Supporting Information

A Computational Study of Cycloaddition Reactions of d^8 Metal Tetroxide (Iron, Ruthenium, Osmium) Complexes with C_{60}.

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(All geometries were calculated B3LYP/LANL2DZ)

Fe-Rea(Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-1.698769	-0.072691	-0.106217
8	-2.593733	-1.412301	-0.259541
8	-2.721138	1.181191	-0.078130
8	-1.057206	0.057594	-1.619787
8	-1.246078	-0.154367	1.477107
7	0.209768	-1.654429	-0.113406
6	0.870443	-1.938530	1.026278
6	0.624428	-2.159663	-1.293555
6	2.006389	-2.769406	1.029279
1	0.472811	-1.474306	1.925451
6	1.743636	-3.007163	-1.376382
1	0.050960	-1.855661	-2.165451
6	2.443802	-3.316223	-0.193147
1	2.524513	-2.976344	1.960498
1	2.049818	-3.408484	-2.337470
1	3.311165	-3.970841	-0.223523
7	0.050053	1.668542	0.136471
6	0.821491	2.005659	-0.915581
6	0.271791	2.207279	1.353472
6	1.877234	2.927233	-0.787184
1	0.577104	1.509689	-1.851636
6	1.298796	3.144716	1.564612
1	-0.378832	1.858137	2.151137
6	2.112956	3.509309	0.473758
1	2.488226	3.175522	-1.649401
1	1.449492	3.571034	2.551603
1	2.913574	4.233062	0.603909

SCF Done: E(RB+HF-LYP) = -920.552849083 A.U.

Fe-Rea(Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-1.257882	-0.050882	-0.081441
8	-2.430559	-1.295447	-0.146283
8	-2.515661	1.104921	-0.196186
8	-0.888408	0.040868	-1.915314
8	-1.135439	-0.121764	1.781092
7	0.236371	-1.548323	-0.143936
6	0.838881	-1.976981	0.997778
6	0.513673	-2.170129	-1.323260
6	1.753453	-3.042456	0.993230
1	0.536538	-1.464894	1.903772
6	1.419060	-3.238852	-1.398467
1	-0.020556	-1.801718	-2.194507
6	2.051051	-3.686103	-0.221913
1	2.205950	-3.361547	1.927971
1	1.607810	-3.710561	-2.357696
1	2.747785	-4.520037	-0.250301
7	0.096049	1.559032	0.175409
6	0.811406	2.032384	-0.880597
6	0.153850	2.209882	1.370301
6	1.617707	3.176869	-0.772402
1	0.683282	1.488214	-1.808766
6	0.942072	3.357136	1.547274
1	-0.459772	1.799003	2.167036
6	1.686019	3.853704	0.458970
1	2.163374	3.529580	-1.643304
1	0.954991	3.850474	2.514058
1	2.293345	4.749251	0.565158

SCF Done: E(UB+HF-LYP) = -920.637297424 A.U.

Ru-Rea(Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
44	-1.378073	-0.056998	-0.091759
8	-2.383103	-1.479430	-0.262049
8	-2.509034	1.277970	-0.064976
8	-0.667646	0.082492	-1.713195
8	-0.880087	-0.146528	1.610175
7	0.465446	-1.734714	-0.102826
6	1.050444	-2.131139	1.051816
6	0.882005	-2.252838	-1.282934
6	2.099110	-3.067779	1.066938
1	0.660410	-1.671313	1.954501
6	1.918409	-3.199459	-1.349384
1	0.375933	-1.879604	-2.168023
6	2.541097	-3.610392	-0.154325
1	2.551827	-3.356904	2.010717
1	2.225265	-3.596796	-2.311781
1	3.350776	-4.335673	-0.174877
7	0.304668	1.763909	0.154899
6	1.004485	2.211824	-0.913896
6	0.513708	2.311290	1.375993
6	1.962615	3.234178	-0.795677
1	0.779644	1.723526	-1.856999
6	1.447778	3.342358	1.573222
1	-0.072689	1.892914	2.188293
6	2.188215	3.808904	0.469232
1	2.512085	3.563804	-1.672464
1	1.587863	3.760980	2.564863
1	2.922797	4.600923	0.592223

SCF Done: E(RB+HF-LYP) = -891.144058551 A.U.

