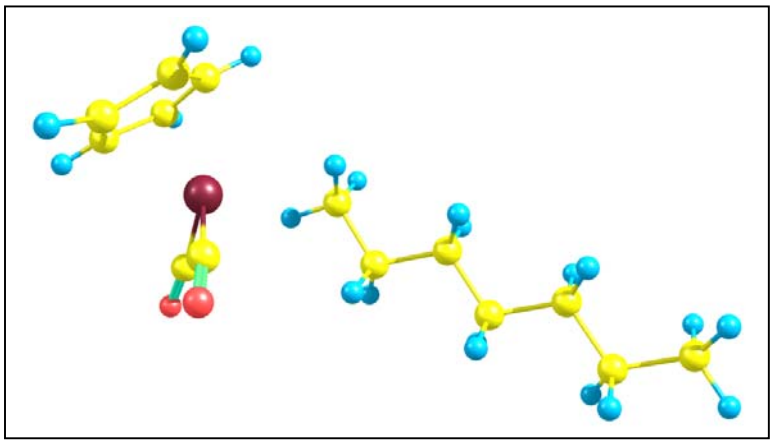
Hexane:

C	-2.895754	-1.109583	1.166780
C	-3.403568	-.182594	.188626
C	-2.962843	-.613179	-1.105668
C	-2.184320	-1.814457	-.934104
C	-2.133934	-2.088105	.462277
H	-3.084843	-1.087850	2.233152
H	-4.071781	.647504	.384585
H	-3.249179	-.168809	-2.051315
H	-1.744895	-2.412998	-1.723111
H	-1.601803	-2.916044	.920799
Re	-1.175057	.044815	.073086
C	-1.206474	1.717484	.951209
O	-1.325954	2.762301	1.482524
C	-.335488	.866257	-1.406237
O	.117324	1.371984	-2.369716
C	1.255560	-.825257	.848053
H	1.399335	-1.472279	1.722051
H	.401855	-.158807	1.209517
H	1.032030	-1.464052	-.009089
C	2.464877	.072162	.581082
H	2.598346	.765454	1.422625
H	2.266028	.685834	-.305068
C	3.747027	-.741071	.373064
H	3.933452	-1.367035	1.258455
H	3.606440	-1.430604	-.472645
C	4.971379	.142313	.109294
H	5.112260	.829516	.956447
H	4.781054	.771914	-.771970
C	6.257802	-.661337	-.109664
H	6.443526	-1.294138	.769568
H	6.117233	-1.344427	-.958988
C	7.476484	.230691	-.365595
H	8.382326	-.366394	-.520468
H	7.326260	.851955	-1.256297
H	7.656041	.900689	.483477

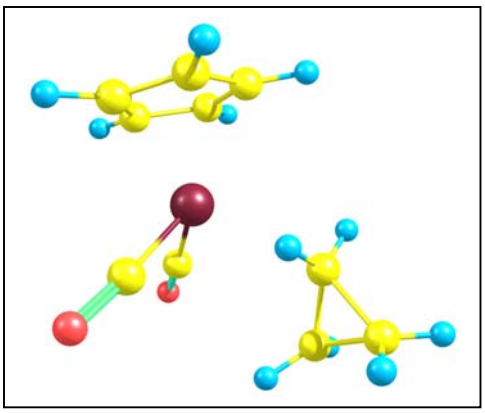


Heptane:

C	-4.487896	-.171675	.155799
C	-3.989415	-.941399	-.945780
C	-3.165320	-1.998072	-.414757
C	-3.148429	-1.847277	1.001697
C	-3.973195	-.745409	1.372687
H	-4.194771	-.419431	2.381689
H	-2.596018	-2.475817	1.693565
H	-2.677160	-2.779739	-.984439
H	-4.262648	-.807685	-1.985591
H	-5.196335	.645180	.086717
Re	-2.268313	.122187	.017922
C	-2.392379	1.971203	.387061
O	-2.568980	3.116250	.600921
C	-1.433192	.534519	-1.625297
O	-.980310	.767864	-2.688099
C	.167585	-.398744	1.040336
C	1.371838	.372293	.497332
C	2.661436	-.451435	.580943
C	3.881594	.299707	.036547
C	5.175265	-.517720	.120526
C	6.397360	.230167	-.423589
C	7.685801	-.593214	-.331845
H	-.694586	.340103	1.159382
H	-.042886	-1.286386	.439781
H	.311150	-.721012	2.078914
H	1.492333	1.307323	1.061047
H	1.176349	.654059	-.543752
H	2.530981	-1.388481	.019318
H	2.847027	-.737968	1.626853
H	4.007793	1.239179	.594252
H	3.695396	.582687	-1.009561
H	5.048532	-1.458197	-.435949
H	5.359991	-.800435	1.167604
H	6.521871	1.170768	.130847
H	6.213249	.510010	-1.470124
H	8.543561	-.037382	-.727226
H	7.907548	-.858470	.708715
H	7.596452	-1.524850	-.903059



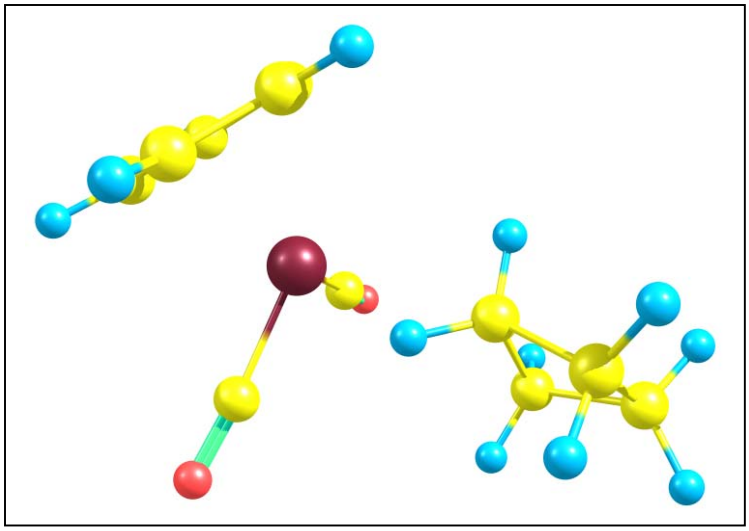
Cyclopropane:



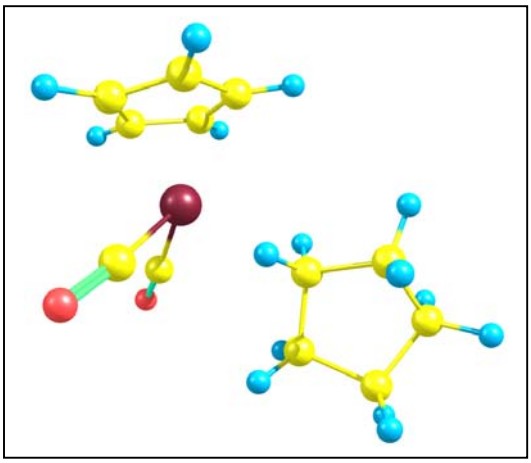
C	-1.190490	-.145956	-1.608051
C	-1.997465	.680561	-.758408
C	-2.289312	-.071912	.438567
C	-1.621258	-1.319469	.329535
C	-.951866	-1.391781	-.933563
H	-.864018	.108494	-2.609591
H	-2.418071	1.642809	-1.023823
H	-2.904723	.256576	1.267830
H	-1.622853	-2.100901	1.083290
H	-.418973	-2.247541	-1.329615
Re	-.002527	.407407	.219603
C	1.516012	.886738	-.791808
O	2.412089	1.189915	-1.496410
C	.036440	2.124340	1.011434
O	.004476	3.209082	1.466963
C	1.234272	-.433204	2.325111
C	2.137959	.628943	2.898550
C	2.602927	-.790926	2.912475
H	.368014	-.755783	2.890214
H	2.605848	1.314733	2.200245
H	1.816457	1.082445	3.832162
H	3.385011	-1.082545	2.216955
H	2.599769	-1.337309	3.851518
H	1.286477	-.699806	1.226960

Cyclobutane:

C	-.916317	.330546	-1.579338
C	-1.939153	.520676	-.594154
C	-2.180746	-.747626	.047391
C	-1.280636	-1.688767	-.526635
C	-.510703	-1.049446	-1.544787
H	-.563421	1.080870	-2.276835
H	-2.499407	1.433674	-.431866
H	-2.922700	-.949585	.810772
H	-1.197361	-2.733152	-.241867
H	.217322	-1.523023	-2.192125
Re	-.014880	.049429	.464002
C	1.544456	1.028837	.040686
O	2.472595	1.672466	-.295988
C	-.333004	1.254924	1.884402
O	-.591352	2.037652	2.726137
C	2.162282	-2.167826	4.038277
C	1.642397	-.792997	3.541134
C	1.008689	-1.525286	2.343412
C	1.983308	-2.713366	2.596337
H	3.167312	-2.207669	4.470311
H	2.460312	-.142479	3.213361
H	.970612	-.220373	4.186675
H	1.248387	-1.116971	1.298480
H	-.028757	-1.814850	2.513590
H	2.902389	-2.609766	2.009316
H	1.587177	-3.725892	2.467342
H	1.457769	-2.636732	4.734186

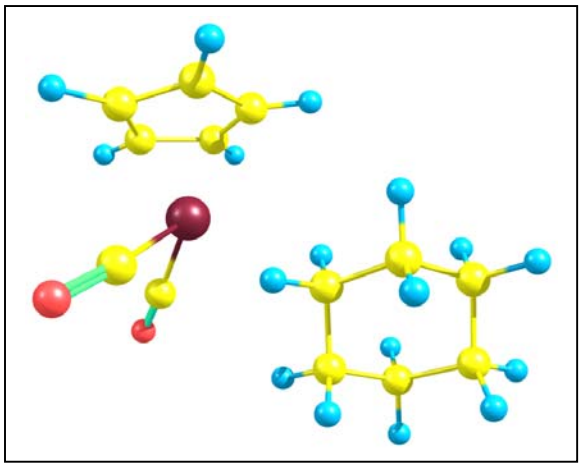


Cyclopentane:



C	-1.316083	.155719	-1.655108
C	-2.017963	.891229	-.644826
C	-2.309367	-.012215	.440887
C	-1.751807	-1.275741	.099994
C	-1.154945	-1.198105	-1.195206
H	-1.023225	.537585	-2.625953
H	-2.360439	1.915463	-.730601
H	-2.865263	.224046	1.340476
H	-1.780669	-2.164119	.723459
H	-.701833	-2.014913	-1.743707
Re	-.003920	.322136	.162998
C	1.532056	.720461	-.858990
O	2.432851	.984388	-1.572142
C	.239470	1.946688	1.099271
O	.322665	2.990076	1.639722
C	3.081432	-1.008766	3.782223
C	2.185640	-2.253801	3.905264
C	1.528320	-2.349149	2.521734
C	1.174280	-.875523	2.228013
C	2.278218	-.021101	2.896721
H	4.017790	-1.284668	3.281018
H	2.742028	-3.157619	4.179243
H	1.413468	-2.092898	4.670130
H	2.254723	-2.723359	1.787984
H	.651593	-3.006710	2.491150
H	.190499	-.648662	2.643660
H	1.249397	-.797950	1.087788
H	1.824286	.781543	3.487610
H	2.912827	.459196	2.144933
H	3.348449	-.579067	4.754093

Cyclohexane

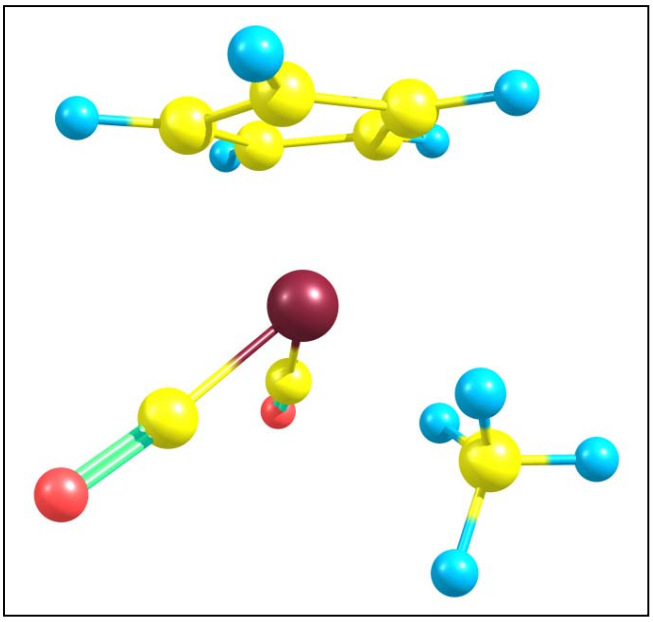


C	.695824	.636109	-2.047673
C	-.559827	.567508	-1.360513
C	-.823214	-.815634	-1.052105
C	.283121	-1.572826	-1.532268
C	1.216550	-.701669	-2.166668
H	1.132119	1.529380	-2.478605
H	-1.233025	1.398621	-1.188105
H	-1.711252	-1.208168	-.571145
H	.396869	-2.648211	-1.435950
H	2.129633	-.994205	-2.670829
Re	1.072373	-.007994	.068253
C	2.596049	1.095028	.235564
O	3.518042	1.828764	.256208
C	.289225	.887643	1.534552
O	-.252840	1.476852	2.399586
C	2.610705	-3.205730	1.218780
C	2.290979	-4.480577	2.011416
C	2.421733	-4.242319	3.521817
C	1.532906	-3.078311	3.980173
C	1.844103	-1.793287	3.200256
C	1.725820	-2.044772	1.692680
H	3.666592	-2.935907	1.365156
H	1.263771	-4.802018	1.782247
H	2.955243	-5.294910	1.693223
H	2.164024	-5.156656	4.072371
H	3.470564	-4.013665	3.761841
H	.476418	-3.345919	3.828672
H	1.661037	-2.900642	5.055905
H	2.866839	-1.460282	3.429148
H	1.169165	-.983035	3.497375
H	.680731	-2.246614	1.435599
H	2.179484	-1.124647	1.184327
H	2.471775	-3.370398	.142572

4-1e. Mononuclear Re, RIMP2.

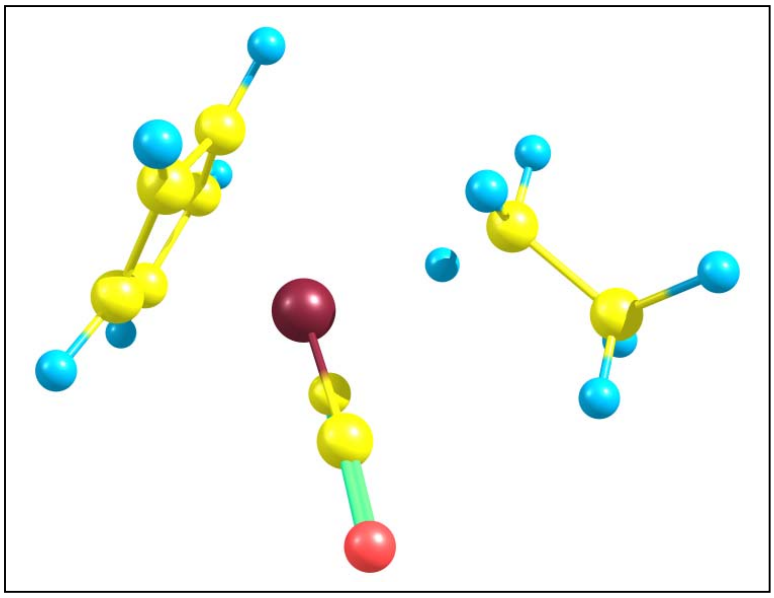
Methane:

C	-1.892969	-1.217253	-.233166
C	-1.521388	-.481497	-1.411445
C	-1.617329	.916426	-1.108480
C	-2.040846	1.049999	.257357
C	-2.167055	-.265340	.787393
H	-1.963279	-2.293737	-.144280
H	-1.321483	-.902949	-2.387963
H	-1.489871	1.725153	-1.816472
H	-2.242904	1.975198	.781098
H	-2.458490	-.502301	1.804957
Re	.044305	.035816	.064492
C	1.157220	1.507986	-.277777
O	1.789745	2.466423	-.571971
C	1.337830	-1.058377	-.743417
O	2.100605	-1.755259	-1.323287
C	.987545	-.738628	2.384953
H	2.003844	-1.116565	2.307303
H	.784104	-.361061	3.388715
H	.944639	.236350	1.790491
H	.277291	-1.528384	2.150741

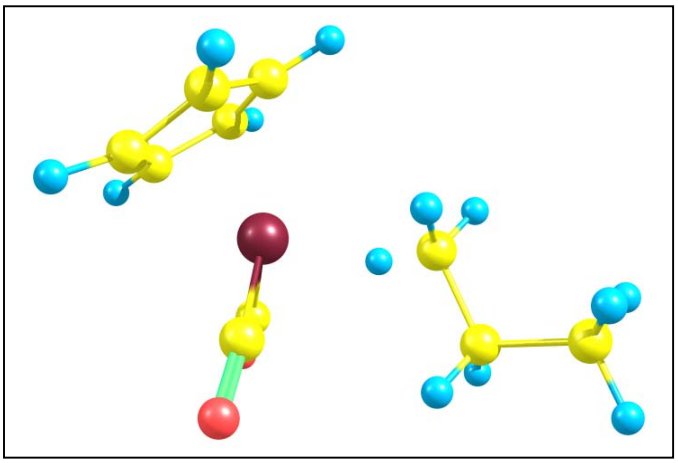


Ethane:

C	1.597655	-1.491673	.820099
C	1.974506	-.112631	.975345
C	2.182913	.438272	-.331706
C	1.926061	-.592313	-1.298010
C	1.530777	-1.755175	-.575180
H	1.406540	-2.198075	1.617730
H	2.182329	.388505	1.911791
H	2.559663	1.430391	-.544930
H	2.030878	-.508508	-2.371813
H	1.255432	-2.704603	-1.021422
Re	.026749	-.028835	-.078423
C	-.491058	1.595144	-.862435
O	-.718358	2.654319	-1.344163
C	-.921469	.478444	1.458342
O	-1.450301	.813585	2.465464
C	-2.040679	-1.509023	-.728881
H	-1.438155	-.628615	-1.161730
H	-1.575492	-2.080546	.074182
H	-2.070631	-2.149739	-1.615582
C	-3.412548	-.981955	-.336487
H	-4.111011	-1.811333	-.194404
H	-3.354812	-.413162	.591793
H	-3.815314	-.326653	-1.112435

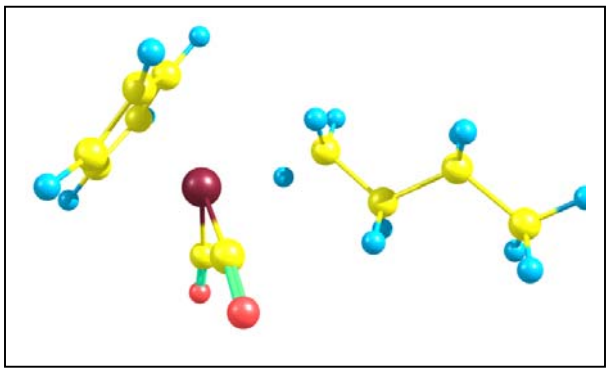


Propane:



C	-1.738990	-1.815525	-.179803
C	-2.407371	-.668608	-.732426
C	-2.673176	.246847	.338327
C	-2.163754	-.325476	1.553052
C	-1.560319	-1.569186	1.209421
H	-1.070760	-2.239567	1.907466
H	-1.437279	-2.704136	-.719279
H	-2.755876	-.565369	-1.751839
H	-3.243746	1.163165	.257373
H	-2.236915	.100600	2.545160
Re	-.479584	.131412	.012672
C	-.287612	1.988834	.191744
O	-.273384	3.170006	.293757
C	.261217	.275558	-1.704354
O	.653921	.354435	-2.820698
C	1.857818	-.663341	.866313
C	3.093573	-.120042	.162854
C	4.247230	-1.114713	.215249
H	2.057311	-.942580	1.906789
H	1.463502	-1.545220	.358778
H	1.137699	.218709	1.041484
H	2.837597	.108175	-.874728
H	3.390820	.825797	.628927
H	4.529254	-1.338530	1.248606
H	5.129425	-.719282	-.295138
H	3.972782	-2.055833	-.27092

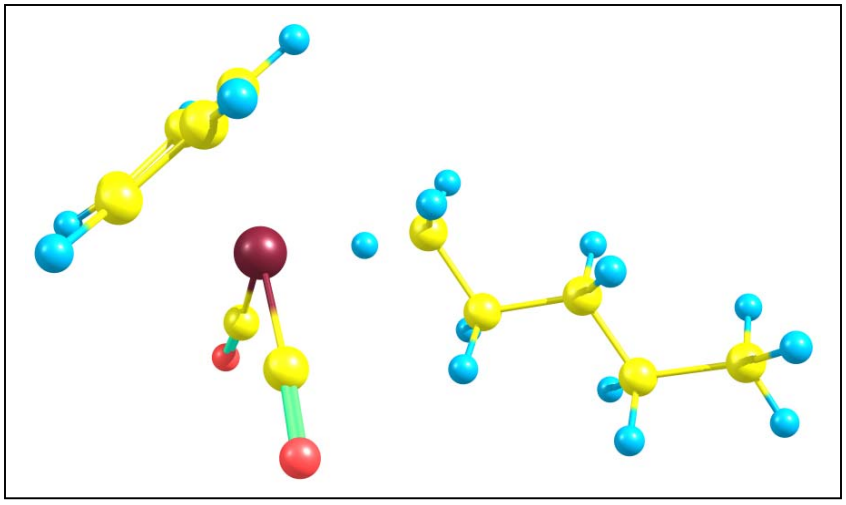
Butane:



C	-1.706337	-1.824147	-.189229
C	-2.383460	-.684135	-.745532
C	-2.667581	.226913	.324277
C	-2.160808	-.341130	1.542115
C	-1.540922	-1.577599	1.201586
H	-1.048908	-2.243195	1.902484
H	-1.390441	-2.708546	-.727520
H	-2.725617	-.583676	-1.767367
H	-3.247842	1.136841	.240140
H	-2.246167	.082869	2.534142
Re	-.470275	.136634	.014802
C	-.299778	1.995777	.196938
O	-.298810	3.176956	.300145
C	.282761	.290853	-1.695830
O	.684781	.375123	-2.808547
C	1.867024	-.633419	.883987
C	3.098028	-.078398	.182416
C	4.269137	-1.053839	.231251
H	2.065836	-.908622	1.925671
H	1.482822	-1.520172	.377192
H	1.136961	.241412	1.057241
H	2.844641	.145585	-.857962
H	3.388559	.871830	.646891
H	4.512822	-1.279950	1.276894
H	3.965987	-2.002354	-.229553
C	5.504412	-.511356	-.478877
H	5.840647	.421408	-.016912
H	6.332534	-1.224195	-.438809
H	5.287464	-.304842	-1.530748