Ru-Rea(Triplet)

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
44	-1.181684	-0.049148	-0.080134
8	-2.457166	-1.398084	-0.259261
8	-2.577053	1.188089	-0.083314
8	-0.594945	0.085038	-1.746021
8	-0.816793	-0.143701	1.650438
7	0.434234	-1.753324	-0.099818
6	0.936445	-2.242653	1.061499
6	0.841655	-2.274701	-1.284241
6	1.887170	-3.276463	1.076111
1	0.557238	-1.777349	1.965466
6	1.783329	-3.314428	-1.346437
1	0.402416	-1.828275	-2.170614
6	2.319454	-3.822035	-0.147216
1	2.273272	-3.638712	2.024079
1	2.084014	-3.709621	-2.311484
1	3.054104	-4.623339	-0.165699
7	0.270003	1.782549	0.148059
6	0.878968	2.320080	-0.938631
6	0.473141	2.327316	1.373894
6	1.734034	3.429204	-0.831578
1	0.662749	1.831220	-1.882988
6	1.308395	3.441215	1.555784
1	-0.039520	1.839110	2.196555
6	1.953784	4.000359	0.435896
1	2.210531	3.828805	-1.721683
1	1.445428	3.852791	2.550644
1	2.610063	4.859889	0.548122

SCF Done: E(UB+HF-LYP) = -891.149926834 A.U.

Os-Rea(Singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z

76	-1.144059	-0.043139	-0.091760
8	-2.165028	-1.461969	-0.252404
8	-2.281495	1.293261	-0.118677
8	-0.443212	0.062512	-1.731436
8	-0.724930	-0.106632	1.643668
7	0.680956	-1.653596	-0.024503
6	1.176220	-2.083708	1.162019
6	1.180118	-2.148166	-1.184335
6	2.211406	-3.030292	1.229441
1	0.721946	-1.641815	2.042274
6	2.209871	-3.102409	-1.194687
1	0.741236	-1.748287	-2.092264
6	2.738659	-3.548656	0.031919
1	2.588298	-3.347166	2.197026
1	2.583251	-3.479501	-2.141432
1	3.540998	-4.281735	0.053590
7	0.542636	1.700023	0.139160
6	1.111448	2.245960	-0.963691
6	0.888695	2.150161	1.370657
6	2.065498	3.272054	-0.869087
1	0.786687	1.828670	-1.910907
6	1.835810	3.172265	1.542653
1	0.393561	1.661255	2.202640
6	2.437408	3.741968	0.404739
1	2.501462	3.685291	-1.773005
1	2.090222	3.506541	2.543515
1	3.176598	4.532271	0.508039

SCF Done: E(RB+HF-LYP) = -888.427132220 A.U.

Os-Rea(Triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z

76	-0.919722	-0.038286	-0.062599
8	-2.212164	-1.376795	-0.239104
8	-2.332483	1.184841	-0.072312
8	-0.356406	0.093950	-1.746817
8	-0.581957	-0.133163	1.683183
7	0.665301	-1.724903	-0.074333
6	1.089960	-2.277794	1.092562
6	1.108232	-2.224393	-1.258217
6	1.987808	-3.355642	1.111721
1	0.687107	-1.827945	1.993526
6	2.002860	-3.303377	-1.311614
1	0.727521	-1.729991	-2.145644
6	2.453414	-3.879765	-0.108592
1	2.305913	-3.770821	2.063206
1	2.331164	-3.678347	-2.275710
1	3.145517	-4.717802	-0.121873
7	0.501527	1.775245	0.154471
6	1.028148	2.370950	-0.948059
6	0.743753	2.299213	1.384908
6	1.829630	3.518385	-0.851926
1	0.784867	1.897520	-1.893142
6	1.532597	3.446850	1.552495
1	0.292486	1.768264	2.216246
6	2.087637	4.068190	0.417614
1	2.234289	3.966062	-1.754487
1	1.700723	3.838897	2.550393
1	2.701646	4.959306	0.519482

SCF Done: E(UB+HF-LYP) = -888.402294572 A.U.

C60-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	1.184276	0.384795	3.350509

6	0.731923	-1.007405	3.350509
6	2.618417	-1.589131	1.842564
6	1.434141	-1.973926	2.612153
6	-1.434141	-1.973926	2.612153
6	0.702218	-2.981331	1.842564
6	-0.731923	-1.007405	3.350509
6	-0.702218	-2.981331	1.842564
6	1.434141	-3.219148	0.597342
6	-1.184276	0.384795	3.350509
6	-2.618417	-2.358721	0.597342
6	-2.618417	-1.589131	1.842564
6	0.731923	-3.447312	-0.597342
6	2.618417	-2.358721	0.597342
6	1.184276	-2.824701	-1.842564
6	-0.731923	-3.447312	-0.597342
6	-1.184276	-2.824701	-1.842564
6	-1.434141	-3.219148	0.597342
6	-3.504765	0.369178	0.597342
6	-2.320489	0.753973	2.612153
6	0.000000	-2.439907	-2.612153
6	-2.320489	-1.999194	-1.842564
6	-2.320489	-0.753973	-2.612153
6	-3.052412	-1.761378	-0.597342
6	-3.504765	-0.369178	-0.597342
6	-2.320489	1.999194	1.842564
6	0.000000	1.245222	3.350509
6	-3.052412	-0.253433	1.842564
6	-3.052412	1.761378	0.597342
6	-3.052412	0.253433	-1.842564
6	3.504765	-0.369178	-0.597342
6	0.000000	-1.245222	-3.350509
6	0.000000	2.439907	2.612153
6	3.052412	1.761378	0.597342
6	2.320489	-0.753973	-2.612153
6	3.052412	-0.253433	1.842564
6	2.320489	-1.999194	-1.842564
6	3.052412	0.253433	-1.842564
6	3.052412	-1.761378	-0.597342
6	2.320489	0.753973	2.612153
6	-1.184276	2.824701	1.842564

6	-0.731923	3.447312	0.597342
6	-2.618417	2.358721	-0.597342
6	-1.434141	3.219148	-0.597342
6	1.434141	3.219148	-0.597342
6	-0.702218	2.981331	-1.842564
6	0.731923	3.447312	0.597342
6	0.702218	2.981331	-1.842564
6	-1.434141	1.973926	-2.612153
6	1.184276	2.824701	1.842564
6	2.618417	1.589131	-1.842564
6	2.618417	2.358721	-0.597342
6	-0.731923	1.007405	-3.350509
6	-2.618417	1.589131	-1.842564
6	-1.184276	-0.384795	-3.350509
6	0.731923	1.007405	-3.350509
6	1.184276	-0.384795	-3.350509
6	1.434141	1.973926	-2.612153
6	3.504765	0.369178	0.597342
6	2.320489	1.999194	1.842564

SCF Done: E(RB+HF-LYP) = -2285.72210837 A.U.

Fe-PC

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.957196	0.686670	0.014212
6	0.956597	-0.735971	-0.006561
8	3.482022	-1.162524	0.001305
26	4.430669	0.150694	-0.010357
8	3.369102	1.374914	-0.006583
6	0.472145	1.427384	-1.158779
6	-0.267772	2.598900	-0.690110
6	-0.268943	2.577360	0.772917
6	0.470736	1.392702	1.208122

6 0.029421 0.673214 2.327935
6 0.029972 -0.793957 2.305969
6 0.473088 -1.479438 1.165289
6 -0.265926 -2.652277 0.695650
6 -0.264717 -2.630764 -0.767158
6 0.475340 -1.444757 -1.200834
6 0.033799 -0.725706 -2.321399
6 0.033248 0.741504 -2.300248
6 -1.150716 1.201446 -3.025568
6 -1.855722 2.331549 -2.579537
6 -1.404206 3.045052 -1.385565
6 -2.589920 3.487152 -0.649201
6 -2.591061 3.466419 0.754468
6 -1.406618 3.002686 1.479426
6 -1.860001 2.254397 2.651243
6 -1.155615 1.111596 3.064635
6 -1.888284 -0.079139 3.498654
6 -1.154674 -1.255675 3.029393
6 -1.857936 -2.386401 2.582079
6 -1.403455 -3.099538 1.388919
6 -2.587834 -3.543163 0.650897
6 -2.586648 -3.522447 -0.752642
6 -1.401129 -3.057232 -1.475297
6 -1.853513 -2.309304 -2.647841
6 -1.149465 -1.165856 -3.060182
6 -1.882461 0.023987 -3.495744
6 -3.286845 0.023379 -3.501216
6 -4.021012 1.200648 -3.033615
6 -3.319149 2.330818 -2.582233
6 -3.773735 3.045629 -1.388415
6 -4.911402 2.601370 -0.694230
6 -4.912527 2.579765 0.769381
6 -3.775998 3.003225 1.478357
6 -3.323546 2.253641 2.651521
6 -4.026230 1.110616 3.067885
6 -3.292681 -0.079883 3.501775
6 -4.025027 -1.257802 3.032752
6 -3.321418 -2.387432 2.582648
6 -3.773430 -3.102721 1.388153
6 -4.910402 -2.659417 0.692098