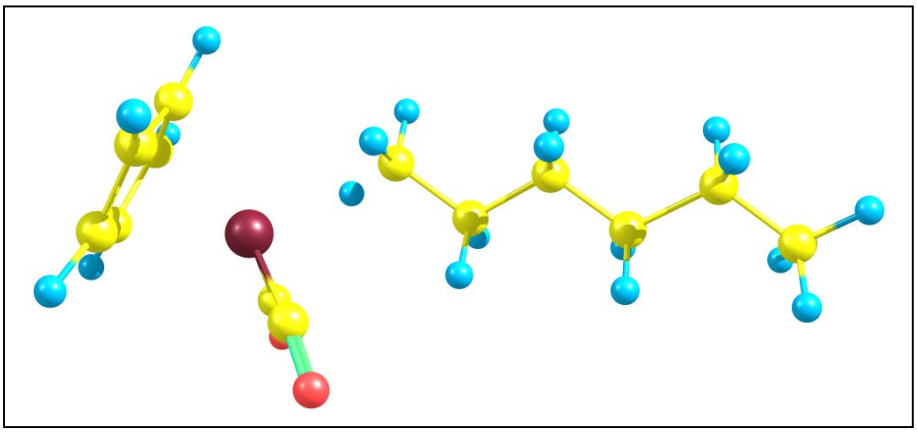
Pentane:

C	3.087322	-.882423	.799102
C	3.494156	-.042362	-.289030
C	2.963199	-.594725	-1.503626
C	2.208287	-1.748349	-1.144334
C	2.310104	-1.964264	.257432
H	3.410914	-.784189	1.827175
H	4.163523	.805136	-.215092
H	3.119442	-.215620	-2.505136
H	1.668298	-2.382511	-1.839028
H	1.888513	-2.792300	.812716
Re	1.291642	.106182	-.043575
C	.507876	.387073	1.636941
O	.083515	.544703	2.733259
C	1.322441	1.966876	-.279262
O	1.448073	3.138251	-.413378
C	-1.089346	-.433756	-.965798
C	-2.267717	.286969	-.327314
C	-3.542436	-.547807	-.384603
C	-4.736127	.150959	.258388
C	-6.007431	-.688775	.205981
H	-.825443	-1.337858	-.414792
H	-.257740	.343954	-1.146890
H	-1.287747	-.725444	-2.003097
H	-2.021776	.519273	.712950
H	-2.429540	1.246069	-.834207
H	-3.781025	-.785586	-1.430201
H	-3.370251	-1.507876	.120750
H	-4.905617	1.109764	-.246291
H	-4.492469	.389301	1.300554
H	-6.848908	-.168703	.671891
H	-5.868741	-1.639028	.730150
H	-6.283666	-.914648	-.828349



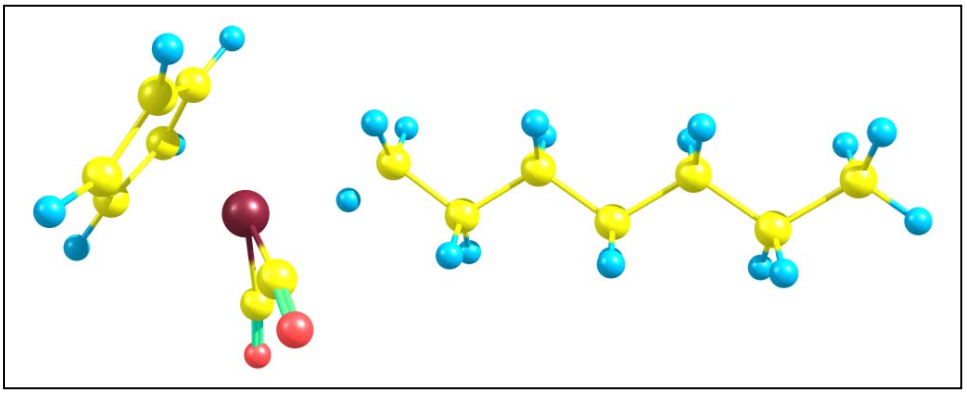
Hexane:

C	-2.838656	-1.097660	1.173402
C	-3.325303	-.149155	.211654
C	-2.902805	-.575692	-1.090270
C	-2.162435	-1.799103	-.936999
C	-2.095678	-2.079185	.454950
H	-3.017244	-1.081425	2.240615
H	-3.975468	.690998	.419588
H	-3.195591	-.122734	-2.028552
H	-1.739646	-2.397159	-1.734074
H	-1.587762	-2.927804	.900115
Re	-1.113834	.013893	.077206
C	-1.119632	1.690311	.918560
O	-1.228559	2.753236	1.432647
C	-.265191	.813392	-1.392064
O	.200557	1.313601	-2.361365
C	1.229663	-.850230	.836949
H	1.385788	-1.504115	1.702119
H	.381723	-.189177	1.254169
H	1.001448	-1.486259	-.019636
C	2.424296	.052208	.564779
H	2.547161	.757613	1.395669
H	2.221858	.651052	-.328006
C	3.709259	-.746247	.373021
H	3.898939	-1.358955	1.264767
H	3.579688	-1.446161	-.463549
C	4.919607	.142317	.104339
H	5.049316	.840186	.942077
H	4.725571	.758582	-.783197
C	6.209882	-.644841	-.099598
H	6.397628	-1.264751	.785787
H	6.079450	-1.338171	-.939513
C	7.413132	.254702	-.359677
H	8.326174	-.329517	-.504532
H	7.257866	.863128	-1.255469
H	7.579545	.934976	.480824

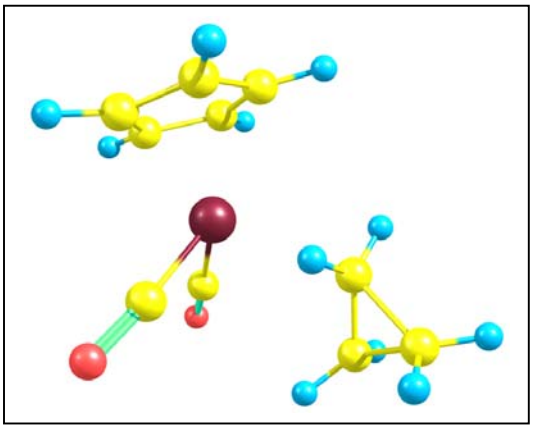


Heptane:

C	-4.407413	-.117040	.169485
C	-3.930817	-.887395	-.941633
C	-3.150547	-1.978222	-.422926
C	-3.117099	-1.835977	.991578
C	-3.916917	-.721602	1.376243
H	-4.127075	-.400610	2.388156
H	-2.592081	-2.493576	1.675883
H	-2.683460	-2.765052	-1.001231
H	-4.210704	-.741461	-1.976851
H	-5.094801	.717041	.109812
Re	-2.200811	.096413	.033344
C	-2.289022	1.939670	.369865
O	-2.449760	3.098509	.562624
C	-1.353677	.491448	-1.592756
O	-.887840	.722021	-2.658897
C	.148198	-.440378	1.033992
C	1.337860	.337488	.490542
C	2.629716	-.468062	.578682
C	3.836228	.289244	.032826
C	5.132733	-.509449	.118811
C	6.341486	.244871	-.425486
C	7.631749	-.561959	-.331161
H	-.708410	.309689	1.215342
H	-.068532	-1.319609	.425220
H	.304960	-.781691	2.063247
H	1.447948	1.276080	1.047228
H	1.139368	.611066	-.549890
H	2.509746	-1.407838	.022794
H	2.818510	-.747214	1.624152
H	3.952378	1.231133	.584931
H	3.646335	.565400	-1.012490
H	5.016129	-1.451937	-.432761
H	5.320281	-.786241	1.165015
H	6.454859	1.187138	.124379
H	6.153358	.519138	-1.470604
H	8.484016	-.002578	-.726951
H	7.854051	-.821196	.708322
H	7.550336	-1.494565	-.897446



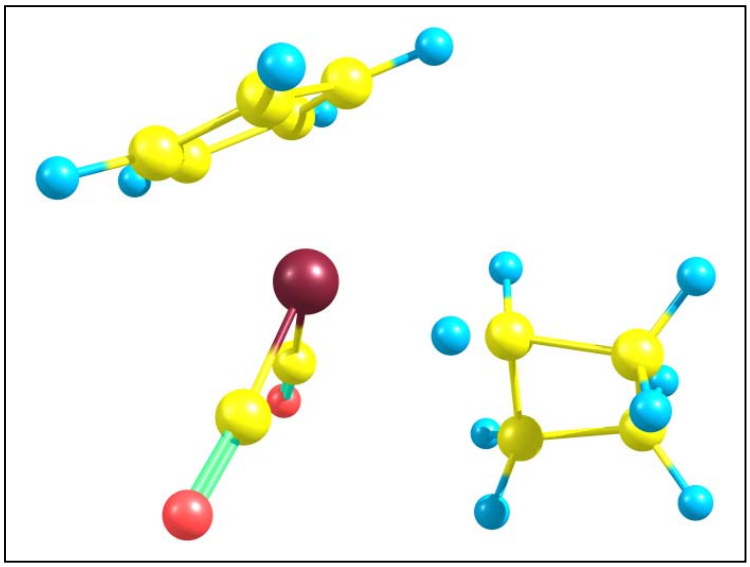
Cyclopropane:



C	-1.158614	-.163604	-1.569749
C	-1.947352	.692227	-.732154
C	-2.254131	-.035537	.471439
C	-1.599217	-1.290627	.386823
C	-.948318	-1.402030	-.880244
H	-.835542	.065870	-2.577318
H	-2.362030	1.649898	-1.018134
H	-2.856388	.319105	1.298284
H	-1.620656	-2.061973	1.148892
H	-.430641	-2.272378	-1.261666
Re	.022815	.391835	.237099
C	1.519095	.865475	-.787459
O	2.409144	1.170347	-1.511180
C	.093643	2.106541	.995430
O	.088373	3.204182	1.440709
C	1.196987	-.438395	2.253827
C	2.030754	.621907	2.918399
C	2.580144	-.754483	2.842802
H	.359747	-.865650	2.789453
H	2.461876	1.382328	2.279403
H	1.663348	.986626	3.871937
H	3.384301	-.949399	2.141186
H	2.590622	-1.371115	3.734907
H	1.336237	-.696240	1.147456

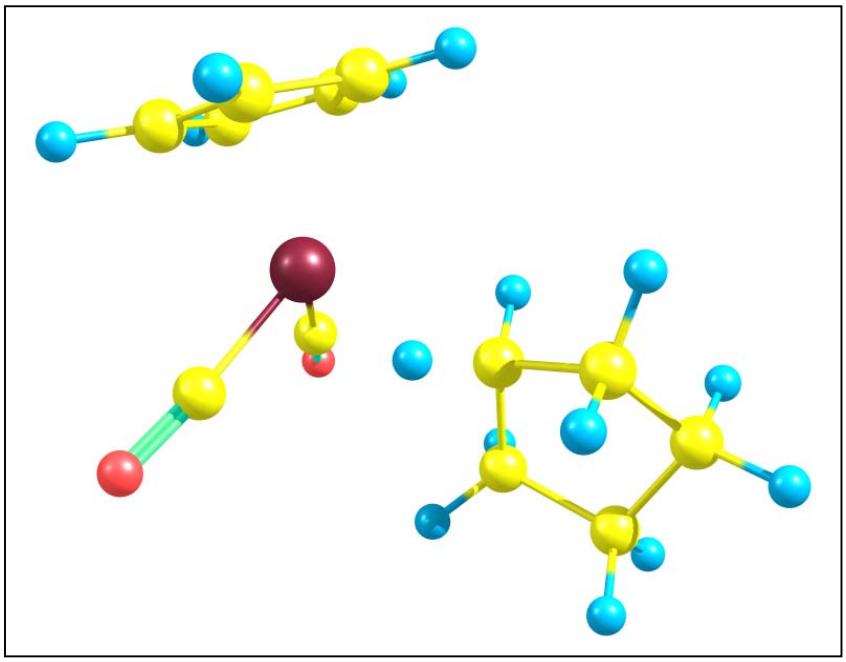
Cyclobutane:

C	-.869148	.286952	-1.544468
C	-1.887222	.527787	-.565545
C	-2.172824	-.719705	.091051
C	-1.288430	-1.691896	-.446675
C	-.504800	-1.098162	-1.481960
H	-.497912	1.010742	-2.258809
H	-2.433613	1.453133	-.437343
H	-2.916399	-.882926	.860840
H	-1.242229	-2.733201	-.147118
H	.210668	-1.605224	-2.116031
Re	.000583	.020945	.494100
C	1.526558	1.029035	.078397
O	2.444590	1.699999	-.259523
C	-.304743	1.208113	1.915535
O	-.557208	1.987149	2.772512
C	2.106324	-2.156351	3.989654
C	1.589742	-.786395	3.499882
C	1.000745	-1.505730	2.283597
C	2.006473	-2.663906	2.534798
H	3.085362	-2.196364	4.474294
H	2.410176	-.129931	3.195515
H	.899295	-.220660	4.128677
H	1.290658	-1.110079	1.228359
H	-.023220	-1.844255	2.435615
H	2.941612	-2.500263	1.991254
H	1.659378	-3.684603	2.353293
H	1.372154	-2.650937	4.632317



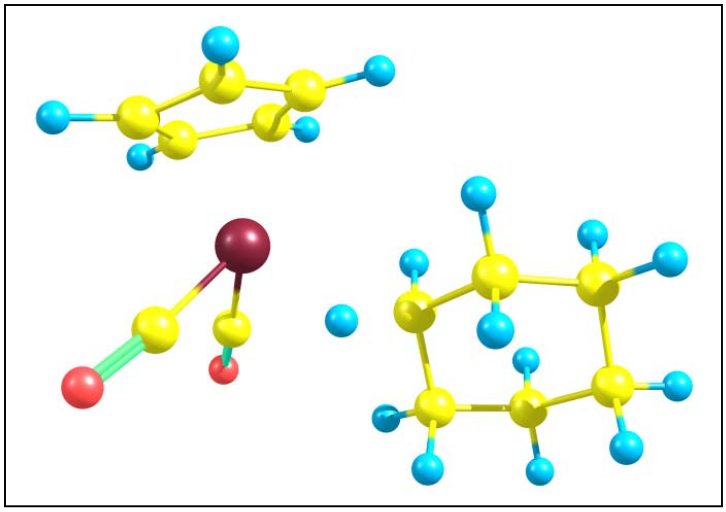
Cyclopentane:

C	-1.288384	.154578	-1.594284
C	-1.983444	.891441	-.580212
C	-2.287283	-.014645	.494934
C	-1.725007	-1.274514	.156569
C	-1.139729	-1.198931	-1.142900
H	-.999114	.536685	-2.565002
H	-2.331533	1.912408	-.668253
H	-2.836546	.222755	1.397154
H	-1.766269	-2.166430	.772199
H	-.689944	-2.015296	-1.692770
Re	.004159	.302246	.214875
C	1.512886	.745978	-.803902
O	2.405513	1.044711	-1.526128
C	.253342	1.904109	1.162872
O	.343487	2.947841	1.717345
C	3.050812	-.996966	3.731410
C	2.169930	-2.245469	3.842433
C	1.534035	-2.344369	2.457129
C	1.159893	-.878559	2.177853
C	2.248137	-.019763	2.845327
H	3.991674	-1.263004	3.237642
H	2.730155	-3.142795	4.122834
H	1.387037	-2.092806	4.595180
H	2.274900	-2.699197	1.730539
H	.669721	-3.014338	2.408951
H	.174889	-.678046	2.601314
H	1.260554	-.828828	1.023721
H	1.785557	.781888	3.427396
H	2.878049	.462260	2.092872
H	3.306999	-.568780	4.704739



Cyclohexane:

C	.739126	.575965	-2.000144
C	-.521942	.520194	-1.321632
C	-.796265	-.856554	-1.011256
C	.314062	-1.620308	-1.464318
C	1.249779	-.762121	-2.110222
H	1.177421	1.461198	-2.442979
H	-1.196585	1.353206	-1.172785
H	-1.686460	-1.240052	-.529114
H	.417674	-2.695325	-1.365283
H	2.164965	-1.063103	-2.603264
Re	1.085655	-.050841	.101239
C	2.565533	1.087656	.271040
O	3.468732	1.856124	.290403
C	.294186	.838844	1.549412
O	-.260228	1.430484	2.415231
C	2.591926	-3.163394	1.189236
C	2.256931	-4.435597	1.965253
C	2.392099	-4.213114	3.470338
C	1.517177	-3.052015	3.938492
C	1.841713	-1.767471	3.178005
C	1.725513	-2.003354	1.675335
H	3.649843	-2.909004	1.338447
H	1.226015	-4.738409	1.735514
H	2.906604	-5.255911	1.638575
H	2.131708	-5.128992	4.013260
H	3.441394	-3.993239	3.708389
H	.460473	-3.307032	3.779453
H	1.641439	-2.888999	5.015186
H	2.865722	-1.447089	3.412439
H	1.175608	-.953045	3.477279
H	.678733	-2.194357	1.419596
H	2.231222	-1.082147	1.190219
H	2.451765	-3.310687	.112515

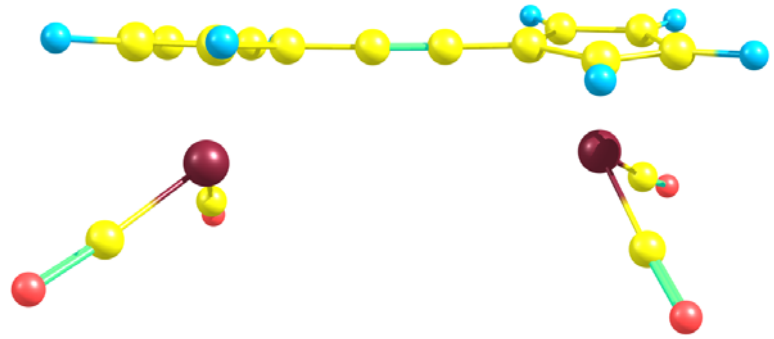


4-2 Binuclear rhenium complexes.

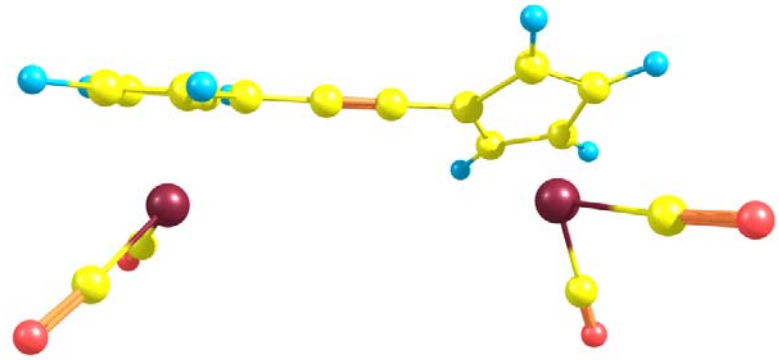
4-2a. Binuclear Re, HF.

Complex:

Re	-3.345239	-0.074239	0.610360
C	-4.236967	1.375836	-0.336002
C	4.200488	-1.714127	0.712047
C	-4.110440	0.440009	2.327352
C	-0.594183	-1.930367	-0.016178
C	-2.029037	-1.941143	-0.032357
C	-2.844331	-1.566191	-1.132343
H	-2.522831	-2.716868	1.984222
H	-2.494051	-1.285432	-2.103139
C	-4.200981	-1.726036	-0.723278
H	-5.063053	-1.568864	-1.337928
C	-4.212823	-2.191557	0.610578
H	-5.083216	-2.454312	1.175001
C	-2.859417	-2.333413	1.044075
C	0.595376	-1.929339	-0.001510
O	4.654012	2.185146	0.988678
O	-4.799896	2.150910	-0.936896
O	-4.598503	0.647074	3.325988
Re	3.345168	-0.074953	-0.636909
H	2.486494	-1.264748	2.081733
C	4.197419	0.444328	-2.310479
C	4.146346	1.397868	0.355427
H	5.088350	-2.453724	-1.178157
C	4.215267	-2.191554	-0.617381
C	2.865185	-2.335913	-1.056520
H	5.059930	-1.554363	1.329490
H	2.532178	-2.731420	-1.992819
C	2.030235	-1.938218	0.017698
O	4.736587	0.655468	-3.281658
C	2.840452	-1.556924	1.115551



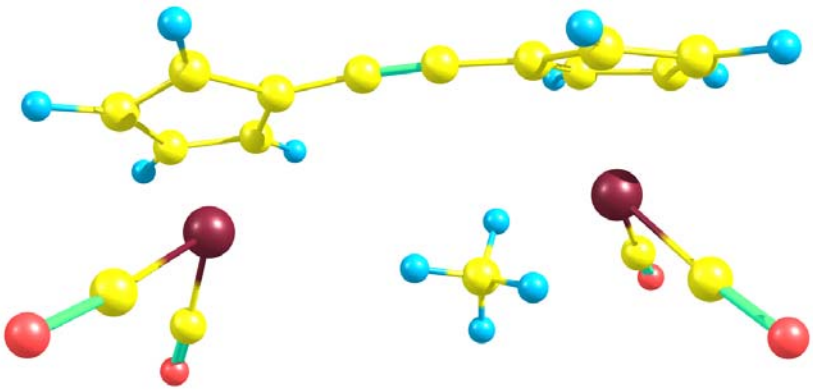
Initial guess



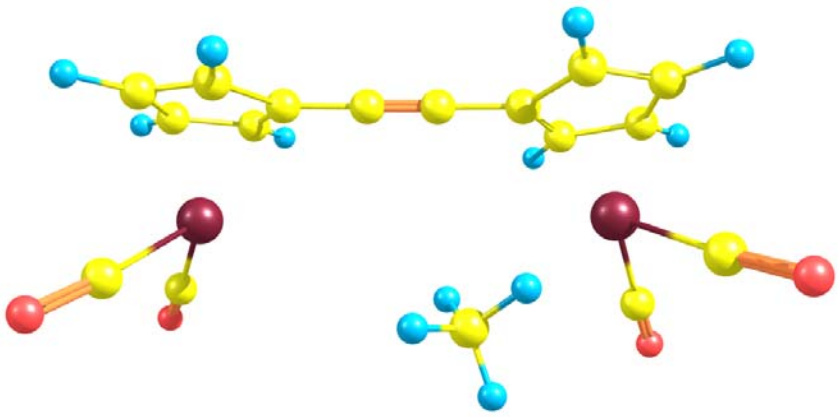
Optimized geometry

Methane:

C	-2.773341	-1.874566	1.153095
C	-1.962432	-1.782745	-0.013353
C	-2.799547	-1.744109	-1.149585
C	-4.150846	-1.806856	-0.690978
C	-4.128038	-1.898334	0.718640
C	-0.528367	-1.774039	-0.035270
C	0.661186	-1.776598	-0.057660
C	2.095331	-1.789906	-0.084682
C	2.942040	-1.642129	1.042885
C	4.287922	-1.707676	0.571893
C	4.259371	-1.893312	-0.828099
C	2.894355	-1.947734	-1.243727
H	-2.416759	-1.992173	2.154524
H	-4.985221	-2.005962	1.350955
H	-5.022324	-1.854035	-1.310044
H	-2.469285	-1.720874	-2.167050
H	2.530835	-2.137131	-2.231705
H	5.112730	-2.031150	-1.459088
H	5.167189	-1.678588	1.181438
H	2.620233	-1.566380	2.060118
Re	3.396788	0.175727	-0.372252
C	4.165796	1.036819	-1.942294
O	4.656434	1.449982	-2.873455
C	4.264249	1.407068	0.862076
O	4.814405	2.043656	1.617807
Re	-3.324165	0.174565	0.132996
C	-4.358114	1.101004	1.488518
O	-5.004728	1.559864	2.296565
C	-4.014399	1.314845	-1.283526
O	-4.448996	1.907290	-2.143991
C	-1.012204	1.962952	0.185456
H	-1.369363	2.936220	-0.117205
H	-0.183590	2.065232	0.875645
H	-1.794524	1.462726	0.787949
H	-0.706407	1.386764	-0.673428