6	-4.909096	-2.637821	-0.771549
6	-3.770924	-3.060332	-1.478553
6	-3.317094	-2.310290	-2.650891
6	-4.020054	-1.167796	-3.068357
6	-5.205136	-0.727179	-2.331998
6	-5.205695	0.737395	-2.310423
6	-5.642162	1.423093	-1.164463
6	-6.094894	0.673226	0.008296
6	-5.644120	1.388262	1.203416
6	-5.209564	0.668952	2.329342
6	-5.209054	-0.795625	2.307784
6	-5.642993	-1.481682	1.161097
6	-6.094373	-0.732209	-0.012443
6	-5.641003	-1.446840	-1.206825
7	6.711563	-1.880441	0.049402
6	7.253022	-2.334536	1.203820
1	6.955615	-1.803217	2.104502
6	8.141597	-3.425307	1.244085
1	8.548926	-3.761410	2.193058
6	8.478589	-4.063429	0.034322
1	9.153570	-4.915435	0.030239
6	7.926591	-3.583343	-1.169699
1	8.164758	-4.045323	-2.123491
6	7.047437	-2.484739	-1.114463
1	6.594218	-2.068650	-2.012211
8	5.252172	0.200731	-1.383652
7	6.703617	2.273871	-0.047991
6	7.224983	2.734236	-1.209315
1	6.918799	2.203243	-2.107291
6	8.104899	3.831890	-1.258973
1	8.497483	4.172683	-2.212522
6	8.453613	4.469925	-0.052506
1	9.123895	5.325570	-0.055376
6	7.919576	3.984878	1.157475
1	8.165755	4.447132	2.108966
6	7.048433	2.879758	1.112341
1	6.609131	2.460034	2.014601
8	5.274984	0.193604	1.347986

SCF Done: E(RB+HF-LYP) = -3206.30728830 A.U.

Ru-PC

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.898862	0.669305	0.012092
6	0.896148	-0.748355	-0.006537
8	3.268851	-1.369327	0.010470
44	4.423495	-0.031673	0.001258
8	3.252636	1.291875	-0.004033
6	0.416777	1.410872	-1.161570
6	-0.317747	2.585432	-0.694674
6	-0.318655	2.565901	0.768490
6	0.415775	1.379414	1.204847
6	-0.023240	0.664513	2.327695
6	-0.025992	-0.802305	2.308219
6	0.410068	-1.488267	1.166495
6	-0.328438	-2.660102	0.698654
6	-0.327403	-2.640557	-0.764530
6	0.412177	-1.456794	-1.199916
6	-0.022858	-0.740217	-2.323341
6	-0.020171	0.726606	-2.303866
6	-1.203294	1.189016	-3.029528
6	-1.905169	2.321965	-2.584794
6	-1.452228	3.035282	-1.391328
6	-2.636569	3.481416	-0.654585
6	-2.637468	3.462589	0.749423
6	-1.454147	2.996800	1.475513
6	-1.908571	2.251881	2.649000
6	-1.207211	1.107397	3.063978
6	-1.942331	-0.081068	3.499907
6	-1.211793	-1.260257	3.032330
6	-1.917398	-2.390536	2.586677
6	-1.465590	-3.105568	1.393823
6	-2.650677	-3.547222	0.655546

6	-2.649697	-3.528404	-0.748452
6	-1.463670	-3.067088	-1.473012
6	-1.913786	-2.320447	-2.647045
6	-1.207540	-1.178633	-3.061127
6	-1.937634	0.012587	-3.498038
6	-3.342449	0.015291	-3.502430
6	-4.073408	1.194936	-3.036130
6	-3.368824	2.324073	-2.586412
6	-3.821404	3.041414	-1.393093
6	-4.959865	2.600515	-0.697796
6	-4.960751	2.580909	0.765882
6	-3.823183	3.002918	1.474312
6	-3.372328	2.254018	2.648783
6	-4.077585	1.113210	3.066906
6	-3.347151	-0.078459	3.502504
6	-4.081949	-1.255330	3.035232
6	-3.381062	-2.387127	2.586428
6	-3.834816	-3.102747	1.392511
6	-4.970701	-2.657510	0.695763
6	-4.969626	-2.637913	-0.767904
6	-3.832749	-3.064255	-1.474849
6	-3.377550	-2.317076	-2.648751
6	-4.077935	-1.173609	-3.067776
6	-5.261796	-0.729047	-2.331098
6	-5.259070	0.735246	-2.311535
6	-5.693462	1.423379	-1.166387
6	-6.147962	0.676214	0.007627
6	-5.695023	1.391768	1.201813
6	-5.262156	0.673132	2.328683
6	-5.264951	-0.791164	2.309135
6	-5.700471	-1.477639	1.163428
6	-6.150610	-0.728758	-0.011179
6	-5.698850	-1.446020	-1.204795
7	5.994799	-2.081322	0.017650
6	6.452412	-2.599125	1.182865
1	6.266494	-2.000350	2.069426
6	7.120770	-3.835412	1.237698
1	7.467724	-4.222532	2.190948
6	7.317872	-4.553438	0.042814
1	7.818882	-5.518251	0.054025

6	6.853418	-4.002902	-1.167240
1	6.987465	-4.522983	-2.110835
6	6.198461	-2.759573	-1.137957
1	5.824338	-2.282821	-2.038826
8	5.137446	-0.043652	-1.609971
7	5.991303	2.014467	-0.017931
6	6.425564	2.544227	-1.186823
1	6.228651	1.950889	-2.074647
6	7.085114	3.785146	-1.243626
1	7.412975	4.181841	-2.199686
6	7.298546	4.495229	-0.046787
1	7.793283	5.463282	-0.059199
6	6.858661	3.932478	1.166779
1	7.006221	4.445961	2.111984
6	6.210464	2.685471	1.139109
1	5.854243	2.199600	2.042387
8	5.143625	-0.008907	1.609642

SCF Done: E(RB+HF-LYP) = -3176.87653000 A.U.

Os-PC

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.872497	0.668431	0.013441
6	0.870283	-0.742836	-0.006220
8	3.277420	-1.382739	0.003484
76	4.431304	-0.043067	0.004828
8	3.272527	1.290307	0.003259
6	0.401953	1.413148	-1.159949
6	-0.329971	2.588909	-0.692314
6	-0.331080	2.568288	0.771504
6	0.400582	1.379903	1.206976
6	-0.034328	0.664625	2.331406
6	-0.036248	-0.801830	2.310860

6	0.396187	-1.485965	1.166446
6	-0.338056	-2.659776	0.697664
6	-0.336849	-2.639142	-0.766159
6	0.398528	-1.452705	-1.200482
6	-0.032528	-0.736194	-2.325670
6	-0.030652	0.730262	-2.304977
6	-1.213493	1.193193	-3.030424
6	-1.915509	2.325628	-2.583872
6	-1.463610	3.038893	-1.389496
6	-2.647909	3.483255	-0.651704
6	-2.648993	3.463377	0.752603
6	-1.465915	2.998242	1.479411
6	-1.919590	2.251592	2.652585
6	-1.218194	1.106944	3.067845
6	-1.952439	-0.082623	3.502673
6	-1.221440	-1.261467	3.034447
6	-1.925781	-2.392033	2.586800
6	-1.473952	-3.106553	1.393134
6	-2.658227	-3.547682	0.653438
6	-2.657073	-3.527811	-0.750890
6	-1.471682	-3.065900	-1.475905
6	-1.921506	-2.317987	-2.649767
6	-1.216408	-1.175207	-3.063930
6	-1.946844	0.016349	-3.499856
6	-3.351539	0.018255	-3.503201
6	-4.082642	1.197151	-3.035479
6	-3.378966	2.326397	-2.584816
6	-3.831913	3.042494	-1.390752
6	-4.969765	2.600169	-0.695719
6	-4.970840	2.579467	0.767864
6	-3.834066	3.001841	1.477010
6	-3.383158	2.252407	2.651269
6	-4.087617	1.110832	3.068417
6	-3.357140	-0.080782	3.503843
6	-4.090611	-1.257740	3.034990
6	-3.389220	-2.388850	2.585428
6	-3.842193	-3.103749	1.390635
6	-4.977754	-2.658389	0.693820
6	-4.976492	-2.637696	-0.769761
6	-3.839764	-3.063098	-1.477133