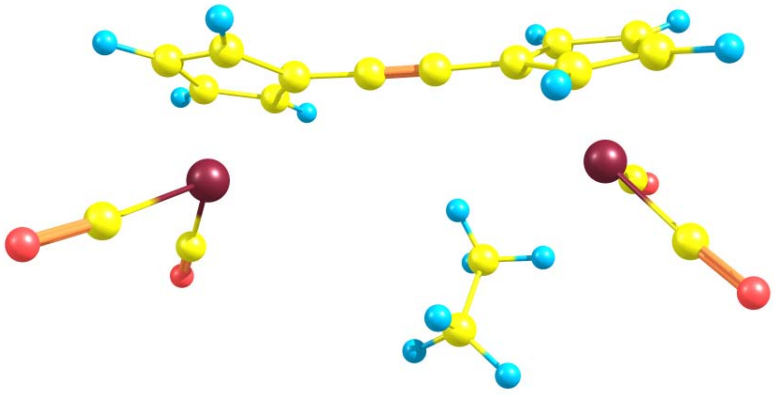
Initial guess



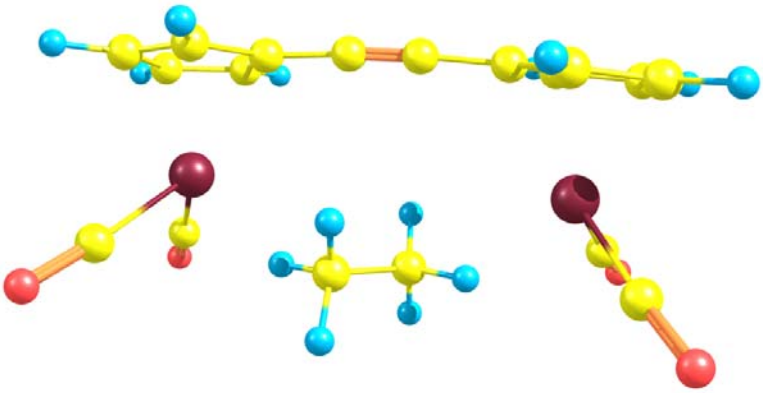
Optimized geometry

Ethane:

C	-4.181042	1.779154	-1.036905
C	-2.787591	1.773520	-1.346276
C	-2.084521	1.869077	-0.120996
C	-3.019422	1.933424	0.943462
C	-4.321732	1.879282	0.364189
H	-4.980831	1.771329	-1.748040
H	-2.346487	1.764439	-2.320765
H	-2.781597	2.070080	1.977430
H	-5.247363	1.955517	0.896230
C	-0.657270	1.867000	0.019578
C	0.524763	1.799668	0.134306
C	1.943500	1.638542	0.268775
C	2.875402	1.628049	-0.796593
C	4.166444	1.406951	-0.228919
C	4.018284	1.287546	1.169943
C	2.635441	1.427774	1.489208
H	2.200239	1.446275	2.466118
H	2.650325	1.814513	-1.825700
H	5.093102	1.396133	-0.764235
H	4.814249	1.165744	1.875157
Re	2.973737	-0.513951	0.194339
C	3.755076	-1.546549	-1.257329
O	4.261185	-2.076015	-2.119519
C	3.574126	-1.784991	1.533868
O	3.975634	-2.455650	2.352706
Re	-3.354719	-0.153791	-0.105401
C	-3.998358	-1.316089	-1.522451
O	-4.414493	-1.916576	-2.387042
C	-4.342656	-1.126666	1.257566
O	-4.963458	-1.615914	2.067082
C	-0.868500	-1.656861	0.566818
C	0.317033	-1.729614	-0.390708
H	0.335240	-0.883082	-1.058991
H	1.239231	-1.784929	0.219049
H	0.308097	-2.635505	-0.983553
H	-1.794079	-1.636262	-0.039241
H	-0.800767	-0.795852	1.213119
H	-0.950652	-2.543077	1.183498



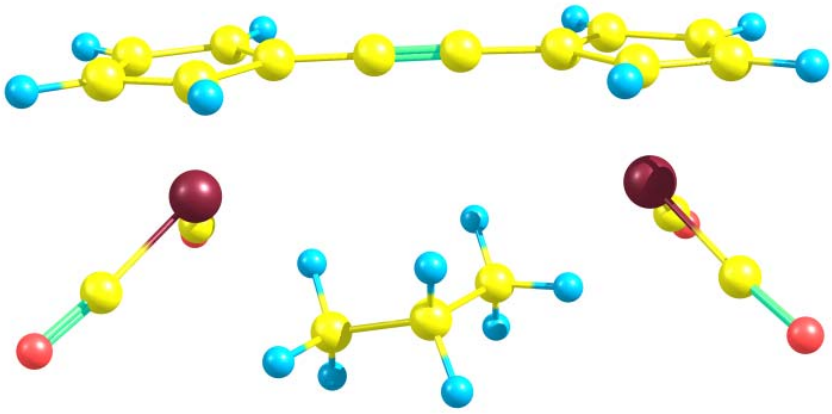
Initial guess



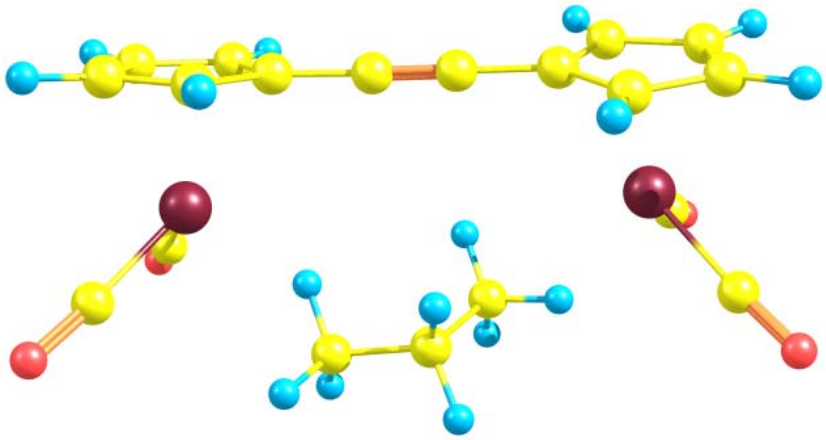
Optimized geometry

Propane:

Re	0.084728	2.943142	-0.633574
C	1.585865	3.559544	0.431744
C	-2.741797	-4.163626	-2.816266
C	-1.165897	4.100032	0.304680
C	-0.631223	0.196684	-2.549539
C	-0.215706	1.569552	-2.570171
C	1.128283	2.031102	-2.539197
H	-2.144860	2.638519	-2.768771
H	2.001250	1.413171	-2.534441
C	1.085308	3.451871	-2.633866
H	1.934906	4.101229	-2.684524
C	-0.266184	3.855578	-2.709288
H	-0.615760	4.858323	-2.841321
C	-1.080010	2.682656	-2.675623
C	-0.985795	-0.939101	-2.557032
O	-5.229871	-3.629936	0.265175
O	2.498850	3.944789	0.979022
O	-1.909003	4.814838	0.770836
Re	-2.305244	-3.465872	-0.668190
H	-3.548012	-2.104068	-3.163902
C	-1.721584	-4.811539	0.599593
C	-4.139358	-3.550932	-0.025889
H	-1.116982	-5.608523	-2.395392
C	-1.438495	-4.590548	-2.476846
C	-0.613720	-3.443819	-2.308854
H	-3.568670	-4.798215	-3.058009
H	0.438344	-3.431321	-2.116656
C	-1.426715	-2.303537	-2.568471
O	-1.357952	-5.651647	1.266346
C	-2.732330	-2.736925	-2.882748
C	-0.234640	0.834473	1.524720
H	-0.907115	1.202229	2.290438
H	0.774471	1.110664	1.790720
H	-0.543943	1.333970	0.584362
C	-0.361303	-0.673959	1.322514
H	0.308964	-0.989664	0.530997
H	-0.035987	-1.174905	2.229685
C	-1.786903	-1.102512	0.985514
H	-2.483896	-0.865985	1.781441
H	-2.139242	-0.638430	0.076426`
H	-1.801919	-2.209331	0.919356



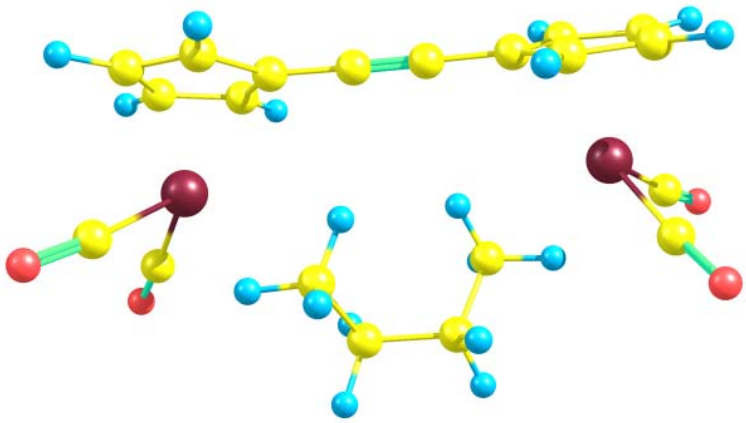
Initial guess



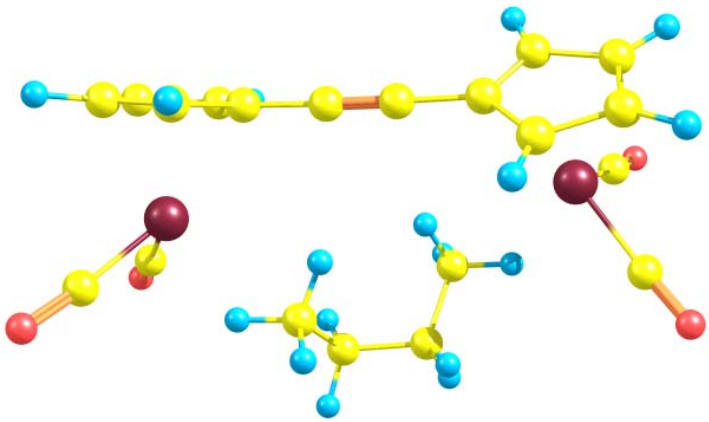
Output geometry

Butane:

Re	0.155951	3.057322	-0.639222
C	1.916482	3.672697	-0.102246
C	-2.513442	-4.260122	-2.904843
C	-0.728547	4.193928	0.660940
C	-0.936901	0.306204	-2.449770
C	-0.652153	1.712816	-2.477525
C	0.587312	2.294406	-2.842849
H	-2.620029	2.606779	-1.981640
H	1.460223	1.759610	-3.153098
C	0.412674	3.709899	-2.822558
H	1.146811	4.435523	-3.105740
C	-0.918015	3.986654	-2.440098
H	-1.365582	4.957354	-2.385463
C	-1.586352	2.745322	-2.219945
C	-1.177821	-0.859526	-2.454945
O	-5.370729	-4.246229	-0.162419
O	2.952645	4.067987	0.124271
O	-1.284765	4.903087	1.346203
Re	-2.420615	-3.585556	-0.712356
H	-3.513517	-2.302800	-3.331132
C	-1.785052	-4.859939	0.602829
C	-4.280235	-3.982774	-0.310231
H	-0.786066	-5.513446	-2.312135
C	-1.217191	-4.539252	-2.418049
C	-0.560189	-3.305591	-2.147094
H	-3.225324	-4.982017	-3.247132
H	0.454139	-3.173090	-1.834474
C	-1.465698	-2.265157	-2.493302
O	-1.375143	-5.652822	1.299700
C	-2.668429	-2.841507	-2.956528
C	-2.346902	-1.279943	1.057550
H	-3.292981	-0.796914	1.273340
H	-2.576708	-2.362754	1.027908
H	-2.005550	-0.918086	0.100134
C	-1.320486	-1.030159	2.165266
H	-1.768998	-1.275745	3.122885
H	-0.474233	-1.700004	2.040133
C	-0.826249	0.422475	2.187190
H	-0.366533	0.635353	3.147327
H	-1.674464	1.095157	2.095749
C	0.186624	0.710693	1.076358
H	1.138967	0.230016	1.269307
H	-0.161267	0.369820	0.113582
H	0.411662	1.794683	1.070097



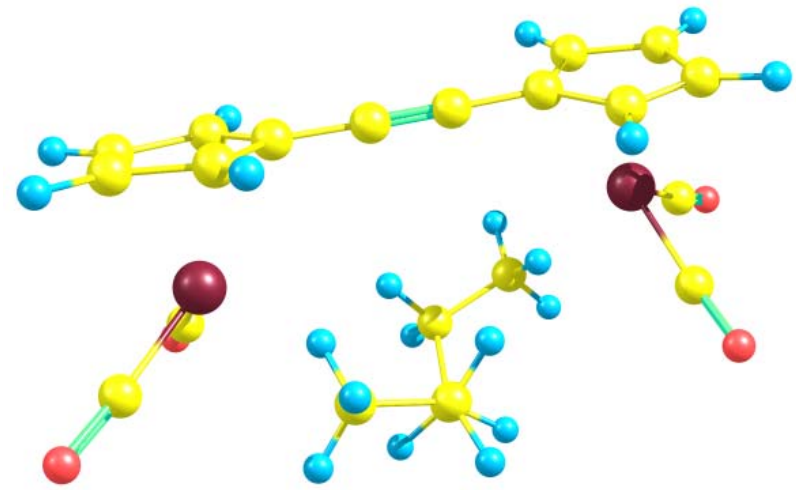
Initial guess



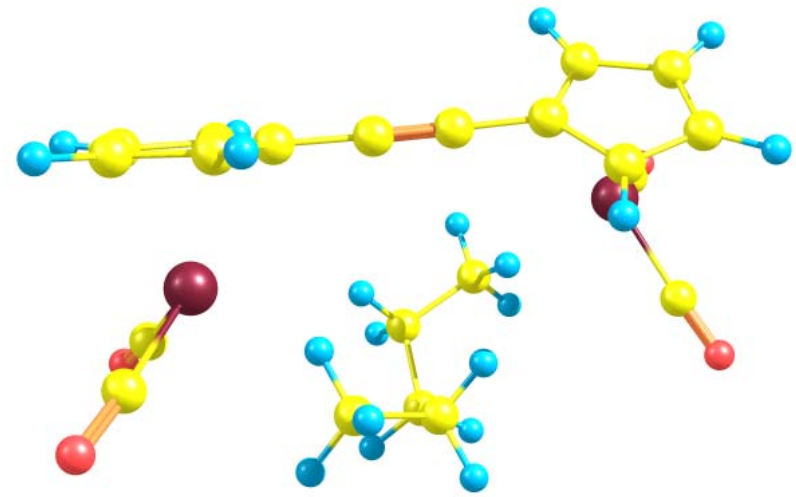
Optimized geometry

Pentane:

Re	0.379781	2.886955	-0.662716
C	2.167927	3.391885	-0.096333
C	-2.696733	-4.185174	-2.910016
C	-0.453519	3.939837	0.739770
C	-0.884336	0.299014	-2.503540
C	-0.525606	1.688561	-2.522076
C	0.741182	2.209461	-2.892673
H	-2.428355	2.678446	-1.962235
H	1.575716	1.635777	-3.236920
C	0.650598	3.630394	-2.817485
H	1.424178	4.321698	-3.081214
C	-0.654743	3.972451	-2.401340
H	-1.042121	4.965262	-2.303253
C	-1.393264	2.764542	-2.218371
C	-1.187947	-0.851048	-2.509345
O	-5.539482	-4.175572	-0.173654
O	3.221722	3.719939	0.154787
O	-0.979183	4.602369	1.492744
Re	-2.621270	-3.405084	-0.752181
H	-3.572352	-2.195791	-3.445675
C	-1.937107	-4.451807	0.732875
C	-4.461859	-3.871219	-0.338265
H	-1.062933	-5.513787	-2.219865
C	-1.436035	-4.522053	-2.370485
C	-0.713439	-3.312928	-2.139656
H	-3.444686	-4.879423	-3.233080
H	0.294239	-3.224421	-1.791614
C	-1.546314	-2.240496	-2.540358
O	-1.493933	-5.112364	1.538835
C	-2.774566	-2.765245	-3.017472
C	-3.204529	-1.066257	1.025831
H	-4.022384	-0.752711	0.392839
H	-2.485467	-1.654628	0.417961
H	-3.593906	-1.700491	1.810918
C	-2.460362	0.140082	1.605169
H	-2.150970	0.795834	0.798441
H	-3.176396	0.704739	2.196093
C	-1.262309	-0.224917	2.493437
H	-1.550901	-1.045272	3.146050
H	-1.038453	0.613644	3.148315
C	0.017092	-0.612815	1.738216
H	0.670819	-1.159160	2.412662
H	-0.212052	-1.291868	0.923891
C	0.815694	0.578176	1.201005
H	0.161517	1.146031	0.506879
H	1.125900	1.235399	2.002235
H	1.691921	0.249376	0.660484



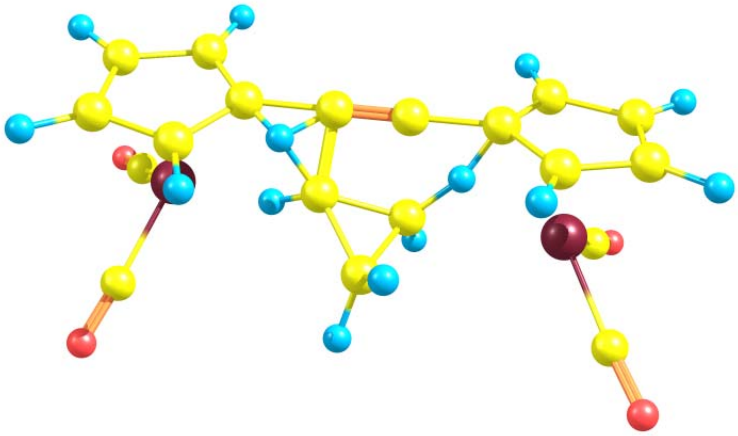
Initial guess



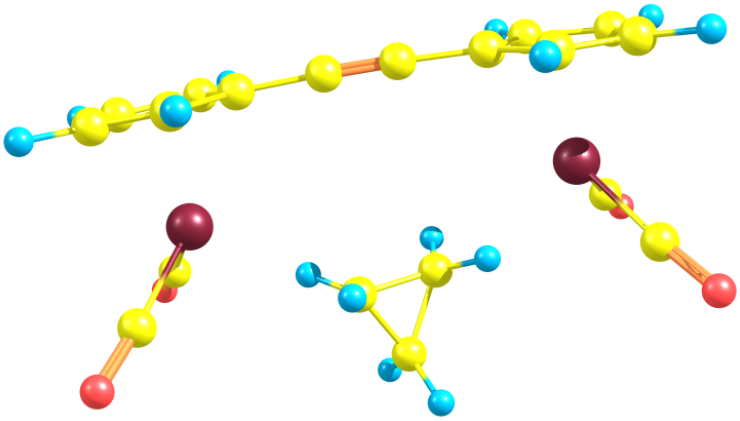
Optimized geometry

Cyclopropane:

C	-0.379078	0.174453	-3.316222
C	0.266844	-0.829576	-2.551635
C	1.544432	-1.082263	-3.108839
C	1.692863	-0.219996	-4.236816
C	0.514875	0.548128	-4.363508
C	-0.277592	-1.467432	-1.388667
C	-0.716910	-1.964364	-0.401830
C	-1.229824	-2.527641	0.812792
C	-2.501243	-2.253594	1.373646
C	-2.600358	-3.001738	2.585298
C	-1.399553	-3.724303	2.757257
C	-0.539363	-3.433558	1.656891
H	-1.377147	0.528495	-3.166238
H	0.307113	1.250587	-5.143967
H	2.527689	-0.201707	-4.906493
H	2.233851	-1.829735	-2.776796
H	0.419074	-3.865263	1.459431
H	-1.192715	-4.414809	3.548494
H	-3.458797	-3.052770	3.222476
H	-3.262661	-1.648363	0.928503
Re	-0.909848	-1.487741	2.934103
C	0.372082	-1.717493	4.376102
O	1.093767	-1.943313	5.218379
C	-1.985837	-0.252485	3.982581
O	-2.681118	0.404826	4.586407
Re	1.555661	1.168414	-2.412219
C	1.143147	3.057676	-2.601430
O	0.865587	4.137628	-2.796229
C	3.466757	1.512120	-2.298680
O	4.588318	1.660170	-2.308964
C	1.469386	1.049201	0.591776
C	1.497504	1.913431	1.813792
C	0.414704	0.893555	1.636934
H	1.133236	1.549432	-0.319919
H	2.267735	1.722238	2.538798
H	1.224835	2.948696	1.717222
H	0.517159	0.004742	2.264056
H	-0.579883	1.230824	1.424685
H	2.210075	0.282205	0.487067



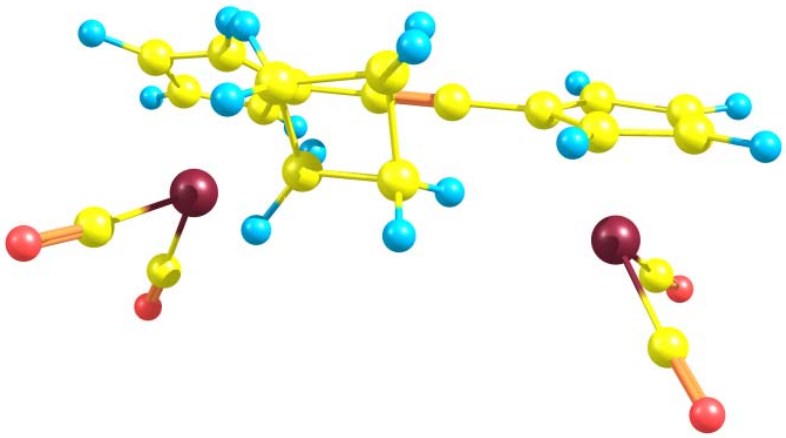
Initial guess



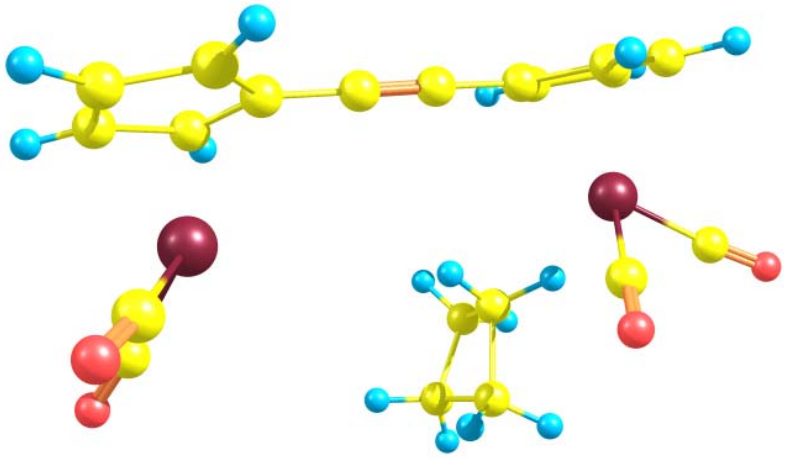
Optimized geometry

Cyclobutane:

C	-0.977035	0.263118	-3.326712
C	-0.468889	-0.778219	-2.481522
C	0.820499	-1.122474	-2.987510
C	1.106451	-0.323753	-4.101097
C	-0.010124	0.551789	-4.308165
C	-1.176478	-1.459058	-1.441868
C	-1.756639	-2.021430	-0.566973
C	-2.455605	-2.704356	0.482277
C	-3.850907	-2.631830	0.729709
C	-4.121004	-3.443271	1.872593
C	-2.903085	-4.000077	2.320332
C	-1.860609	-3.542770	1.455446
H	-1.946354	0.709821	-3.245341
H	-0.122997	1.249044	-5.111995
H	1.986978	-0.378447	-4.707435
H	1.461724	-1.872404	-2.569858
H	-0.829465	-3.826242	1.489046
H	-2.790621	-4.694804	3.126422
H	-5.088511	-3.637610	2.287149
H	-4.566692	-2.121184	0.120757
Re	-2.801167	-1.737914	2.628967
C	-1.768784	-1.818677	4.276233
O	-1.174104	-1.964556	5.228213
C	-4.264001	-0.766975	3.471273
O	-5.172411	-0.282154	3.939522
Re	0.857548	1.142310	-2.256434
C	-0.189850	2.317779	-1.118745
O	-0.867930	2.973221	-0.493275
C	1.963306	2.613607	-2.880579
O	2.579619	3.452902	-3.324754
C	3.705574	-0.172911	0.491352
C	3.559492	0.472856	1.888238
C	2.500495	1.432524	1.298190
C	2.343669	0.454007	0.119609
H	4.518593	0.268093	-0.073622
H	4.445640	0.916610	2.325142
H	3.124972	-0.213269	2.606542
H	2.937957	2.373168	0.984246
H	1.617894	1.639415	1.890446
H	2.352652	0.913257	-0.893839
H	1.522682	-0.233476	0.252606
H	3.787457	-1.251652	0.435954



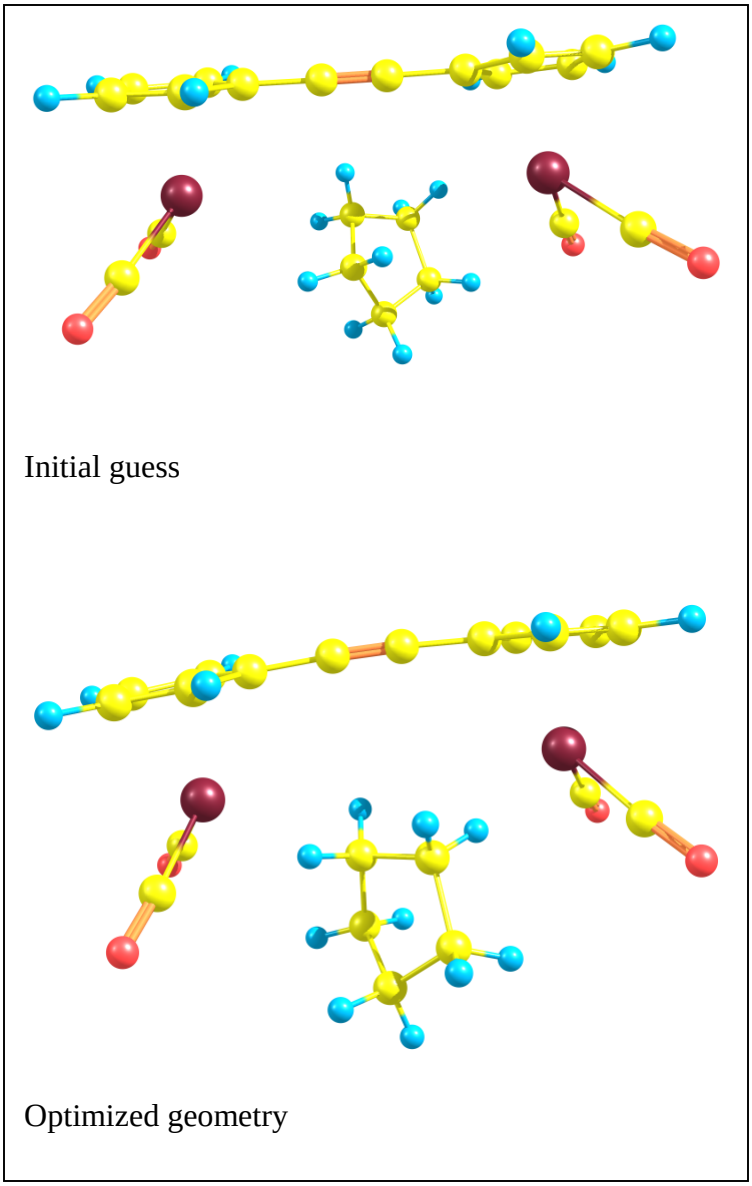
Initial guess



Optimized geometry

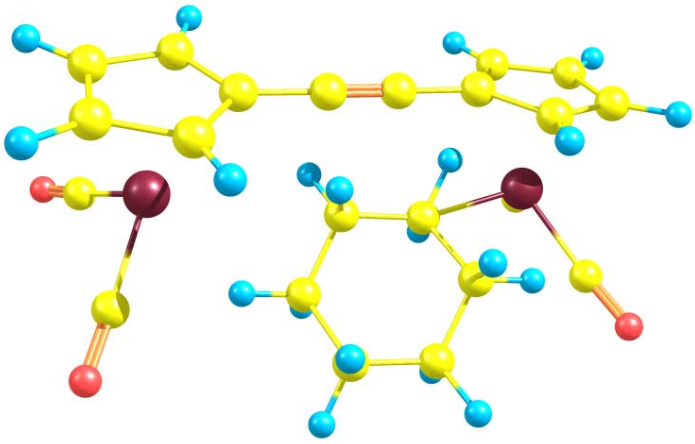
Cyclopentane:

C	0.012859	0.908107	-2.866461
C	0.523674	-0.226495	-2.187601
C	1.694523	-0.671319	-2.849511
C	1.913143	0.203623	-3.955496
C	0.883282	1.169192	-3.966241
C	-0.034560	-0.810626	-1.003195
C	-0.466110	-1.263726	0.008124
C	-0.945050	-1.769248	1.261425
C	-2.000845	-1.211419	2.021836
C	-2.129197	-1.995348	3.207781
C	-1.162074	-3.022866	3.164578
C	-0.417949	-2.888490	1.955425
H	-0.894234	1.422919	-2.628858
H	0.748262	1.932209	-4.704640
H	2.690250	0.108782	-4.685340
H	2.263523	-1.540970	-2.596299
H	0.346809	-3.544089	1.595424
H	-1.042491	-3.800403	3.890430
H	-2.870516	-1.864087	3.968511
H	-2.619903	-0.391425	1.724116
Re	-0.051890	-1.014063	3.338241
C	1.310359	-1.668488	4.559995
O	2.060084	-2.124841	5.274577
C	-0.595844	0.382854	4.571292
O	-0.997620	1.157477	5.292963
Re	2.151874	1.510508	-2.077291
C	2.057849	3.449373	-2.145647
O	1.960546	4.571544	-2.258183
C	4.092529	1.520638	-2.118970
O	5.219505	1.479304	-2.221256
C	2.087039	0.529696	1.903136
C	1.834435	1.701145	0.934596
C	2.489978	2.902958	1.615782
C	3.767957	2.305910	2.212416
C	3.338472	0.918348	2.731119
H	2.189103	-0.412056	1.388706
H	1.206020	0.495536	2.577089
H	2.414303	1.473801	0.014103
H	0.792754	1.835417	0.689120
H	1.836808	3.262187	2.407747
H	2.673189	3.730111	0.941065
H	4.517728	2.201639	1.433137
H	4.198789	2.923014	2.992177
H	4.127488	0.183311	2.626681
H	3.091669	0.968086	3.784879

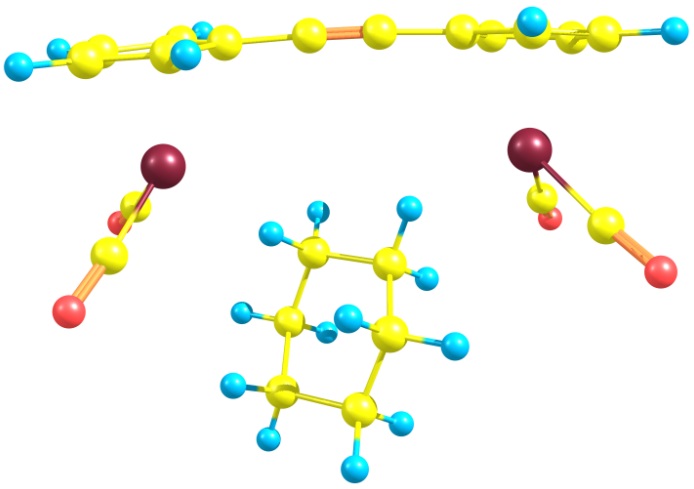


Cyclohexane:

C	-.161466	-.109533	-3.285842
C	.420340	-1.017127	-2.367592
C	1.795679	-1.168435	-2.675414
C	2.068602	-.338482	-3.803072
C	.871460	.310459	-4.176502
C	-.263863	-1.665712	-1.288633
C	-.815054	-2.176778	-.367520
C	-1.455276	-2.742195	.783344
C	-2.756649	-2.421852	1.239581
C	-2.979362	-3.164135	2.438788
C	-1.824236	-3.931826	2.703577
C	-.868365	-3.674551	1.676507
H	-1.197068	.154163	-3.332921
H	.747773	.959688	-5.017405
H	3.006570	-.262902	-4.313177
H	2.475515	-1.834985	-2.187960
H	.086037	-4.141681	1.554240
H	-1.707052	-4.627856	3.508259
H	-3.887417	-3.182909	3.004956
H	-3.455642	-1.786140	.738119
Re	-1.263734	-1.715462	2.917364
C	-.101151	-1.981571	4.452599
O	.551381	-2.222584	5.345342
C	-2.372747	-.430586	3.864368
O	-3.089223	.259629	4.404223
Re	1.487330	1.099356	-2.109388
C	.909328	2.923575	-2.445562
O	.551536	3.960631	-2.724646
C	3.312583	1.643999	-1.738371
O	4.404736	1.908178	-1.597817
C	.890727	3.038515	1.237748
C	2.304492	3.078660	1.826648
C	2.454331	2.115284	3.008066
C	2.030096	.690856	2.635538
C	.608215	.679773	2.067994
C	.470825	1.614488	.860401
H	.182328	3.415005	1.973569
H	3.025564	2.817575	1.055703
H	2.541471	4.091179	2.139536
H	3.481493	2.114724	3.360164
H	1.841310	2.463436	3.837725
H	2.715730	.285986	1.893889
H	2.091079	.043673	3.504375
H	-.082456	1.025393	2.831447
H	.332130	-.343924	1.772862
H	1.148473	1.228689	.068810
H	-.539007	1.595402	.472195
H	.820475	3.694860	.377663



Initial guess

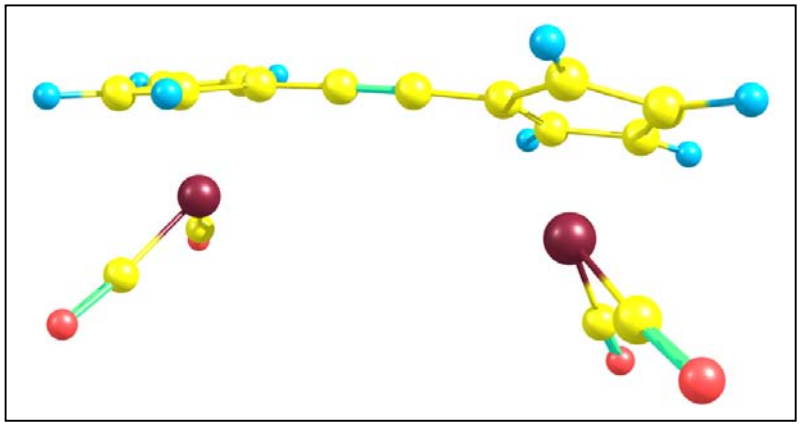


Optimized geometry

4-2b. Binuclear Re, DFT(B3LYP).

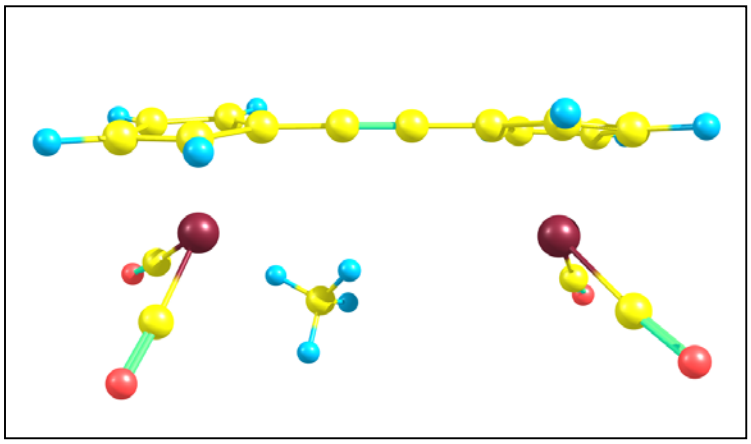
Complex:

Re	-3.183251	-0.104452	0.489715
C	-3.910591	1.280986	-0.609992
C	4.212576	-1.733083	0.611549
C	-3.912151	0.670409	2.077557
C	-0.607044	-2.157317	0.017208
C	-2.024499	-2.117706	0.037958
C	-2.858385	-1.804910	-1.087631
H	-2.509958	-2.589961	2.177954
H	-2.513312	-1.647995	-2.099352
C	-4.211557	-1.745767	-0.613328
H	-5.089693	-1.569292	-1.218398
C	-4.210772	-2.061597	0.790599
H	-5.089655	-2.159837	1.413046
C	-2.855289	-2.306542	1.194506
C	0.608264	-2.153310	-0.015675
O	4.461688	2.039081	1.331500
O	-4.413326	2.044134	-1.333630
O	-4.413993	1.046320	3.060261
Re	3.179282	-0.087384	-0.480929
H	2.517479	-1.645980	2.101327
C	3.880429	0.693847	-2.079091
C	3.936983	1.286058	0.612807
H	5.088391	-2.133606	-1.418782
C	4.210437	-2.039532	-0.794412
C	2.854290	-2.287563	-1.196290
H	5.091372	-1.555850	1.215531
H	2.507944	-2.566363	-2.180739
C	2.025435	-2.106741	-0.038298
O	4.366550	1.073037	-3.068300
C	2.860876	-1.796149	1.087980



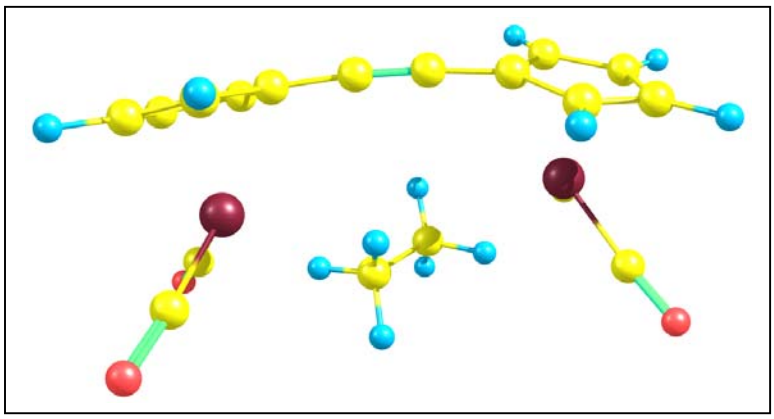
Methane:

C	-2.740496	-1.869508	1.147720
C	-1.958564	-1.815305	-0.072960
C	-2.859979	-1.736703	-1.175562
C	-4.199985	-1.709281	-0.655961
C	-4.113009	-1.816059	0.772920
C	-0.543681	-1.837054	-0.136274
C	0.672195	-1.830821	-0.150564
C	2.090050	-1.831455	-0.146897
C	2.914343	-1.604315	1.009273
C	4.277664	-1.583728	0.565318
C	4.293912	-1.821332	-0.853687
C	2.936901	-1.993733	-1.292746
H	-2.339124	-1.986038	2.144070
H	-4.956482	-1.866312	1.448762
H	-5.108528	-1.709855	-1.241859
H	-2.572338	-1.678429	-2.216296
H	2.602702	-2.212903	-2.296433
H	5.180204	-1.931005	-1.463406
H	5.150190	-1.470112	1.193546
H	2.555562	-1.482524	2.021412
Re	3.348914	0.159573	-0.466052
C	4.090882	0.988682	-2.021002
O	4.596558	1.397493	-2.988505
C	4.171792	1.427088	0.700958
O	4.731627	2.109554	1.463485
Re	-3.251565	0.187124	0.134704
C	-4.440289	1.141832	1.272194
O	-5.219086	1.643364	1.982184
C	-3.708446	1.346194	-1.312212
O	-4.024136	1.975063	-2.241879
C	-1.026324	1.746078	0.490512
H	-1.251744	2.535498	-0.222471
H	-0.475106	2.155112	1.343757
H	-1.961714	1.389523	1.032065
H	-0.446685	0.944715	0.035055



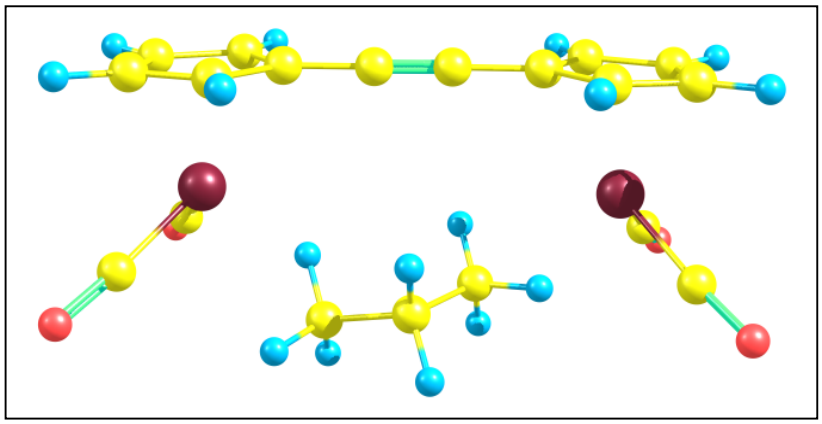
Ethane:

C	-4.140699	1.567467	-1.198842
C	-2.734492	1.622561	-1.468849
C	-2.071623	1.907597	-0.221046
C	-3.061276	2.048605	0.800726
C	-4.346379	1.814806	0.198740
H	-4.922221	1.406671	-1.928981
H	-2.250103	1.516389	-2.428482
H	-2.863802	2.279818	1.837966
H	-5.304524	1.894413	0.693428
C	-0.665334	1.948401	-0.026738
C	0.535677	1.879956	0.140473
C	1.924054	1.671928	0.351045
C	2.946270	1.726671	-0.644917
C	4.182685	1.333859	-0.023915
C	3.919237	1.081022	1.362331
C	2.523636	1.283836	1.605301
H	2.008394	1.208785	2.551796
H	2.801523	1.999382	-1.680707
H	5.153900	1.319074	-0.497056
H	4.660237	0.815035	2.103788
Re	2.880551	-0.502711	0.129276
C	3.574585	-1.357857	-1.431942
O	4.059789	-1.793236	-2.398594
C	3.532525	-1.911976	1.232149
O	3.990628	-2.703516	1.957499
Re	-3.262667	-0.150625	-0.028356
C	-4.048176	-1.454279	-1.172790
O	-4.582397	-2.174578	-1.919835
C	-4.054046	-0.972277	1.503114
O	-4.587401	-1.384199	2.454762
C	-0.846171	-1.492463	0.520733
C	0.340334	-1.565098	-0.445876
H	0.393193	-0.679253	-1.078304
H	1.258442	-1.723383	0.199652
H	0.308669	-2.448174	-1.089644
H	-1.773509	-1.505269	-0.131563
H	-0.775431	-0.619666	1.168752
H	-0.938506	-2.385073	1.144686



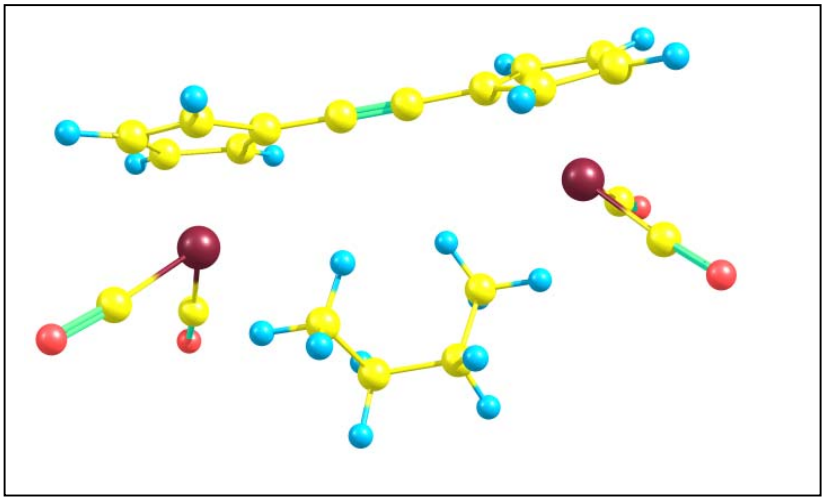
Propane:

Re	0.021141	2.914051	-0.622568
C	1.366390	3.573440	0.550276
C	-2.922063	-4.097857	-2.694545
C	-1.277262	4.075604	0.157260
C	-0.592871	0.191028	-2.592567
C	-0.133762	1.533172	-2.581142
C	1.232580	1.956459	-2.398278
H	-2.014390	2.686073	-2.949363
H	2.083952	1.299047	-2.292657
C	1.244631	3.386352	-2.449329
H	2.121909	4.015419	-2.381962
C	-0.098812	3.846942	-2.660315
H	-0.398671	4.875352	-2.807979
C	-0.949343	2.692269	-2.765093
C	-0.992610	-0.956132	-2.610928
O	-5.036361	-3.745303	0.558628
O	2.243381	4.002648	1.190249
O	-2.076282	4.837941	0.532549
Re	-2.230301	-3.441084	-0.650263
H	-3.670754	-1.986570	-2.974187
C	-1.535710	-4.756003	0.538366
C	-3.951369	-3.605322	0.153126
H	-1.314357	-5.637415	-2.417175
C	-1.593872	-4.594501	-2.478444
C	-0.693407	-3.478690	-2.438802
H	-3.808915	-4.701616	-2.828087
H	0.381682	-3.514977	-2.334803
C	-1.480692	-2.287656	-2.613646
O	-1.092373	-5.622638	1.182976
C	-2.850591	-2.666546	-2.792354
C	-0.374267	0.907502	1.432338
H	-1.089210	1.179622	2.215656
H	0.606091	1.283425	1.720201
H	-0.786370	1.421893	0.508177
C	-0.329535	-0.599159	1.160287
H	0.313768	-0.793835	0.295276
H	0.137623	-1.091851	2.022436
C	-1.718109	-1.196510	0.917867
H	-2.384283	-1.069586	1.776670
H	-2.198537	-0.755406	0.044359
H	-1.567215	-2.321611	0.852790