6	-3.385051	-2.314863	-2.650711
6	-4.085826	-1.171427	-3.068958
6	-5.269592	-0.727968	-2.331536
6	-5.267722	0.736095	-2.310875
6	-5.702346	1.422986	-1.165280
6	-6.156432	0.674767	0.008057
6	-5.704215	1.389604	1.202790
6	-5.271410	0.670500	2.329170
6	-5.273341	-0.793566	2.308526
6	-5.707974	-1.479308	1.162252
6	-6.158236	-0.729895	-0.011800
6	-5.706053	-1.445916	-1.205839
7	5.989051	-1.964649	0.010876
6	6.440426	-2.471729	1.183298
1	6.216979	-1.880700	2.065505
6	7.142717	-3.686736	1.242618
1	7.481656	-4.066844	2.201097
6	7.380067	-4.393518	0.048628
1	7.905387	-5.345087	0.065526
6	6.922954	-3.850401	-1.167561
1	7.087308	-4.362011	-2.110868
6	6.232238	-2.627756	-1.147031
1	5.859421	-2.155087	-2.050038
8	5.099314	-0.042578	-1.637440
7	5.970939	1.900586	-0.015513
6	6.407348	2.417698	-1.189807
1	6.172581	1.834577	-2.074369
6	7.111745	3.632381	-1.250261
1	7.440550	4.018749	-2.209935
6	7.367591	4.330323	-0.054874
1	7.899249	5.278689	-0.071587
6	6.920081	3.782038	1.162410
1	7.096771	4.288482	2.106461
6	6.225491	2.560498	1.142108
1	5.859485	2.086351	2.047142
8	5.096079	-0.029092	1.648929

SCF Done: E(RB+HF-LYP) = -3174.15350799 A.U.

[6,5]-Fe-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.053397	-0.734794	-0.076896
6	-1.053648	0.737791	-0.095459
8	-3.283355	1.263463	-0.074970
26	-4.306243	-0.004640	-0.046880
8	-3.283446	-1.273352	-0.077324
6	-0.571317	-1.445271	-1.201784
6	0.259172	-2.631226	-1.014218
6	0.603853	-3.048700	0.278720
6	0.128976	-2.298628	1.448337
6	-0.663072	-1.162325	1.270050
6	-0.443323	0.028479	2.080601
6	-0.661801	1.198662	1.240193
6	0.131159	2.338194	1.389748
6	0.606987	3.057642	0.201465
6	0.261255	2.608615	-1.080575
6	-0.571046	1.419305	-1.238206
6	-0.107001	0.679239	-2.388272
6	-0.107558	-0.735187	-2.370435
6	1.026246	-1.475650	-2.930827
6	1.251460	-2.649525	-2.086429
6	2.558719	-3.078057	-1.815059
6	2.921003	-3.511078	-0.466301
6	1.964434	-3.497972	0.560501
6	2.329139	-3.028860	1.898479
6	1.192306	-2.288960	2.447964
6	1.408449	-1.143172	3.233751
6	0.569833	0.040115	3.052626
6	1.409703	1.226667	3.203810
6	1.194650	2.352423	2.389342
6	2.332215	3.076731	1.821196
6	1.968065	3.512141	0.471857
6	2.924637	3.499196	-0.554886