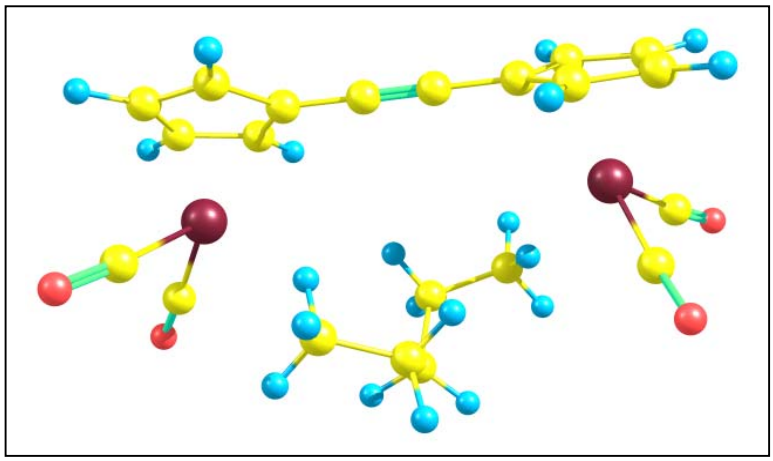


Butane:

Re	0.079091	3.038560	-0.616262
C	1.668796	3.808506	0.087368
C	-2.720046	-4.217563	-2.807987
C	-0.996060	4.074462	0.568576
C	-0.886033	0.296987	-2.498494
C	-0.566131	1.680125	-2.513522
C	0.742976	2.242609	-2.733489
H	-2.564916	2.632643	-2.205741
H	1.642728	1.677594	-2.930482
C	0.601586	3.668146	-2.712985
H	1.389686	4.385356	-2.897138
C	-0.775626	3.984728	-2.468850
H	-1.207091	4.975494	-2.458888
C	-1.501575	2.749041	-2.362408
C	-1.162244	-0.886926	-2.503609
O	-5.302789	-4.150131	0.067946
O	2.661113	4.320957	0.427227
O	-1.696279	4.758970	1.203297
Re	-2.385368	-3.565748	-0.682776
H	-3.654130	-2.195176	-3.173129
C	-1.743232	-4.867464	0.546628
C	-4.182363	-3.911954	-0.153315
H	-0.991172	-5.575697	-2.358116
C	-1.381707	-4.569966	-2.433383
C	-0.626955	-3.364089	-2.257415
H	-3.507974	-4.908034	-3.073971
H	0.425114	-3.281676	-2.024924
C	-1.509695	-2.263288	-2.533038
O	-1.318755	-5.721330	1.220440
C	-2.796266	-2.784274	-2.881429
C	-2.229958	-1.366470	1.011860
H	-3.226551	-1.003959	1.279019
H	-2.322419	-2.496220	0.997239
H	-1.962199	-0.934252	0.046550
C	-1.195589	-1.046082	2.102391
H	-1.605228	-1.338804	3.076253
H	-0.293726	-1.653637	1.952297
C	-0.815474	0.445994	2.125384
H	-0.371392	0.697550	3.095830
H	-1.718846	1.061717	2.030779
C	0.182935	0.799308	1.013118
H	1.187799	0.428621	1.239340
H	-0.112843	0.381776	0.049476
H	0.306134	1.927945	1.016309



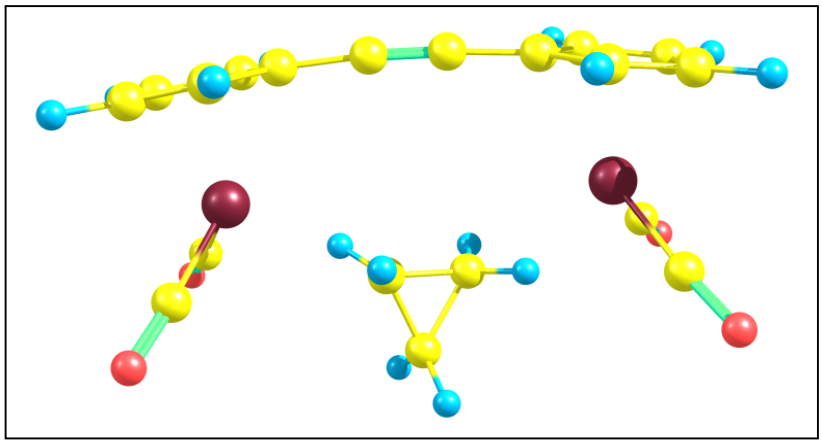
Pentane:



Re	0.240756	2.917776	-0.656883
C	1.768485	3.715476	0.148497
C	-2.735805	-4.187693	-2.787625
C	-0.903243	3.813446	0.578525
C	-0.812075	0.296731	-2.541168
C	-0.424904	1.661378	-2.571861
C	0.921416	2.156316	-2.772522
H	-2.370745	2.726768	-2.306332
H	1.791128	1.545241	-2.966988
C	0.857454	3.581053	-2.737138
H	1.690537	4.256104	-2.879861
C	-0.502017	3.976139	-2.504680
H	-0.875699	4.990085	-2.493095
C	-1.299279	2.781326	-2.442189
C	-1.142550	-0.871459	-2.511975
O	-5.742825	-3.813558	-0.313064
O	2.726860	4.240431	0.559474
O	-1.644171	4.416583	1.249004
Re	-2.736170	-3.314988	-0.716195
H	-3.518814	-2.196771	-3.510371
C	-2.290928	-4.431355	0.758823
C	-4.600297	-3.602268	-0.418420
H	-1.174097	-5.524402	-1.886437
C	-1.499135	-4.525461	-2.142365
C	-0.744597	-3.320127	-1.957099
H	-3.492958	-4.887640	-3.112588
H	0.244822	-3.232529	-1.532782
C	-1.528626	-2.236982	-2.488580
O	-1.968398	-5.181286	1.593985
C	-2.745694	-2.769691	-3.018745
C	-3.162174	-1.141106	1.170515
H	-4.069409	-0.766588	0.694734
H	-2.514186	-1.623041	0.372048
H	-3.430753	-1.888321	1.918657
C	-2.323712	-0.006064	1.779047
H	-2.160215	0.775216	1.027312
H	-2.937852	0.453322	2.564335
C	-0.981740	-0.459575	2.384683
H	-1.134387	-1.412119	2.909299
H	-0.671606	0.260994	3.153452
C	0.167475	-0.619532	1.370785
H	0.932088	-1.284710	1.793571
H	-0.189407	-1.112172	0.458074
C	0.877322	0.693884	1.008367
H	0.069648	1.391273	0.612306
H	1.303333	1.183757	1.886734
H	1.667915	0.531481	0.276354

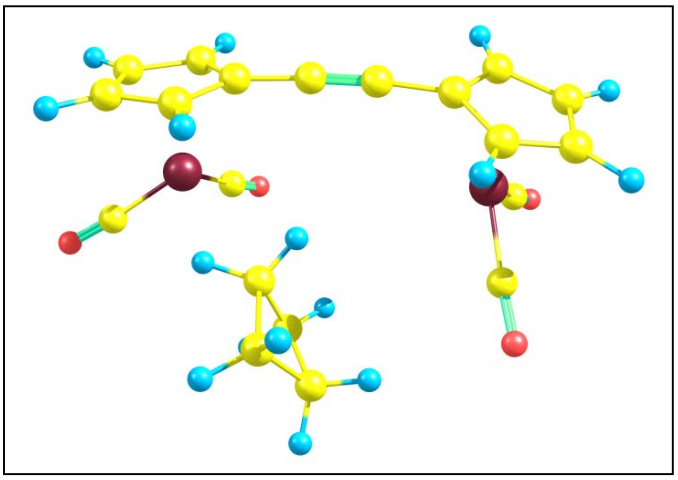
Cyclopropane:

C	-0.386323	0.181565	-3.355581
C	0.235065	-0.883172	-2.615474
C	1.555001	-1.094069	-3.133353
C	1.767759	-0.128490	-4.176415
C	0.572469	0.651610	-4.312550
C	-0.326576	-1.543522	-1.491637
C	-0.769799	-2.036204	-0.474627
C	-1.239584	-2.551652	0.760242
C	-2.505948	-2.254528	1.368199
C	-2.536043	-2.914795	2.641784
C	-1.300287	-3.622295	2.808780
C	-0.498826	-3.411406	1.636459
H	-1.398199	0.535297	-3.220157
H	0.406014	1.424510	-5.049924
H	2.648573	-0.051082	-4.798270
H	2.250838	-1.848921	-2.796641
H	0.473450	-3.834316	1.430068
H	-1.045812	-4.260822	3.643392
H	-3.368910	-2.924457	3.331291
H	-3.296540	-1.668015	0.923004
Re	-0.866989	-1.414172	2.840011
C	0.433166	-1.586870	4.222784
O	1.205700	-1.804222	5.069724
C	-1.906544	-0.234997	3.915151
O	-2.620323	0.412255	4.572995
Re	1.502497	1.106122	-2.310709
C	1.173508	2.979040	-2.444972
O	0.942689	4.108653	-2.624968
C	3.367628	1.424675	-2.053872
O	4.521767	1.568472	-1.970277
C	1.284299	0.889377	0.490401
C	1.491044	1.818278	1.653501
C	0.311590	0.866376	1.639989
H	0.827866	1.358903	-0.420746
H	2.321899	1.607786	2.320433
H	1.270305	2.874166	1.527932
H	0.458461	0.038017	2.378655
H	-0.676709	1.290452	1.523533
H	1.956591	0.051130	0.370086



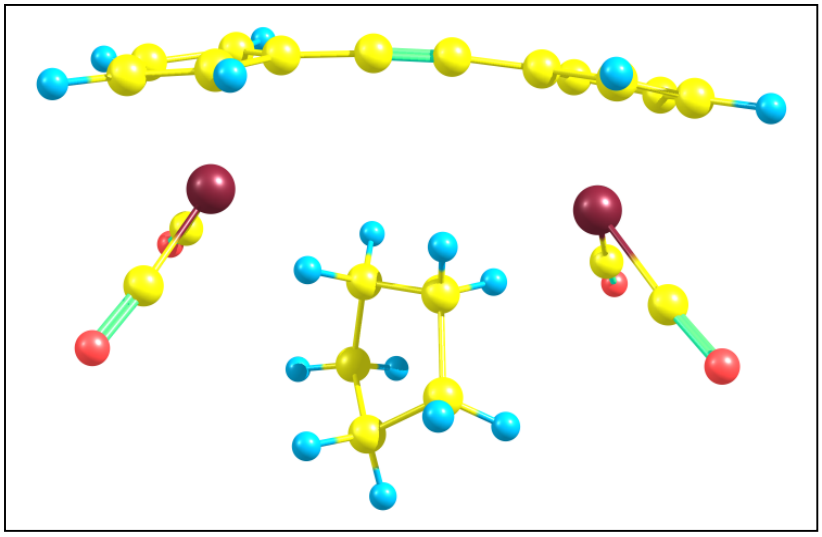
Cyclobutane:

C	-0.909504	0.298187	-3.486649
C	-0.451810	-0.840828	-2.724295
C	0.909378	-1.102106	-3.155913
C	1.250968	-0.194391	-4.178090
C	0.139070	0.705805	-4.368574
C	-1.149816	-1.544611	-1.720043
C	-1.702409	-2.134494	-0.808537
C	-2.278621	-2.746448	0.330420
C	-3.634569	-2.573899	0.794221
C	-3.725657	-3.194721	2.079984
C	-2.441896	-3.755795	2.408896
C	-1.555195	-3.506180	1.303968
H	-1.895694	0.737183	-3.421725
H	0.071022	1.482542	-5.117460
H	2.195046	-0.154584	-4.703466
H	1.541240	-1.885886	-2.758991
H	-0.515461	-3.790088	1.223591
H	-2.216164	-4.335053	3.293088
H	-4.619750	-3.272530	2.683629
H	-4.424876	-2.077593	0.250240
Re	-2.241568	-1.536068	2.351496
C	-0.850832	-1.453635	3.653960
O	0.006771	-1.527046	4.444887
C	-3.402553	-0.449346	3.412150
O	-4.171237	0.135053	4.066631
Re	0.810874	1.077320	-2.234505
C	-0.303744	2.257354	-1.237951
O	-1.052859	2.947006	-0.669304
C	2.022655	2.503067	-2.603253
O	2.754462	3.353614	-2.921445
C	3.021971	-0.478918	0.774028
C	2.673452	0.140597	2.157635
C	1.764210	1.178983	1.439619
C	1.775323	0.253694	0.202829
H	3.956297	-0.079216	0.367228
H	3.508197	0.534805	2.744137
H	2.095097	-0.543842	2.785465
H	2.285773	2.121395	1.246764
H	0.790519	1.400818	1.884961
H	2.058063	0.762666	-0.784841
H	0.905420	-0.399393	0.139771
H	3.038348	-1.569413	0.685983



Cyclopentane:

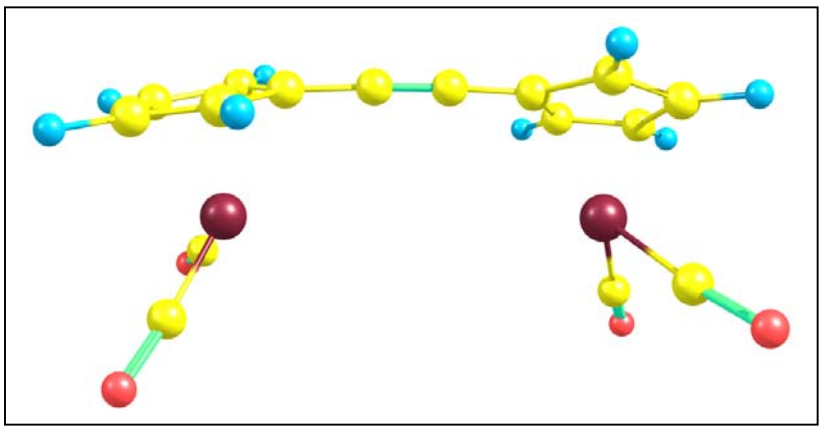
C	0.007508	0.823347	-2.915972
C	0.546492	-0.295385	-2.202402
C	1.807752	-0.656013	-2.789256
C	2.061292	0.271930	-3.853443
C	0.956936	1.183199	-3.931427
C	-0.031241	-0.894580	-1.053636
C	-0.485426	-1.350244	-0.024317
C	-0.956020	-1.801807	1.235717
C	-2.014298	-1.198877	1.991113
C	-2.088349	-1.884985	3.251461
C	-1.101031	-2.924454	3.253301
C	-0.401981	-2.884949	2.001386
H	-0.948032	1.289031	-2.721655
H	0.831239	1.960003	-4.672740
H	2.908900	0.252768	-4.525348
H	2.424557	-1.492082	-2.493577
H	0.380965	-3.551885	1.670138
H	-0.950733	-3.651371	4.039647
H	-2.816680	-1.701845	4.029334
H	-2.636539	-0.381463	1.656676
Re	-0.050041	-0.927705	3.266301
C	1.265061	-1.481712	4.529084
O	2.025031	-1.899870	5.310223
C	-0.597967	0.492864	4.411922
O	-1.031618	1.312446	5.121205
Re	2.051165	1.541670	-1.988563
C	1.787040	3.429402	-2.021560
O	1.584613	4.572500	-2.141049
C	3.939446	1.788589	-1.991016
O	5.098122	1.901618	-2.081349
C	2.015277	0.447280	1.847431
C	1.800118	1.668306	0.920412
C	2.557172	2.806707	1.615955
C	3.825444	2.115029	2.148077
C	3.354239	0.706495	2.595391
H	1.980906	-0.499725	1.312489
H	1.174770	0.524566	2.608204
H	2.381940	1.410487	-0.025263
H	0.753860	1.874752	0.702103
H	1.942829	3.176344	2.448203
H	2.763747	3.651301	0.952834
H	4.562425	2.030228	1.339973
H	4.299865	2.672038	2.961646
H	4.091362	-0.066045	2.356742
H	3.196401	0.669829	3.677089



4-2c. Binuclear Re, DFT(BP86).

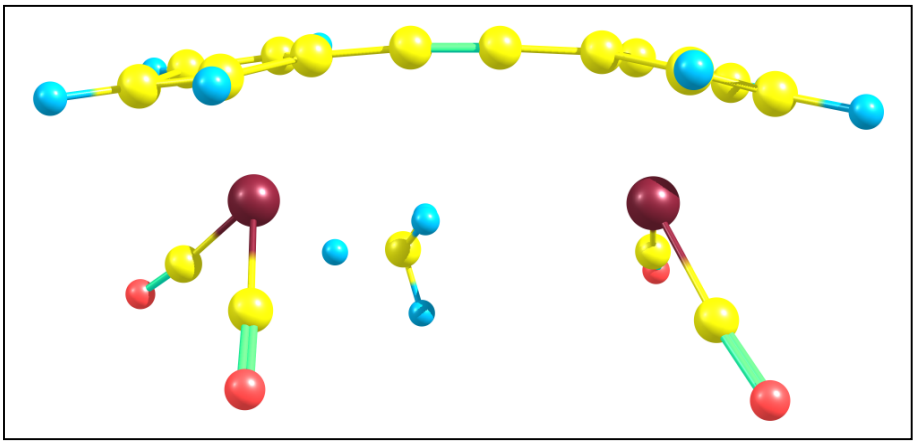
Complex:

Re	-3.102035	-0.142472	0.470439
C	-3.799902	1.290175	-0.582420
C	4.208353	-1.685867	0.643635
C	-3.755823	0.646000	2.081059
C	-0.613962	-2.230409	0.011760
C	-2.029526	-2.174383	0.019987
C	-2.853068	-1.824127	-1.120486
H	-2.544562	-2.628076	2.175657
H	-2.491735	-1.671098	-2.136522
C	-4.209110	-1.698445	-0.643922
H	-5.083891	-1.474708	-1.254424
C	-4.228261	-2.017651	0.772762
H	-5.120551	-2.071861	1.397115
C	-2.879232	-2.338279	1.180777
C	0.616403	-2.227718	-0.021078
O	4.299872	2.098414	1.296680
O	-4.300153	2.095915	-1.284805
O	-4.231746	1.032068	3.089555
Re	3.100037	-0.129695	-0.470104
H	2.487382	-1.665390	2.131896
C	3.749068	0.663644	-2.080823
C	3.798647	1.297665	0.589267
H	5.125941	-2.052171	-1.395959
C	4.231948	-2.001154	-0.773812
C	2.884684	-2.324837	-1.185742
H	5.081027	-1.460475	1.256568
H	2.553449	-2.613302	-2.182161
C	2.031698	-2.165713	-0.026945
O	4.221963	1.052247	-3.089723
C	2.851603	-1.815363	1.116421

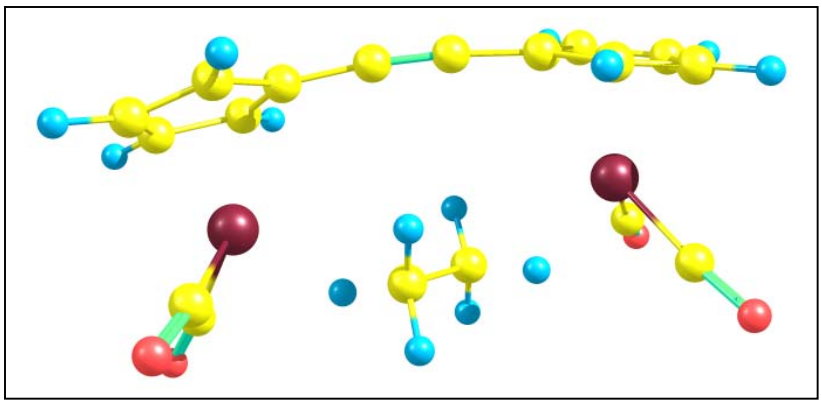


Methane:

C	-2.646156	-1.761079	1.284308
C	-1.970579	-1.950979	-0.009275
C	-2.991799	-1.837366	-1.029984
C	-4.264337	-1.611764	-0.388718
C	-4.036827	-1.605952	1.044898
C	-0.578164	-2.078421	-0.180423
C	0.653062	-2.079883	-0.251812
C	2.065507	-2.015299	-0.281850
C	2.895572	-1.758570	0.879472
C	4.220573	-1.451506	0.398816
C	4.219093	-1.573270	-1.047332
C	2.893983	-1.954362	-1.470399
H	-2.148572	-1.780393	2.253947
H	-4.802444	-1.448169	1.806092
H	-5.232637	-1.553863	-0.885255
H	-2.818386	-1.930113	-2.102332
H	2.560093	-2.139173	-2.490098
H	5.091041	-1.471114	-1.693201
H	5.094152	-1.242917	1.016816
H	2.552223	-1.756000	1.913386
Re	2.925052	0.133302	-0.456433
C	3.439200	1.258126	-1.911839
O	3.830030	1.871232	-2.842901
C	3.426018	1.449271	0.827843
O	3.803410	2.185743	1.672346
Re	-2.955465	0.177718	0.017257
C	-4.291558	1.420281	0.559335
O	-5.185374	2.107369	0.906637
C	-2.745684	1.143596	-1.613400
O	-2.640813	1.663462	-2.666206
C	-0.770144	1.363773	0.885078
H	-0.472390	2.362802	0.535319
H	-0.386923	1.156862	1.894706
H	-1.918499	1.465229	1.044714
H	-0.396044	0.601844	0.183657



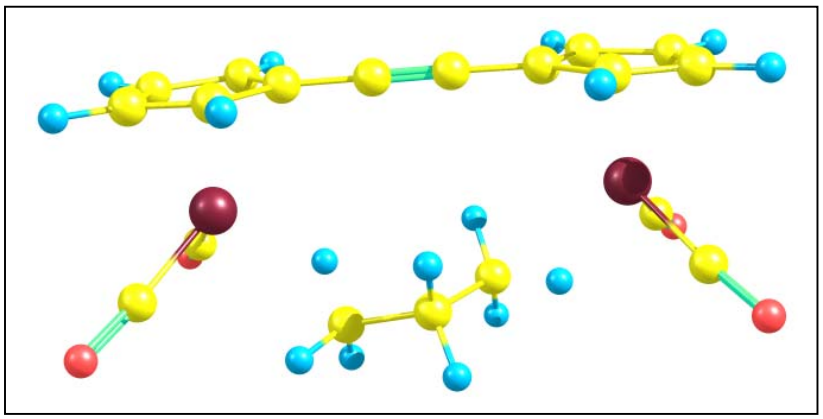
Ethane:



C	-4.139509	1.518207	-1.216731
C	-2.724516	1.610174	-1.484940
C	-2.069257	1.916961	-0.226452
C	-3.074648	2.046222	0.798944
C	-4.358143	1.771215	0.189443
H	-4.921153	1.329848	-1.953270
H	-2.227179	1.496838	-2.447009
H	-2.882940	2.283286	1.845123
H	-5.328194	1.826037	0.683511
C	-0.664237	1.972466	-0.025895
C	0.549868	1.905401	0.146444
C	1.935872	1.681290	0.354820
C	2.963405	1.720296	-0.652113
C	4.200263	1.287346	-0.036414
C	3.934850	1.035009	1.361336
C	2.539646	1.275934	1.616592
H	2.021716	1.208012	2.572062
H	2.813728	1.986335	-1.698215
H	5.176358	1.250120	-0.518290
H	4.678756	0.740461	2.102186
Re	2.841630	-0.488538	0.121092
C	3.469160	-1.334831	-1.469512
O	3.929451	-1.770288	-2.465120
C	3.511671	-1.933844	1.161405
O	3.989023	-2.763017	1.854575
Re	-3.221639	-0.146013	-0.030973
C	-3.945295	-1.465619	-1.193445
O	-4.446647	-2.203982	-1.967716
C	-4.032033	-0.983984	1.477214
O	-4.586096	-1.409927	2.428555
C	-0.868173	-1.420854	0.578644
C	0.332086	-1.486716	-0.380831
H	0.371626	-0.599894	-1.028599
H	1.241741	-1.629389	0.317614
H	0.328481	-2.388117	-1.013309
H	-1.795511	-1.507172	-0.103240
H	-0.830500	-0.522327	1.210064
H	-0.948092	-2.304301	1.232230

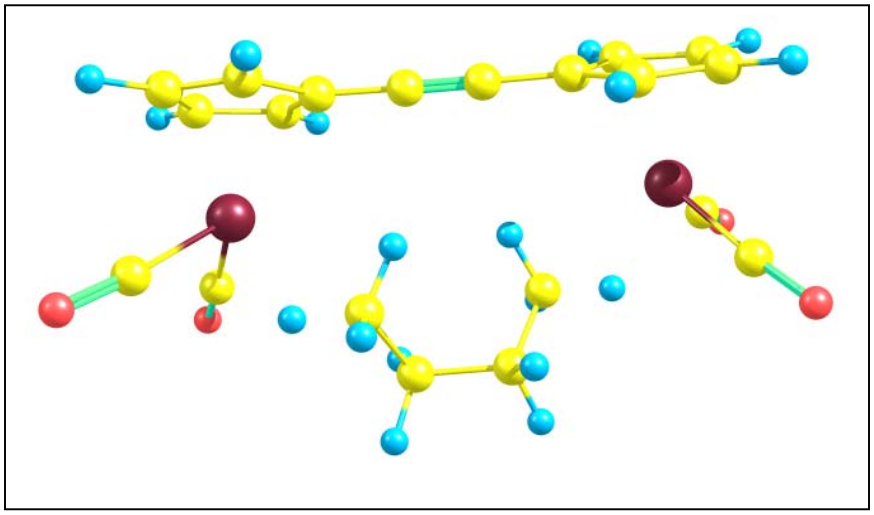
Propane:

Re	0.037516	2.894781	-0.619542
C	1.381020	3.526569	0.568411
C	-2.932659	-4.108394	-2.651625
C	-1.247144	4.052438	0.181723
C	-0.587195	0.204677	-2.587782
C	-0.124084	1.544529	-2.572030
C	1.254793	1.965916	-2.390504
H	-2.020824	2.713239	-2.916633
H	2.111189	1.299439	-2.292207
C	1.266357	3.405981	-2.412312
H	2.150485	4.039319	-2.331542
C	-0.087537	3.875985	-2.616255
H	-0.387788	4.916213	-2.745358
C	-0.945099	2.717587	-2.742839
C	-0.993091	-0.954915	-2.604483
O	-5.001862	-3.810494	0.609959
O	2.269007	3.949258	1.223687
O	-2.048335	4.825737	0.574384
Re	-2.213507	-3.420127	-0.643676
H	-3.693319	-1.987061	-2.947536
C	-1.467608	-4.697486	0.552605
C	-3.915107	-3.635304	0.181838
H	-1.312348	-5.657705	-2.359817
C	-1.592447	-4.606586	-2.435524
C	-0.684321	-3.483025	-2.424115
H	-3.827824	-4.719958	-2.765597
H	0.399445	-3.514739	-2.315204
C	-1.480007	-2.285615	-2.598033
O	-0.984557	-5.554391	1.207594
C	-2.863746	-2.670090	-2.767602
C	-0.402721	0.905662	1.343143
H	-1.124228	1.200937	2.123926
H	0.589540	1.272975	1.636286
H	-0.829464	1.410953	0.394551
C	-0.370725	-0.608751	1.083547
H	0.279240	-0.820550	0.215980
H	0.095172	-1.097086	1.960571
C	-1.769290	-1.193396	0.846528
H	-2.456294	-1.008218	1.690492
H	-2.233271	-0.785184	-0.063389
H	-1.646509	-2.345151	0.883377

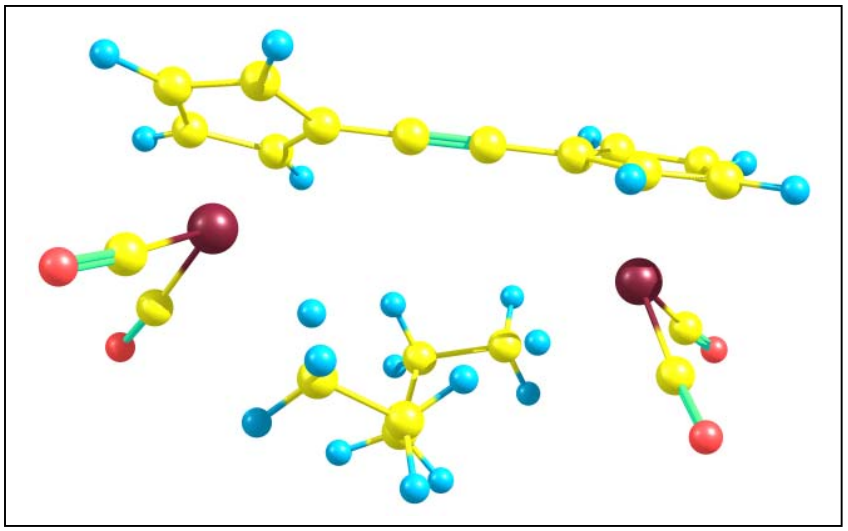


Butane:

Re	0.064194	3.025676	-0.614237
C	1.623447	3.819794	0.121869
C	-2.767549	-4.223711	-2.769719
C	-1.048856	4.029053	0.560594
C	-0.880494	0.299717	-2.493425
C	-0.552710	1.680039	-2.502353
C	0.776150	2.239031	-2.700840
H	-2.563903	2.654024	-2.219137
H	1.682738	1.661538	-2.877709
C	0.642064	3.673861	-2.675301
H	1.445284	4.393171	-2.837473
C	-0.747697	4.002973	-2.452678
H	-1.174642	5.005380	-2.444583
C	-1.489801	2.764799	-2.369166
C	-1.157010	-0.898290	-2.501641
O	-5.283854	-4.139591	0.105973
O	2.613404	4.353634	0.484463
O	-1.782371	4.704394	1.193738
Re	-2.365274	-3.553635	-0.680116
H	-3.691969	-2.174248	-3.119418
C	-1.714253	-4.847787	0.550432
C	-4.151156	-3.898376	-0.125048
H	-1.034682	-5.613586	-2.344713
C	-1.415554	-4.594499	-2.418926
C	-0.633097	-3.390466	-2.272255
H	-3.578172	-4.911885	-3.008561
H	0.433090	-3.319599	-2.058283
C	-1.515475	-2.271038	-2.528866
O	-1.281830	-5.710571	1.232577
C	-2.827614	-2.781193	-2.851789
C	-2.209694	-1.379315	0.965026
H	-3.217651	-1.018819	1.227503
H	-2.297186	-2.528591	0.986861
H	-1.936814	-0.950815	-0.012043
C	-1.178671	-1.046715	2.061927
H	-1.590830	-1.347300	3.042604
H	-0.261469	-1.648330	1.914040
C	-0.818336	0.454923	2.086370
H	-0.371466	0.712003	3.064463
H	-1.735817	1.066539	1.995140
C	0.177268	0.819884	0.968981
H	1.194022	0.451960	1.189997
H	-0.122292	0.402586	-0.005216
H	0.303852	1.967732	1.006914

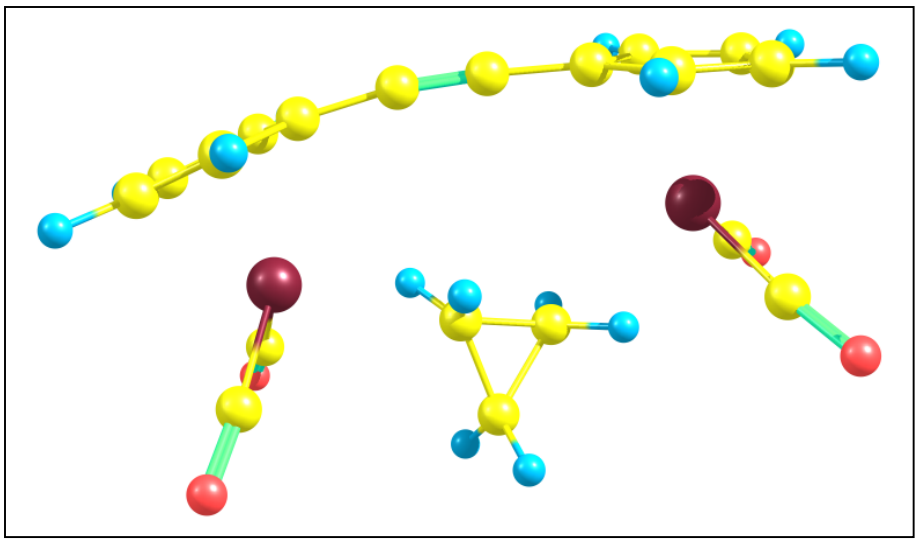


Pentane:



Re	0.223962	2.910189	-0.650198
C	1.710663	3.734583	0.196970
C	-2.767427	-4.196535	-2.755776
C	-0.954723	3.773785	0.572275
C	-0.817298	0.308032	-2.525317
C	-0.415328	1.666767	-2.555723
C	0.953627	2.148367	-2.734395
H	-2.364231	2.770664	-2.319170
H	1.826849	1.518751	-2.902395
C	0.907999	3.581134	-2.694932
H	1.761110	4.250545	-2.812853
C	-0.459699	4.000537	-2.484236
H	-0.819716	5.028819	-2.476495
C	-1.281839	2.810272	-2.446512
C	-1.153527	-0.872805	-2.494881
O	-5.746939	-3.801030	-0.273522
O	2.659926	4.284163	0.637008
O	-1.725406	4.367835	1.242300
Re	-2.731684	-3.308193	-0.707995
H	-3.555594	-2.191007	-3.483772
C	-2.277365	-4.414760	0.768222
C	-4.590907	-3.589996	-0.391342
H	-1.196642	-5.546635	-1.844319
C	-1.518689	-4.539551	-2.109594
C	-0.750128	-3.329874	-1.938305
H	-3.537289	-4.901211	-3.070317
H	0.245736	-3.241288	-1.506925
C	-1.542265	-2.236222	-2.468563
O	-1.942034	-5.172739	1.611417
C	-2.772312	-2.771786	-2.998141
C	-3.160721	-1.167201	1.154454
H	-4.075786	-0.803651	0.666177
H	-2.484110	-1.647916	0.352031
H	-3.421548	-1.918254	1.913899
C	-2.317370	-0.020497	1.746173
H	-2.166391	0.764324	0.981703
H	-2.931656	0.443295	2.541742
C	-0.961157	-0.465442	2.337875
H	-1.099488	-1.428429	2.866637
H	-0.643764	0.261666	3.110832
C	0.175855	-0.612379	1.301899
H	0.958997	-1.281743	1.708005
H	-0.196046	-1.105454	0.383877
C	0.877724	0.712670	0.943981
H	0.024483	1.427538	0.623616
H	1.346582	1.181997	1.822246
H	1.636341	0.574007	0.161954

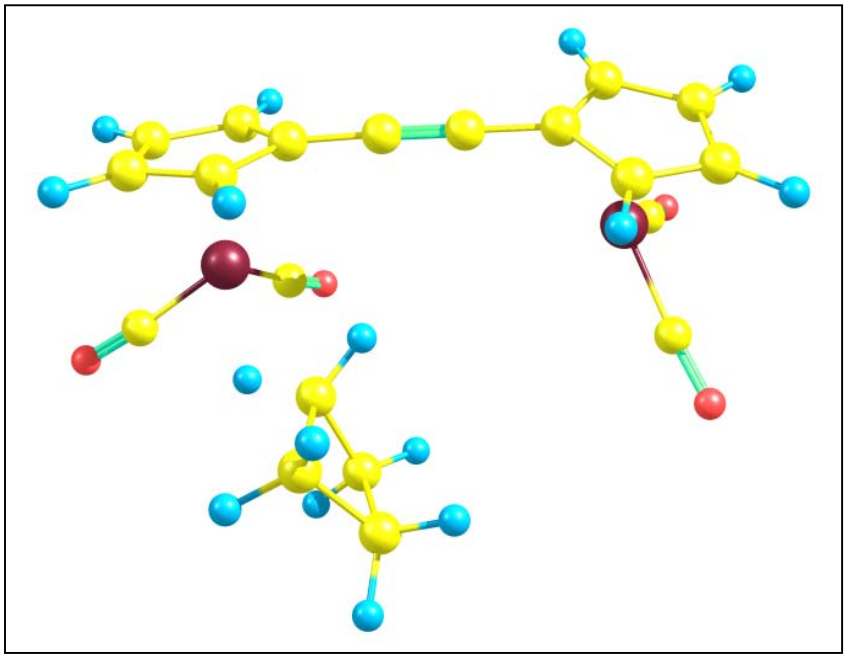
Cyclopropane:



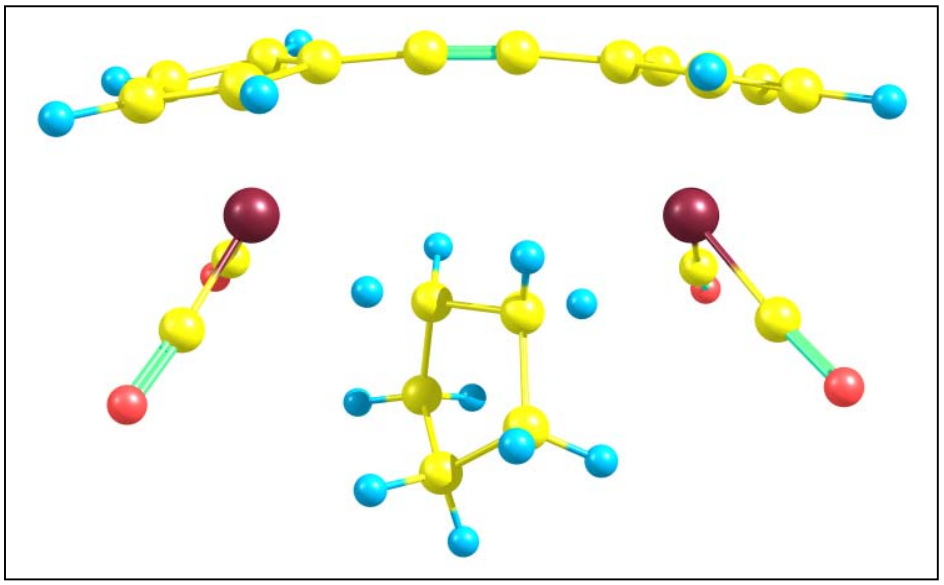
C	-0.368521	0.184397	-3.411961
C	0.243956	-0.908910	-2.680877
C	1.604915	-1.068418	-3.139426
C	1.854686	-0.033672	-4.118536
C	0.639909	0.730033	-4.288210
C	-0.337252	-1.594136	-1.581107
C	-0.771343	-2.051856	-0.528569
C	-1.210973	-2.524681	0.731740
C	-2.477621	-2.219571	1.359109
C	-2.474965	-2.841290	2.662523
C	-1.215722	-3.529437	2.829874
C	-0.433549	-3.346022	1.629810
H	-1.399286	0.519434	-3.305574
H	0.495037	1.543054	-5.000167
H	2.776461	0.098401	-4.684565
H	2.309253	-1.818445	-2.782071
H	0.545608	-3.771426	1.413803
H	-0.932858	-4.137017	3.689865
H	-3.301167	-2.840874	3.373965
H	-3.286819	-1.647944	0.906668
Re	-0.830869	-1.327161	2.793808
C	0.460723	-1.480779	4.180376
O	1.236892	-1.698621	5.044123
C	-1.893707	-0.175515	3.865249
O	-2.635635	0.455108	4.534335
Re	1.425264	1.069878	-2.212783
C	1.081341	2.940964	-2.257412
O	0.849267	4.091588	-2.393295
C	3.261031	1.413162	-1.825020
O	4.418976	1.578245	-1.667946
C	1.077773	0.633185	0.398409
C	1.570480	1.622671	1.412100
C	0.255548	0.884716	1.665478
H	0.454045	1.006995	-0.489804
H	2.448827	1.342631	2.002217
H	1.493283	2.689163	1.181117
H	0.409726	0.209133	2.572202
H	-0.667298	1.463232	1.615671
H	1.559349	-0.341534	0.323117

Cyclobutane:

C	-0.913676	0.269704	-3.335364
C	-0.392197	-0.845712	-2.551384
C	0.978914	-1.059026	-3.010181
C	1.260054	-0.166921	-4.079222
C	0.102158	0.688224	-4.264918
C	-1.048174	-1.543058	-1.515940
C	-1.604336	-2.125725	-0.582819
C	-2.264655	-2.768962	0.489198
C	-3.693438	-2.724844	0.741696
C	-3.923813	-3.344744	2.023161
C	-2.646908	-3.796640	2.548228
C	-1.623534	-3.468249	1.580113
H	-1.922234	0.675570	-3.254751
H	-0.012895	1.451624	-5.034505
H	2.197649	-0.103257	-4.631291
H	1.658178	-1.810755	-2.604334
H	-0.556284	-3.670173	1.659026
H	-2.504690	-4.357955	3.471537
H	-4.893919	-3.501375	2.495296
H	-4.437428	-2.290097	0.075522
Re	-2.660631	-1.591649	2.490084
C	-1.651380	-1.382563	4.093382
O	-1.031914	-1.373054	5.100314
C	-4.122376	-0.612061	3.219611
O	-5.096876	-0.110637	3.661197
Re	0.809559	1.129749	-2.172938
C	-0.320454	2.257946	-1.137717
O	-1.091571	2.927520	-0.546819
C	1.860884	2.642618	-2.654241
O	2.492785	3.559197	-3.046903
C	3.410161	-0.348468	0.297422
C	3.278761	0.054976	1.799623
C	2.226123	1.136774	1.401581
C	2.053259	0.377646	0.056804
H	4.251004	0.168022	-0.196701
H	4.193571	0.409565	2.302490
H	2.831771	-0.753392	2.402556
H	2.693716	2.125242	1.255279
H	1.331782	1.254533	2.033982
H	2.156942	1.101244	-0.857756
H	1.196944	-0.314065	0.058538
H	3.459110	-1.422763	0.051687



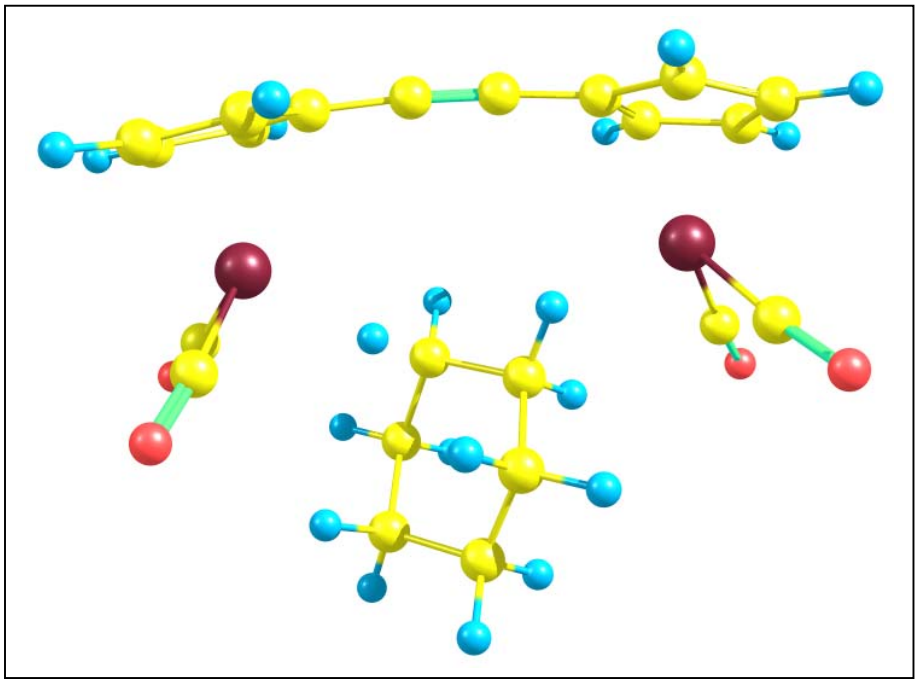
Cyclopentane:



C	0.014714	0.851639	-2.915118
C	0.560290	-0.281730	-2.207668
C	1.846236	-0.619267	-2.786787
C	2.110441	0.345277	-3.826948
C	0.988336	1.252729	-3.905549
C	-0.018881	-0.898100	-1.068483
C	-0.469516	-1.357930	-0.023520
C	-0.925392	-1.800262	1.244682
C	-2.005042	-1.206871	1.995782
C	-2.055507	-1.867400	3.281903
C	-1.035681	-2.890602	3.301373
C	-0.336144	-2.862881	2.039623
H	-0.952827	1.311747	-2.718412
H	0.867776	2.052706	-4.636033
H	2.980644	0.355412	-4.484445
H	2.478468	-1.452794	-2.484576
H	0.471934	-3.518845	1.717798
H	-0.859380	-3.594885	4.114890
H	-2.791201	-1.682688	4.064920
H	-2.640836	-0.394041	1.647665
Re	-0.048714	-0.876945	3.246690
C	1.224423	-1.360920	4.574825
O	1.968596	-1.746748	5.407958
C	-0.630992	0.599370	4.298267
O	-1.095717	1.463732	4.956343
Re	2.024687	1.553221	-1.938176
C	1.718430	3.433324	-1.911159
O	1.489697	4.588542	-2.003863
C	3.903385	1.848418	-1.914545
O	5.074538	1.988122	-1.995263
C	1.969746	0.368771	1.847224
C	1.757037	1.571751	0.887088
C	2.536629	2.716479	1.553163
C	3.815787	2.022921	2.074240
C	3.358583	0.601777	2.518545
H	1.864967	-0.609659	1.354957
H	1.176917	0.557579	2.674161
H	2.362663	1.241540	-0.054438
H	0.702302	1.780782	0.665051
H	1.932006	3.105676	2.395809
H	2.738384	3.552330	0.864382
H	4.552740	1.948120	1.253740
H	4.295410	2.583772	2.893933
H	4.075824	-0.176282	2.206367
H	3.270760	0.530844	3.615085

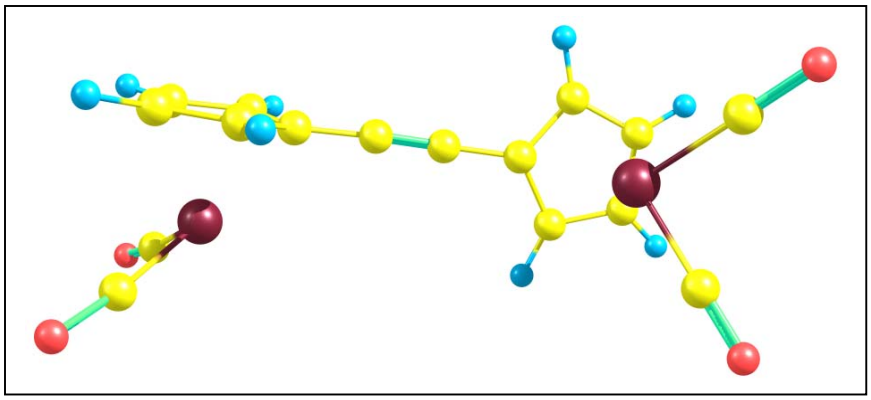
Cyclohexane:

C	-.111279	.081104	-3.314264
C	.335825	-.974442	-2.428375
C	1.732237	-1.240311	-2.685075
C	2.170831	-.303762	-3.694042
C	1.033160	.500176	-4.086084
C	-.426060	-1.595449	-1.408255
C	-1.003297	-2.093137	-.446490
C	-1.579499	-2.631883	.730238
C	-2.797437	-2.181250	1.371246
C	-2.918547	-2.909685	2.611848
C	-1.792746	-3.811741	2.725656
C	-.975211	-3.663114	1.543136
H	-1.124454	.475858	-3.370498
H	1.032089	1.255508	-4.871523
H	3.160483	-.268863	-4.149734
H	2.330025	-2.003319	-2.188493
H	-.064125	-4.206289	1.296478
H	-1.640166	-4.544767	3.518277
H	-3.743791	-2.834457	3.320816
H	-3.485699	-1.436676	.974062
Re	-1.048641	-1.719368	2.847937
C	.271546	-2.130457	4.158998
O	1.050951	-2.481806	4.974175
C	-1.878728	-.491797	4.042155
O	-2.484453	.207399	4.777947
Re	1.575542	.984072	-1.967156
C	1.316656	2.846932	-2.234952
O	1.131916	3.984081	-2.502521
C	3.371036	1.275782	-1.408392
O	4.518860	1.406362	-1.158656
C	.557797	2.873154	1.059354
C	1.950307	3.128503	1.666909
C	2.196576	2.259472	2.915349
C	1.973528	.759085	2.623968
C	.571493	.548979	2.026534
C	.342812	1.380716	.748410
H	-.224639	3.174785	1.786523
H	2.722476	2.901542	.906982
H	2.059453	4.199709	1.917521
H	3.223317	2.417229	3.293300
H	1.508322	2.573700	3.726284
H	2.736096	.397491	1.905347
H	2.087212	.162624	3.545881
H	-.185438	.882986	2.757898
H	.421386	-.564264	1.797879
H	1.155372	1.023894	-.002465
H	-.651150	1.179050	.318544
H	.405895	3.477594	.150100



4-2d. Binuclear Re, RIMP2.