6	2.561710	3.032530	-1.892306
6	1.253875	2.598646	-2.152779
6	1.027567	1.404101	-2.967187
6	2.115090	0.691744	-3.489020
6	2.114383	-0.777928	-3.470378
6	3.476796	-1.224703	-3.189925
6	3.693655	-2.350402	-2.378745
6	4.760982	-2.336306	-1.379208
6	4.283470	-3.052639	-0.196733
6	4.633156	-2.604052	1.084388
6	3.635559	-2.590866	2.154841
6	3.861103	-1.396439	2.968921
6	2.771720	-0.687647	3.496729
6	2.772472	0.776400	3.478118
6	3.862578	1.470481	2.932730
6	3.638177	2.644137	2.088681
6	4.635676	2.629335	1.018280
6	4.286640	3.046136	-0.273746
6	4.763121	2.299407	-1.437638
6	3.695819	2.289456	-2.437190
6	3.477918	1.143962	-3.219866
6	4.318426	-0.038668	-3.033714
6	5.341552	-0.027098	-2.075450
6	5.567260	-1.199357	-1.231024
6	5.932857	-0.730522	0.105093
6	5.474098	-1.417539	1.238675
6	4.996610	-0.672549	2.401411
6	4.997333	0.731325	2.383663
6	5.475501	1.446316	1.202501
6	5.933511	0.730441	0.086642
6	5.568325	1.165817	-1.260836
7	-5.889750	2.228887	0.008149
6	-6.366595	2.696518	1.182869
1	-6.098834	2.121998	2.067013
6	-7.165885	3.849765	1.262174
1	-7.528594	4.193792	2.225250
6	-7.475838	4.535857	0.073240
1	-8.088259	5.432640	0.098811
6	-6.982038	4.044164	-1.149486
1	-7.199211	4.541810	-2.088919

6	-6.189908	2.883676	-1.135624
1	-5.787022	2.455621	-2.050775
8	-5.086109	0.001680	-1.444653
7	-5.892451	-2.220692	-0.003629
6	-6.288207	-2.796491	-1.160367
1	-5.968510	-2.300188	-2.074103
6	-7.072584	-3.962129	-1.187139
1	-7.369140	-4.395149	-2.136831
6	-7.454387	-4.543623	0.036205
1	-8.057050	-5.447184	0.051712
6	-7.045131	-3.938848	1.239239
1	-7.319851	-4.353389	2.203577
6	-6.262204	-2.774042	1.172402
1	-5.921805	-2.259587	2.068307
8	-5.005796	-0.006451	1.395135

SCF Done: E(RB+HF-LYP) = -3206.30339151 A.U.

[6,6]-Fe-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.018032	0.688001	0.010630
6	1.013564	-0.712064	-0.006348
8	3.352134	-1.274749	0.003180
26	4.339307	-0.001673	0.000712
8	3.352543	1.272456	-0.001110
6	0.578221	1.433931	-1.164345
6	-0.140374	2.613191	-0.698771
6	-0.141333	2.595623	0.764627
6	0.576604	1.405373	1.202530
6	0.152434	0.695900	2.322893
6	0.147856	-0.769727	2.305282
6	0.567402	-1.454697	1.168126
6	-0.157868	-2.629402	0.701821

6	-0.156983	-2.611771	-0.761577
6	0.569037	-1.426243	-1.198664
6	0.150711	-0.713825	-2.319413
6	0.155559	0.751758	-2.301930
6	-1.020093	1.215705	-3.029565
6	-1.714842	2.343332	-2.584319
6	-1.263562	3.060186	-1.393564
6	-2.444653	3.505796	-0.655501
6	-2.445549	3.489005	0.740311
6	-1.265436	3.025617	1.468874
6	-1.718150	2.280265	2.641491
6	-1.023946	1.142162	3.060188
6	-1.758550	-0.045128	3.496313
6	-1.031467	-1.226211	3.031650
6	-1.732781	-2.349445	2.585561
6	-1.284676	-3.069146	1.395378
6	-2.467649	-3.507267	0.655900
6	-2.466761	-3.490426	-0.739899
6	-1.282912	-3.034532	-1.467079
6	-1.729451	-2.286295	-2.640174
6	-1.027559	-1.152624	-3.058082
6	-1.754116	0.039295	-3.495066
6	-3.148876	0.043679	-3.494446
6	-3.875858	1.223291	-3.028308
6	-3.175305	2.345821	-2.583527
6	-3.626237	3.064167	-1.392378
6	-4.756445	2.627136	-0.700249
6	-4.757328	2.609504	0.760929
6	-3.627996	3.029672	1.464869
6	-3.178643	2.282829	2.638993
6	-3.879754	1.149840	3.055529
6	-3.153303	-0.040681	3.494070
6	-3.887127	-1.215707	3.027014
6	-3.193204	-2.342682	2.583087
6	-3.647259	-3.058167	1.391382
6	-4.773832	-2.613943	0.697919
6	-4.772858	-2.596305	-0.763248
6	-3.645376	-3.023623	-1.465833
6	-3.189915	-2.279645	-2.639441
6	-3.883332	-1.142242	-3.056784