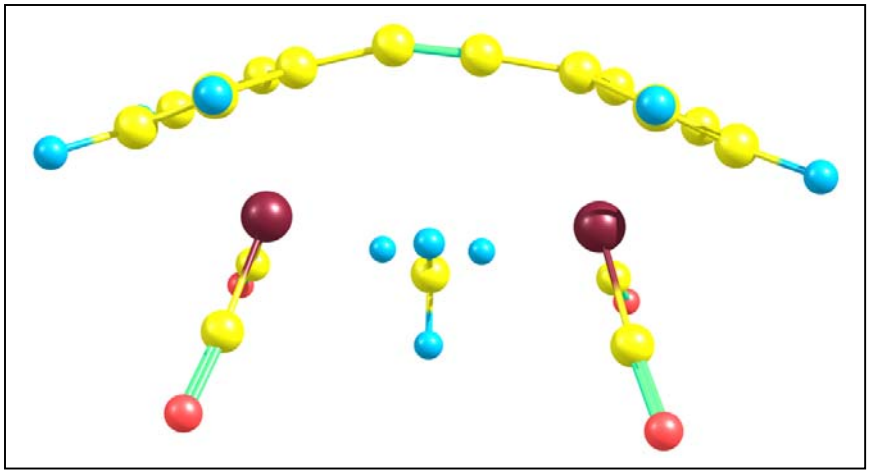
Complex:



Re	-3.519449	-.323761	1.023513
C	-4.481266	1.260154	.674430
C	4.150613	-1.148422	.887952
C	-4.572914	-.630031	2.556056
C	-.609762	-1.621914	-.071766
C	-2.020642	-1.597797	-.148360
C	-2.777630	-.842463	-1.103233
H	-2.595260	-3.243843	1.262541
H	-2.370146	-.142730	-1.821537
C	-4.157573	-1.168298	-.895055
H	-4.992813	-.797530	-1.475797
C	-4.232560	-2.184989	.119931
H	-5.132045	-2.707184	.420632
C	-2.897448	-2.498164	.538392
C	.611256	-1.622200	.042413
O	5.022306	2.247959	-.340539
O	-5.147652	2.183752	.357643
O	-5.298257	-.917233	3.444367
Re	3.525123	-.328227	-1.044725
H	2.349672	-.119124	1.784068
C	4.648459	-.615381	-2.530784
C	4.408141	1.295097	-.675387
H	5.142288	-2.698133	-.400984
C	4.237404	-2.177955	-.112946
C	2.908786	-2.500698	-.542199
H	4.978373	-.769389	1.473867
H	2.616351	-3.257958	-1.258183
C	2.021549	-1.594816	.127191
O	5.417127	-.887907	-3.386831
C	2.766487	-.827883	1.079982

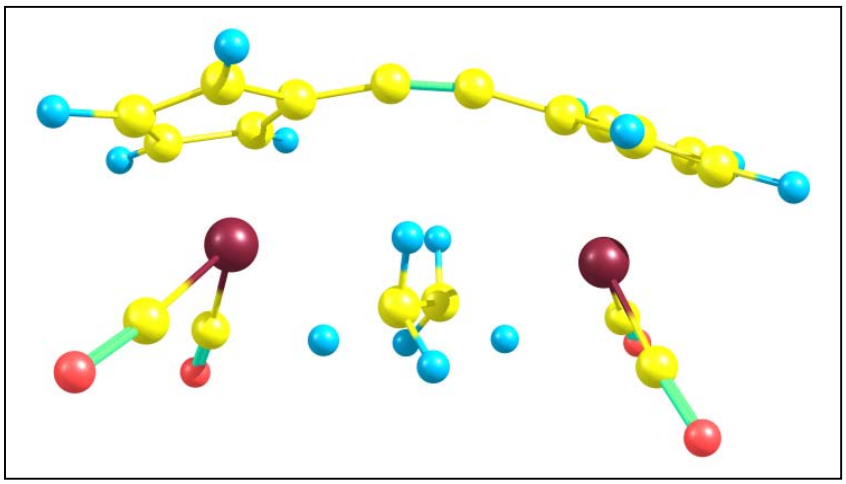
Methane:

C	-2.805370	-1.878211	1.254931
C	-2.033060	-2.142106	.071199
C	-2.856790	-1.938866	-1.082103
C	-4.114573	-1.433347	-.616602
C	-4.083111	-1.408301	.817741
C	-.656737	-2.452881	.047061
C	.566280	-2.321298	.005318
C	1.953949	-2.090568	-.041656
C	2.754242	-1.723309	1.097237
C	3.977279	-1.185880	.586625
C	3.934284	-1.226933	-.846393
C	2.684778	-1.809056	-1.240579
H	-2.466947	-2.012562	2.274308
H	-4.918518	-1.153382	1.457910
H	-4.983220	-1.229720	-1.229478
H	-2.559874	-2.110833	-2.109254
H	2.349059	-2.019661	-2.248289
H	4.755634	-.979580	-1.506468
H	4.829469	-.874716	1.177870
H	2.485245	-1.880511	2.133707
Re	2.382566	.188567	-.131899
C	2.599196	1.390522	-1.565460
O	2.816059	2.102632	-2.484128
C	2.988976	1.552906	1.007715
O	3.473304	2.354062	1.732973
Re	-2.620780	.077419	.030725
C	-3.236766	1.382017	1.234118
O	-3.720286	2.139258	2.005681
C	-3.009684	1.279570	-1.365106
O	-3.331482	1.987721	-2.256009
C	-.150139	.938471	-.168443
H	-.177684	1.922698	-.623324
H	.685028	.893595	.621755
H	-.933194	.876989	.675474
H	-.160920	.145714	-.913989



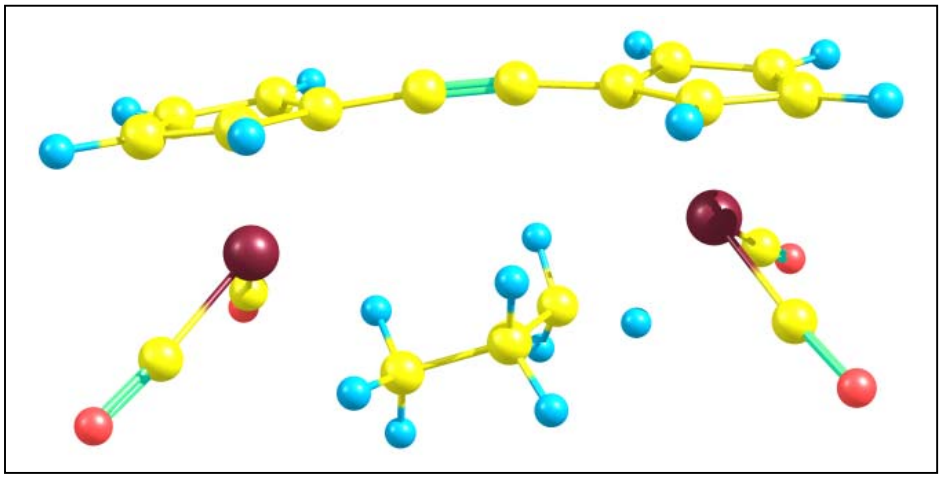
Ethane:

C	-4.061081	1.333104	-1.122842
C	-2.673348	1.571407	-1.394196
C	-2.050226	1.899218	-.148514
C	-3.053027	1.968913	.875736
C	-4.291105	1.576338	.270601
H	-4.824221	1.116694	-1.859508
H	-2.174230	1.510403	-2.353315
H	-2.889622	2.261307	1.905245
H	-5.258146	1.564535	.757708
C	-.668238	2.135240	.019224
C	.548180	2.062931	.176270
C	1.898693	1.677928	.322618
C	2.889097	1.673171	-.713412
C	4.087013	1.130063	-.142537
C	3.849073	.870907	1.246524
C	2.498339	1.245016	1.549373
H	2.010120	1.212373	2.515289
H	2.742566	2.010394	-1.731796
H	5.041566	1.035787	-.644583
H	4.594200	.549202	1.963096
Re	2.599113	-.510256	.036808
C	3.424896	-1.482327	-1.346274
O	4.032539	-2.025567	-2.203792
C	2.942513	-1.929999	1.216779
O	3.239938	-2.760438	2.007588
Re	-2.982221	-.208627	.061078
C	-3.359537	-1.545426	-1.202637
O	-3.663193	-2.316549	-2.049132
C	-3.998450	-1.148969	1.334537
O	-4.720142	-1.662100	2.119343
C	-.646317	-1.073001	.724673
C	.162356	-1.123283	-.560133
H	.217105	-.159871	-1.064661
H	1.156226	-1.690535	-.421032
H	-.270063	-1.821045	-1.286766
H	-1.698930	-1.529243	.603303
H	-.594133	-.106533	1.223253
H	-.291733	-1.809515	1.455862



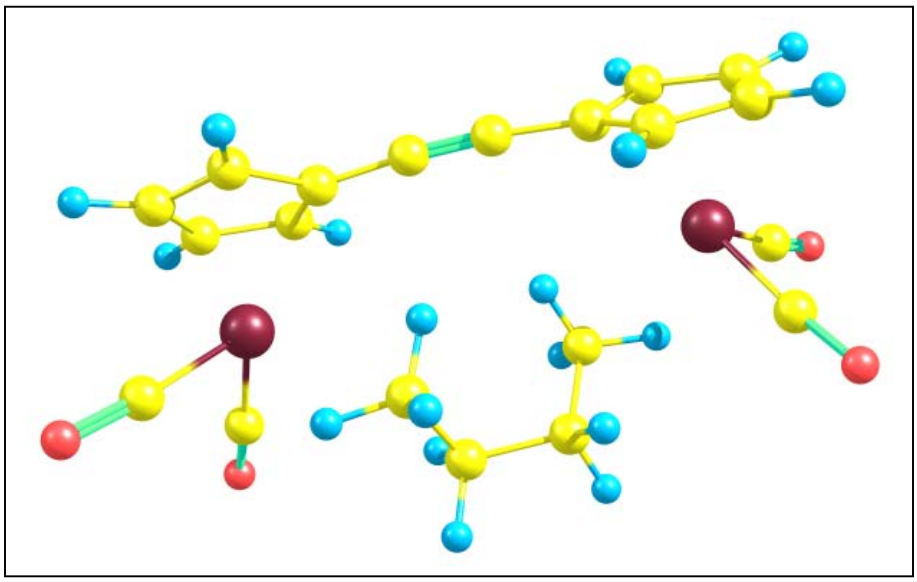
Propane:

Re	.005235	2.775416	-.563781
C	1.226348	3.544676	.641526
C	-2.852820	-4.080377	-2.546069
C	-1.363415	3.763298	.268341
C	-.558031	.222327	-2.616700
C	-.122534	1.556856	-2.486651
C	1.249070	1.985696	-2.349059
H	-2.012693	2.698798	-2.851005
H	2.112121	1.335780	-2.281924
C	1.234087	3.413118	-2.315869
H	2.103797	4.053607	-2.233304
C	-.114389	3.866304	-2.500869
H	-.424521	4.895821	-2.621324
C	-.944167	2.711563	-2.674198
C	-.960942	-.936845	-2.636940
O	-5.027513	-3.965869	.523080
O	2.031226	4.081432	1.324332
O	-2.225503	4.443672	.709108
Re	-2.259149	-3.252658	-.572804
H	-3.617765	-2.015174	-3.044963
C	-1.470113	-4.363585	.719382
C	-3.949061	-3.650390	.151836
H	-1.234401	-5.574158	-2.114239
C	-1.531801	-4.539775	-2.231230
C	-.651202	-3.409493	-2.242045
H	-3.717345	-4.713182	-2.702799
H	.418889	-3.413629	-2.076420
C	-1.453342	-2.248866	-2.489126
O	-.957688	-5.140317	1.452994
C	-2.801479	-2.664614	-2.755110
C	-.087267	.677450	1.136517
H	-.466949	.969982	2.118328
H	.984400	.863355	1.108108
H	-.726510	1.305333	.417772
C	-.414996	-.771081	.780223
H	.099690	-1.051699	-.141714
H	-.022710	-1.417829	1.573536
C	-1.908588	-1.002388	.614856
H	-2.491338	-.492758	1.393683
H	-2.291534	-.632448	-.338098
H	-2.213242	-2.069378	.927619



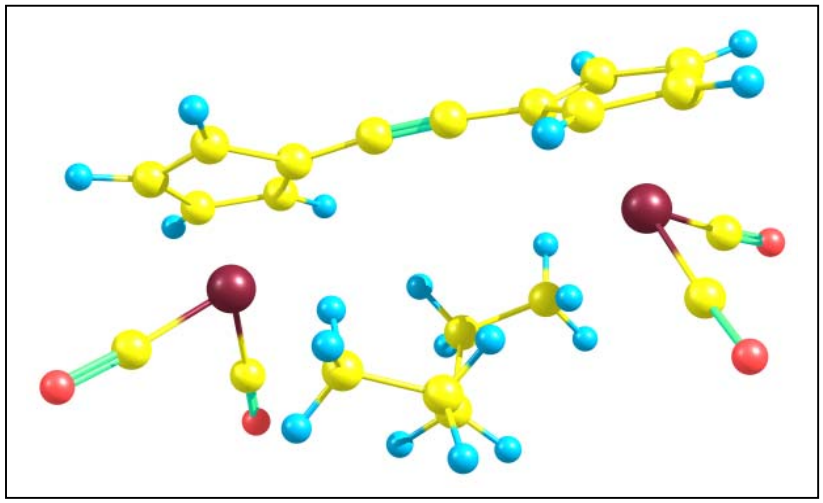
Butane:

Re	.161783	2.859326	-.564988
C	1.780278	3.620083	.006078
C	-2.553675	-4.274408	-2.670775
C	-.719648	3.796781	.802265
C	-.919212	.322706	-2.536937
C	-.625489	1.697451	-2.411632
C	.606785	2.330012	-2.789679
H	-2.625394	2.530579	-1.839455
H	1.492361	1.824345	-3.152655
C	.432604	3.736286	-2.585391
H	1.161947	4.503904	-2.812535
C	-.915374	3.971548	-2.156567
H	-1.374309	4.942345	-2.019495
C	-1.587982	2.707735	-2.094716
C	-1.155362	-.882215	-2.542472
O	-5.188128	-4.479109	.008225
O	2.794354	4.168251	.278149
O	-1.314756	4.449317	1.591513
Re	-2.402171	-3.393478	-.641115
H	-3.535208	-2.344606	-3.314298
C	-1.700235	-4.426181	.760626
C	-4.115512	-4.018835	-.190957
H	-.812252	-5.508550	-1.977287
C	-1.241360	-4.530106	-2.152502
C	-.550514	-3.279173	-2.046245
H	-3.277439	-5.029844	-2.949841
H	.471584	-3.120298	-1.726077
C	-1.472588	-2.253320	-2.434139
O	-1.220343	-5.144075	1.571477
C	-2.684400	-2.865571	-2.894000
C	-2.407388	-1.160729	.714091
H	-3.291514	-.529279	.855552
H	-2.884696	-2.196712	.813912
H	-1.985077	-.890327	-.254308
C	-1.401206	-.998256	1.848263
H	-1.900653	-1.206246	2.801194
H	-.608302	-1.746211	1.741576
C	-.798149	.406270	1.878332
H	-.308169	.577616	2.843384
H	-1.590901	1.156807	1.793252
C	.218701	.611563	.760756
H	1.114711	-.002831	.902871
H	-.185307	.346248	-.216783
H	.674925	1.655540	.879304



Pentane:

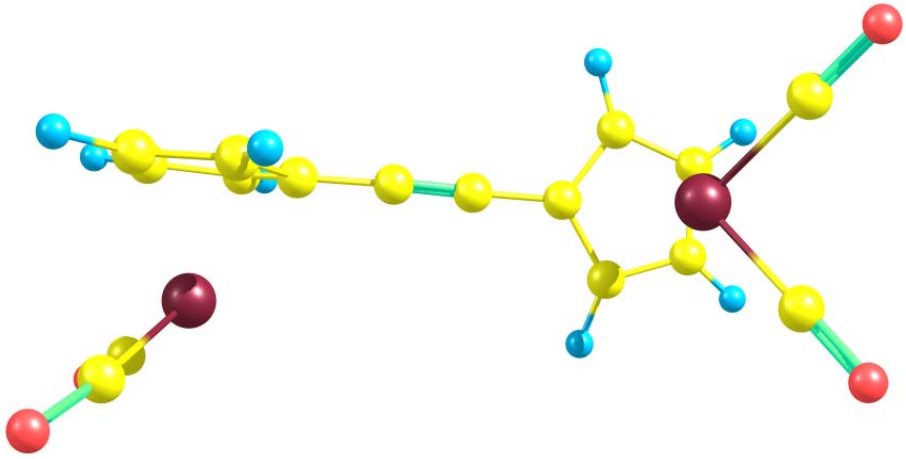
Re	.362139	2.657461	-.506521
C	2.014959	3.302476	.115868
C	-2.827025	-4.170670	-2.634865
C	-.482837	3.398431	.997880
C	-.956841	.346925	-2.504518
C	-.560530	1.694202	-2.356717
C	.706795	2.250963	-2.758502
H	-2.462091	2.656865	-1.667572
H	1.538360	1.696362	-3.173898
C	.653265	3.651617	-2.474850
H	1.439262	4.368786	-2.677420
C	-.655174	3.971303	-1.979872
H	-1.028991	4.966168	-1.774992
C	-1.427681	2.764411	-1.970141
C	-1.287759	-.834420	-2.516424
O	-5.230680	-4.364032	.341412
O	3.053882	3.775595	.430052
O	-1.061617	3.915590	1.894114
Re	-2.527235	-3.284860	-.608147
H	-3.772097	-2.201765	-3.202849
C	-1.703322	-4.204198	.807263
C	-4.184144	-3.915952	.015657
H	-1.102494	-5.478095	-2.038777
C	-1.503276	-4.482738	-2.181482
C	-.760027	-3.260167	-2.108708
H	-3.597590	-4.894789	-2.868729
H	.278884	-3.143009	-1.826251
C	-1.662168	-2.191528	-2.419151
O	-1.148491	-4.848640	1.632204
C	-2.919320	-2.756814	-2.832737
C	-3.163609	-1.019201	.621228
H	-3.760868	-.912885	-.283829
H	-2.335748	-1.820042	.587038
H	-3.816093	-1.305520	1.447360
C	-2.365399	.249972	.922607
H	-1.857021	.591227	.016044
H	-3.082210	1.036839	1.187898
C	-1.347685	.065131	2.049499
H	-1.803157	-.535309	2.847072
H	-1.107385	1.038928	2.491493
C	-.055385	-.603084	1.571194
H	.466124	-1.064512	2.418132
H	-.286301	-1.415363	.871833
C	.913677	.386885	.925511
H	.313527	.840530	.067143
H	1.254395	1.128930	1.645025
H	1.777754	-.092661	.463039



4-2e. Binuclear Re, SOS-MP2

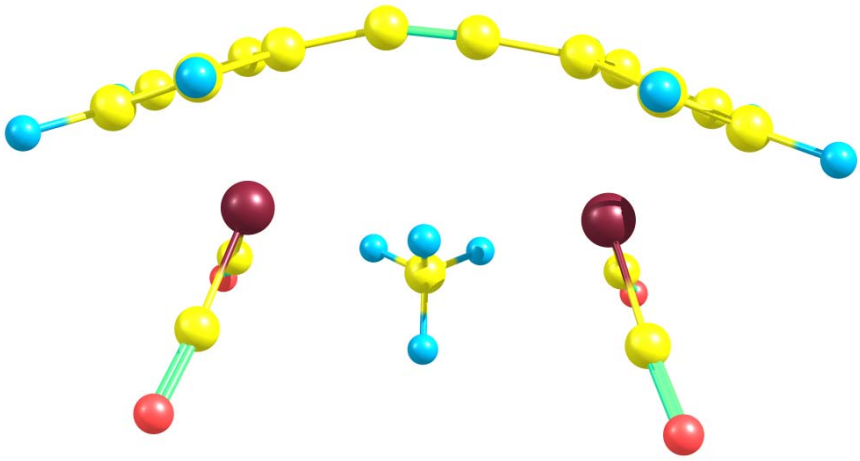
Complex

Re	-3.520144	-.303747	1.010827
C	-4.462978	1.305197	.652619
C	4.164802	-1.185536	.900678
C	-4.533115	-.567402	2.594654
C	-.607242	-1.660746	-.079698
C	-2.030714	-1.645619	-.173822
C	-2.786948	-.881487	-1.122964
H	-2.616574	-3.244795	1.286909
H	-2.377441	-.200743	-1.859355
C	-4.171842	-1.202085	-.911323
H	-5.007008	-.828554	-1.491926
C	-4.251840	-2.197982	.122246
H	-5.155230	-2.703697	.441609
C	-2.914078	-2.507766	.550808
C	.608050	-1.661914	.046814
O	4.939776	2.316515	-.324448
O	-5.102958	2.240700	.343236
O	-5.217411	-.818605	3.516150
Re	3.527224	-.313747	-1.036625
H	2.356851	-.178304	1.817703
C	4.634846	-.555071	-2.558937
C	4.367135	1.345172	-.654134
H	5.163737	-2.701170	-.423866
C	4.254988	-2.197494	-.116241
C	2.924654	-2.513442	-.558544
H	4.992331	-.806120	1.488089
H	2.636084	-3.263698	-1.284618
C	2.030789	-1.644110	.150206
O	5.377744	-.789938	-3.438620
C	2.775034	-.870880	1.097227



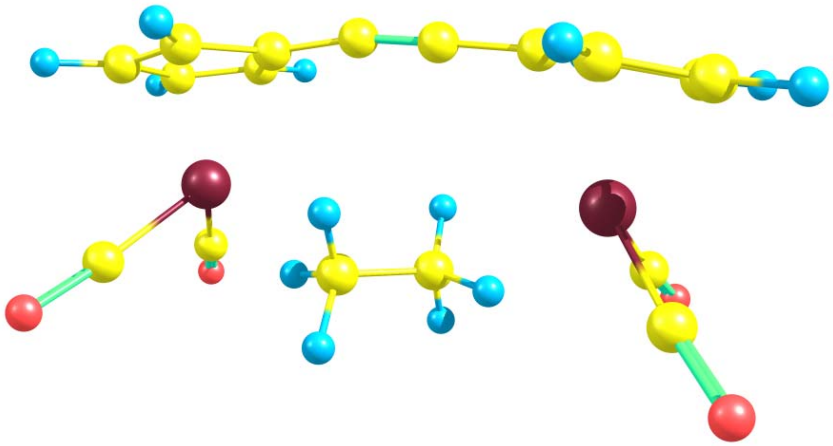
Methane:

C	-2.812108	-1.898885	1.281317
C	-2.052953	-2.145544	.086248
C	-2.890546	-1.942766	-1.055948
C	-4.164975	-1.487105	-.569569
C	-4.116601	-1.471877	.863911
C	-.656717	-2.429930	.041745
C	.560570	-2.309416	-.014175
C	1.959521	-2.061940	-.082676
C	2.789656	-1.740275	1.046756
C	4.030897	-1.246107	.523034
C	3.962318	-1.265210	-.909217
C	2.678068	-1.789275	-1.290304
H	-2.459090	-2.033493	2.296549
H	-4.949635	-1.243562	1.518445
H	-5.043939	-1.294733	-1.172971
H	-2.603807	-2.100610	-2.088995
H	2.319694	-1.973466	-2.296190
H	4.777493	-1.028798	-1.582456
H	4.902060	-.971949	1.106434
H	2.532399	-1.898350	2.086978
Re	2.471881	.227521	-.147116
C	2.733249	1.452569	-1.570888
O	2.970521	2.163624	-2.476150
C	3.089647	1.549748	1.058086
O	3.564468	2.313543	1.816482
Re	-2.705628	.092431	.073340
C	-3.299834	1.373959	1.333084
O	-3.754740	2.107032	2.133060
C	-3.157994	1.297535	-1.318623
O	-3.511309	1.992611	-2.198330
C	-.151821	1.008141	-.207521
H	-.190310	1.991221	-.670345
H	.707462	.968014	.535521
H	-.944109	.939978	.605821
H	-.167575	.215783	-.952164



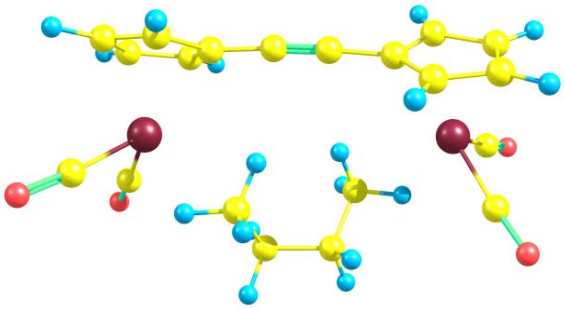
Ethane:

C	-4.175091	1.625487	-1.035073
C	-2.777921	1.764187	-1.345296
C	-2.079671	1.872021	-.099950
C	-3.030487	1.885771	.974409
C	-4.329788	1.706084	.387588
H	-4.982546	1.571917	-1.755526
H	-2.325504	1.787245	-2.329517
H	-2.800553	2.023486	2.024280
H	-5.273571	1.713971	.919939
C	-.665623	1.995597	.040186
C	.544583	1.863375	.156441
C	1.953687	1.683993	.274585
C	2.867836	1.596386	-.823425
C	4.153398	1.250241	-.277139
C	4.021922	1.148594	1.146348
C	2.656069	1.424932	1.499079
H	2.236060	1.484501	2.495857
H	2.631454	1.795783	-1.861976
H	5.080848	1.176758	-.832325
H	4.834315	.977376	1.842755
Re	2.833832	-.500720	.198696
C	3.526420	-1.579537	-1.196744
O	4.022865	-2.186978	-2.072477
C	3.441500	-1.776410	1.457209
O	3.893491	-2.501432	2.266573
Re	-3.210735	-.177282	-.112251
C	-3.819816	-1.327639	-1.486787
O	-4.260782	-1.965546	-2.371787
C	-4.174444	-1.203665	1.154254
O	-4.836302	-1.767467	1.946119
C	-.884518	-1.413613	.574086
C	.341284	-1.491662	-.341913
H	.400761	-.617177	-.990288
H	1.215340	-1.637039	.368655
H	.343215	-2.388553	-.967091
H	-1.777219	-1.554630	-.112721
H	-.877426	-.495188	1.162069
H	-.951310	-2.260524	1.262935



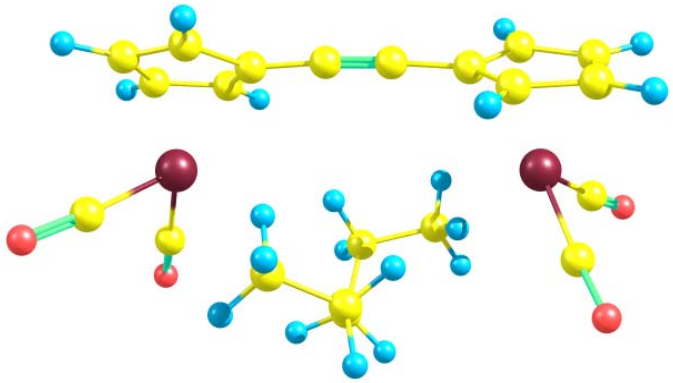
Butane:

Re	.158686	2.943037	-.579810
C	1.801744	3.674149	.001300
C	-2.586266	-4.276277	-2.740919
C	-.738918	3.950997	.745285
C	-.918277	.318336	-2.523177
C	-.617130	1.708858	-2.438360
C	.635545	2.315683	-2.790621
H	-2.618137	2.578378	-1.921901
H	1.523274	1.790867	-3.122300
C	.466561	3.734921	-2.654146
H	1.210115	4.487350	-2.889771
C	-.886965	3.995487	-2.259240
H	-1.340032	4.974628	-2.160155
C	-1.572270	2.735630	-2.158137
C	-1.162829	-.879816	-2.529202
O	-5.235654	-4.445863	.009860
O	2.823555	4.188478	.278446
O	-1.331396	4.636585	1.496293
Re	-2.403337	-3.478823	-.655726
H	-3.571059	-2.314251	-3.287975
C	-1.708734	-4.603067	.696127
C	-4.150270	-4.040463	-.194909
H	-.840224	-5.542582	-2.117692
C	-1.265705	-4.555856	-2.257583
C	-.566785	-3.309330	-2.107828
H	-3.322278	-5.016576	-3.031288
H	.464904	-3.169792	-1.807658
C	-1.484548	-2.266833	-2.462656
O	-1.245234	-5.365125	1.464308
C	-2.715383	-2.853761	-2.899930
C	-2.371155	-1.225854	.818640
H	-3.286122	-.638146	.955248
H	-2.748708	-2.292232	.904856
H	-1.950503	-.948759	-.149208
C	-1.369558	-1.008604	1.958661
H	-1.863809	-1.225687	2.914098
H	-.544991	-1.726206	1.861170
C	-.817228	.424974	1.979597
H	-.335054	.618811	2.946165
H	-1.641242	1.143849	1.889989
C	.198046	.669941	.857776
H	1.119225	.093339	1.001745
H	-.202267	.395467	-.119433
H	.567734	1.738490	.956037



Pentane:

Re	.377693	2.716916	-.532237
C	2.051230	3.341964	.091739
C	-2.847119	-4.177670	-2.712281
C	-.477684	3.519308	.952284
C	-.946738	.335489	-2.519239
C	-.548558	1.699699	-2.405321
C	.734538	2.235404	-2.785133
H	-2.449941	2.686328	-1.748688
H	1.566309	1.667183	-3.183453
C	.680051	3.649389	-2.556015
H	1.474532	4.356409	-2.765487
C	-.631001	3.987528	-2.081051
H	-1.002301	4.989356	-1.902593
C	-1.409489	2.779155	-2.037756
C	-1.275527	-.841430	-2.533694
O	-5.251825	-4.405273	.308243
O	3.093545	3.788520	.406382
O	-1.051355	4.067926	1.822352
Re	-2.535422	-3.343601	-.642104
H	-3.778751	-2.183622	-3.226375
C	-1.688701	-4.281031	.766116
C	-4.207447	-3.970001	-.015333
H	-1.131803	-5.514897	-2.149689
C	-1.523616	-4.512575	-2.273714
C	-.767609	-3.293776	-2.173190
H	-3.630055	-4.888560	-2.949744
H	.275996	-3.194549	-1.898327
C	-1.655401	-2.213832	-2.475410
O	-1.127223	-4.924373	1.576607
C	-2.930566	-2.754381	-2.867645
C	-3.174175	-1.044260	.705949
H	-3.824101	-.902495	-.158626
H	-2.351144	-1.818649	.544476
H	-3.772196	-1.401126	1.547937
C	-2.404830	.239651	1.048303
H	-1.926884	.636588	.146035
H	-3.142265	.990698	1.362857
C	-1.357621	.046591	2.156908
H	-1.789360	-.581819	2.948342
H	-1.133524	1.017181	2.619183
C	-.046896	-.585091	1.655717
H	.487208	-1.046786	2.496890
H	-.260290	-1.393772	.945277
C	.906753	.434133	1.017274
H	.320770	.895414	.161345
H	1.226633	1.181999	1.743007
H	1.786930	-.033917	.569494



4-3. Monuclear manganese complex.

4-3a. Mononuclear manganese, BP86.

Complex:

C	3.544063	-0.812374	0.734233
C	3.867309	0.126557	-0.302586
C	3.256161	-0.333439	-1.529668
C	2.549043	-1.535247	-1.223245
C	2.725969	-1.854440	0.159083
H	3.867512	-0.749222	1.773523
H	4.478970	1.021117	-0.182471
H	3.310510	0.153892	-2.503316
H	1.913035	-2.085575	-1.922462
H	2.321868	-2.722328	0.680260
Mn	1.798080	0.087318	0.010845
C	1.153311	0.209716	1.659722
O	0.804596	0.283726	2.781536
C	1.698638	1.838333	-0.262787
O	1.730759	3.001674	-0.439363

Methane:

C	-1.787875	-1.220441	-0.215533
C	-1.479336	-0.459294	-1.403257
C	-1.544579	0.933509	-1.067899
C	-1.886687	1.045182	0.328697
C	-2.022622	-0.284605	0.836508
H	-1.830192	-2.307165	-0.135255
H	-1.253899	-0.868670	-2.388854
H	-1.376288	1.763552	-1.755312
H	-2.018640	1.969377	0.891437
H	-2.217954	-0.544182	1.879517
Mn	-0.005970	0.004860	0.027438
C	1.026723	1.404080	-0.296821
O	1.650376	2.361066	-0.585413
C	1.135901	-1.093027	-0.765275
O	1.843140	-1.819416	-1.364173
C	0.891123	-0.664936	2.331581
H	1.979575	-0.789754	2.421963
H	0.434363	-0.454786	3.312032
H	0.725672	0.292433	1.740546
H	0.448685	-1.575780	1.907317

Cyclobutane:

C	-0.865528	0.224385	-1.499949
C	-1.907661	0.442871	-0.539999
C	-2.075139	-0.771753	0.222919
C	-1.122703	-1.715274	-0.266792
C	-0.376173	-1.121726	-1.332989
H	-0.510426	0.949559	-2.233573
H	-2.479236	1.363694	-0.417887
H	-2.796033	-0.934071	1.024774
H	-0.952310	-2.714428	0.140656
H	0.417902	-1.596491	-1.909657
Mn	-0.085476	0.069674	0.456705
C	1.334332	0.986820	-0.056860
O	2.240793	1.618719	-0.467166
C	-0.472212	1.254721	1.712455
O	-0.782728	2.067752	2.506557
C	2.156114	-2.195164	3.912705
C	1.728639	-0.755164	3.491931
C	0.980966	-1.390497	2.289941
C	1.848231	-2.678390	2.462321
H	3.185266	-2.334979	4.284380
H	2.591053	-0.153257	3.156725
H	1.131257	-0.155686	4.198188
H	1.187070	-0.911076	1.267921
H	-0.081821	-1.573135	2.500335
H	2.749214	-2.649025	1.825268
H	1.350956	-3.654650	2.329677
H	1.452219	-2.630157	4.643632

Heptane:

C	-4.909852	-.184361	-.213337
C	-4.403727	-1.118045	-1.126452
C	-3.563084	-2.020197	-.420834
C	-3.576162	-1.635692	.935215
C	-4.390748	-.494295	1.072684
H	-4.639280	-.001111	1.991741
H	-3.056697	-2.133486	1.732115
H	-3.077020	-2.884260	-.829254
H	-4.629370	-1.157860	-2.174540
H	-5.590358	.612958	-.441610
Mn	-2.557944	.054739	-.229471
C	-2.510421	2.004349	.098855
O	-2.583496	3.100171	.300749
C	-1.446937	.032170	-1.865030
O	-.886268	-.043434	-2.827827
C	.457419	-.375970	1.559203
C	1.660123	.434830	1.076827
C	2.887400	-.432157	.790483
C	4.095855	.371279	.306718
C	5.323122	-.496049	.021210
C	6.532338	.306316	-.462764
C	7.754300	-.566802	-.745825
H	-.394311	.268024	1.767940
H	.158548	-1.115195	.820086
H	.683202	-.911145	2.476576
H	1.912137	1.182616	1.825172
H	1.390696	.984438	.176701
H	2.630627	-1.181967	.043831
H	3.155870	-.980257	1.691967
H	4.351160	1.120904	1.053818
H	3.825645	.919395	-.594353
H	5.068276	-1.245940	-.725918
H	5.594052	-1.044399	.922014
H	6.789302	1.055270	.283384
H	6.263738	.853667	-1.363824
H	8.594335	.030335	-1.086916
H	8.069198	-1.101562	.145881
H	7.539619	-1.304582	-1.513824

4-4. Binuclear manganese complexes.

4-4a. Binuclear manganese, BP86.

Complex:

Mn	-3.390144	0.176207	-0.141270
C	-4.687606	-0.067091	-1.329874
C	4.151020	-1.383017	-1.042905
C	-3.761533	1.898419	0.092477
C	-0.567162	-1.042228	0.240363
C	-1.871732	-1.029946	0.798211
C	-2.974757	-1.864656	0.374732
H	-1.764079	0.712280	2.225149
H	-2.907194	-2.697609	-0.324009
C	-4.151394	-1.381243	1.044757
H	-5.154910	-1.797399	0.948946
C	-3.782525	-0.270665	1.875017
H	-4.457037	0.301759	2.512455
C	-2.365218	-0.054053	1.736663
C	0.567037	-1.042552	-0.237925
O	5.589228	-0.273763	2.056734
O	-5.586037	-0.278560	-2.058871
O	-4.016464	3.022116	0.327179
Mn	3.390536	0.176168	0.141241
H	2.907183	-2.697364	0.328077
C	3.759837	1.898542	-0.094730
C	4.689797	-0.064248	1.328406
H	4.456335	0.297672	-2.513342
C	3.782011	-0.273644	-1.874707
C	2.364803	-0.056592	-1.736039
H	5.154467	-1.799317	-0.946932
H	1.763653	0.709191	-2.225372
C	1.871507	-1.031032	-0.796000
O	4.013209	3.022336	-0.330633
C	2.974629	-1.865262	-0.371695

Ethane:

Mn	3.062958	-0.406678	0.248330
C	4.131707	1.257111	-0.488574
C	2.915082	1.691443	0.126643
C	1.796860	1.134676	-0.613371
C	2.374791	0.335070	-1.679001
C	3.788641	0.432039	-1.624549
H	4.491298	-0.063552	-2.295117
H	5.138992	1.524375	-0.167906
H	2.828908	2.346427	0.994090
H	1.796506	-0.263110	-2.385270
C	4.544407	-1.338253	0.522760
O	5.573241	-1.886466	0.686462
C	2.739193	-0.299963	1.985714
O	2.539960	-0.160324	3.137100
Mn	-3.618039	0.170193	0.728798
C	-2.797793	2.100868	1.285930
C	-2.172905	1.643139	0.059315
C	-3.255602	1.447633	-0.892928
C	-4.491353	1.797159	-0.259385
C	-4.197151	2.229626	1.089829
H	-2.262318	2.269772	2.223467
H	-4.923457	2.555015	1.834991
H	-5.476416	1.772541	-0.726357
H	-3.131971	1.106647	-1.921031
C	-3.232789	-1.214449	-0.310167
O	-2.979861	-2.084254	-1.062126
C	-5.196283	-0.496961	1.198527
O	-6.279922	-0.877752	1.451580
C	-0.787906	1.469176	-0.168837
C	0.418025	1.329561	-0.369989
C	0.974572	-3.212359	-1.149358
H	-0.096856	-3.477960	-1.155466
H	1.198465	-2.705618	-2.104210
H	1.561894	-4.146196	-1.117399
C	1.286737	-2.310200	0.053105
H	1.115672	-2.819095	1.016173
H	2.415982	-2.124471	0.031472
H	0.682613	-1.390781	0.044949

Propane:

Mn	0.127533	2.813423	-0.798245
C	1.167907	3.561760	0.420272
C	-3.556677	-3.713949	-2.116343
C	-1.206391	3.916086	-0.410960
C	-0.607294	0.186935	-2.542237
C	0.072605	1.427894	-2.527907
C	1.435295	1.644455	-2.067991
H	-1.491559	2.867751	-3.259251
H	2.123106	0.863040	-1.745850
C	1.708840	3.043535	-2.186242
H	2.651910	3.530795	-1.934678
C	0.531313	3.703943	-2.673823
H	0.429466	4.771899	-2.869216
C	-0.479001	2.703264	-2.890319
C	-1.189679	-0.896067	-2.497401
O	-3.742831	-4.886253	1.251665
O	1.900301	4.103691	1.166929
O	-2.067009	4.697524	-0.227601
Mn	-2.056916	-3.360256	-0.624291
H	-3.984211	-1.517151	-1.853777
C	-0.570451	-4.158473	-0.078847
C	-3.054161	-4.247256	0.543301
H	-2.237169	-5.494509	-2.561558
C	-2.345594	-4.415943	-2.443026
C	-1.312921	-3.439120	-2.643316
H	-4.520547	-4.177529	-1.901283
H	-0.271237	-3.638436	-2.895571
C	-1.872727	-2.132817	-2.420060
O	0.416515	-4.734043	0.204163
C	-3.279490	-2.318305	-2.077060
C	-1.012042	0.988019	0.708184
H	-1.648626	1.443858	1.485498
H	-0.088032	1.657134	0.647933
H	-1.585852	0.950425	-0.228653
C	-0.507229	-0.406147	1.114940
H	0.239334	-0.766384	0.385779
H	0.008944	-0.341249	2.091428
C	-1.645970	-1.433535	1.226429
H	-2.507715	-1.055373	1.804849
H	-2.077635	-1.622988	0.193470
H	-1.303252	-2.361675	1.705666

Butane:

Mn	0.185243	2.814620	-0.814187
C	1.875189	2.365418	-1.092409
C	-1.640754	-4.564820	-2.472948
C	0.666433	4.178617	0.208012
C	-1.030596	0.342548	-2.414208
C	-1.028210	1.752878	-2.277961
C	-0.149352	2.714469	-2.906944
H	-2.643201	2.068132	-0.725198
H	0.628786	2.472605	-3.631594
C	-0.480512	4.021151	-2.423817
H	-0.007982	4.954738	-2.730734
C	-1.579062	3.886852	-1.496467
H	-2.053795	4.699341	-0.945026
C	-1.893346	2.509880	-1.383601
C	-1.080598	-0.888570	-2.418711
O	-5.161434	-2.657733	-1.541868
O	2.992454	2.090957	-1.338793
O	0.966256	5.139413	0.818600
Mn	-2.375584	-3.363253	-0.891025
H	-2.684926	-3.005733	-3.725062
C	-2.898757	-4.727314	0.110577
C	-4.054315	-2.923765	-1.245550
H	-0.141519	-5.256275	-0.925319
C	-0.586530	-4.439033	-1.494315
C	-0.273307	-3.063853	-1.359033
H	-2.103145	-5.494864	-2.804760
H	0.446330	-2.627559	-0.664392
C	-1.091970	-2.299556	-2.290514
O	-3.224024	-5.688424	0.707452
C	-1.943571	-3.254286	-2.964999
C	-2.294483	-1.419238	0.834055
H	-3.325498	-1.105277	1.067094
H	-2.319924	-2.561732	0.799285
H	-2.009791	-0.961783	-0.125670
C	-1.313318	-1.036214	1.960143
H	-1.737392	-1.345566	2.933441
H	-0.363332	-1.593700	1.845089
C	-1.016539	0.482265	1.977201
H	-0.645798	0.779825	2.975637
H	-1.959873	1.040746	1.819201
C	0.023669	0.879922	0.910515
H	1.041379	0.565981	1.195522
H	-0.205562	0.430018	-0.067756
H	0.049581	2.022523	0.887017

Pentane:

Mn	0.254320	2.882364	-0.651929
C	1.743064	3.583640	0.000501
C	-2.852417	-4.157033	-2.671298
C	-0.749126	3.753930	0.519573
C	-0.821248	0.287435	-2.291975
C	-0.431871	1.648716	-2.333725
C	0.904871	2.153577	-2.579693
H	-2.383545	2.710714	-1.975103
H	1.786172	1.542947	-2.774020
C	0.828764	3.584640	-2.560924
H	1.663402	4.268855	-2.719243
C	-0.525017	3.970824	-2.290428
H	-0.900169	4.992279	-2.223550
C	-1.312393	2.774408	-2.166505
C	-1.171550	-0.890430	-2.276017
O	-5.516461	-3.918589	-0.269344
O	2.737500	4.091781	0.372775
O	-1.435216	4.392017	1.232378
Mn	-2.661479	-3.351779	-0.736178
H	-3.642126	-2.102590	-3.223075
C	-2.147874	-4.395117	0.598494
C	-4.375563	-3.673877	-0.424044
H	-1.302665	-5.583267	-1.872287
C	-1.602584	-4.558303	-2.092595
C	-0.807949	-3.380214	-1.871241
H	-3.660873	-4.825811	-2.968455
H	0.196864	-3.335561	-1.452954
C	-1.581501	-2.246772	-2.316461
O	-1.785466	-5.149733	1.426779
C	-2.849167	-2.725675	-2.810592
C	-3.083697	-1.212698	0.870714
H	-3.883711	-0.916691	0.176585
H	-2.291524	-1.830690	0.332252
H	-3.515121	-1.837584	1.667270
C	-2.346944	0.011734	1.452719
H	-2.101182	0.720776	0.640063
H	-3.064392	0.538047	2.111000
C	-1.070141	-0.340347	2.246780
H	-1.254220	-1.251438	2.848990
H	-0.851643	0.466572	2.973484
C	0.170993	-0.547859	1.351192
H	0.931991	-1.139227	1.896475
H	-0.097497	-1.144333	0.458180
C	0.849113	0.767673	0.919932
H	0.031588	1.413378	0.452665
H	1.235814	1.323741	1.788428
H	1.672651	0.590911	0.214023

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