6	-5.063222	-0.695620	-2.320979
6	-5.058628	0.766455	-2.303351
6	-5.489170	1.451885	-1.166411
6	-5.943187	0.708175	0.006563
6	-5.490642	1.423412	1.197694
6	-5.061527	0.710665	2.318299
6	-5.066159	-0.751410	2.300695
6	-5.499682	-1.434104	1.163244
6	-5.947590	-0.687551	-0.010275
6	-5.498172	-1.405627	-1.200891
7	5.915060	-2.332268	0.007123
6	6.410274	-2.823379	1.165201
1	6.181734	-2.250500	2.060283
6	7.177810	-3.993083	1.223214
1	7.554128	-4.348203	2.175341
6	7.442759	-4.681974	0.032716
1	8.033919	-5.591547	0.042446
6	6.933975	-4.177535	-1.171062
1	7.117173	-4.678635	-2.114218
6	6.175484	-3.001440	-1.138577
1	5.764019	-2.569775	-2.047001
8	5.134221	-0.005907	-1.387759
7	5.910704	2.334505	-0.008479
6	6.381352	2.842091	-1.169876
1	6.143540	2.275629	-2.066593
6	7.135708	4.020500	-1.229459
1	7.492391	4.388560	-2.184274
6	7.413328	4.701092	-0.037053
1	7.994880	5.616999	-0.047940
6	6.929652	4.180187	1.170188
1	7.123182	4.674587	2.114895
6	6.182989	2.996255	1.139115
1	5.790566	2.551643	2.049951
8	5.135836	0.001737	1.388472

SCF Done: E(RB+HF-LYP) = -3206.30575503   A.U.

[6,5]-Ru-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.095729	-0.739603	-0.084234
6	-1.095228	0.743091	-0.102603
8	-3.260958	1.331774	-0.095235
44	-4.441409	0.001451	-0.051876
8	-3.261533	-1.329287	-0.100622
6	-0.577877	-1.444935	-1.204297
6	0.262708	-2.627083	-1.015553
6	0.608611	-3.048224	0.275788
6	0.129382	-2.294363	1.441071
6	-0.675398	-1.163371	1.263627
6	-0.446724	0.028539	2.071528
6	-0.673443	1.199937	1.233861
6	0.132050	2.334217	1.382847
6	0.612228	3.057517	0.198766
6	0.265251	2.604833	-1.081541
6	-0.577393	1.419490	-1.240558
6	-0.103556	0.679455	-2.386160
6	-0.104159	-0.734838	-2.368406
6	1.036122	-1.472689	-2.925893
6	1.261201	-2.647102	-2.084475
6	2.570654	-3.078686	-1.815233
6	2.933354	-3.513693	-0.466590
6	1.971831	-3.497060	0.557922
6	2.335545	-3.026302	1.895113
6	1.196264	-2.284579	2.439539
6	1.412992	-1.140928	3.227414
6	0.572600	0.040175	3.041880
6	1.414392	1.224592	3.197628
6	1.199000	2.348319	2.381256
6	2.339104	3.074483	1.818081
6	1.975971	3.511533	0.469462
6	2.937472	3.502061	-0.555127
6	2.574038	3.033366	-1.892328
6	1.263981	2.596572	-2.150512

6	1.037619	1.401632	-2.961981
6	2.127688	0.691460	-3.484715
6	2.126919	-0.777255	-3.466161
6	3.490894	-1.225076	-3.188554
6	3.708596	-2.353115	-2.378743
6	4.777685	-2.339602	-1.378407
6	4.297790	-3.056634	-0.195474
6	4.646823	-2.606989	1.087746
6	3.644964	-2.591957	2.155711
6	3.870647	-1.397125	2.971249
6	2.778122	-0.687511	3.496074
6	2.778980	0.776445	3.477492
6	3.872340	1.471322	2.935107
6	3.648004	2.645434	2.089624
6	4.649741	2.632403	1.021618
6	4.301405	3.050265	-0.272534
6	4.780101	2.302708	-1.436862
6	3.711023	2.292255	-2.437150
6	3.492129	1.144516	-3.218416
6	4.334092	-0.038626	-3.032875
6	5.359848	-0.027117	-2.074265
6	5.585551	-1.200968	-1.229270
6	5.950647	-0.731519	0.108683
6	5.489450	-1.419601	1.243270
6	5.009722	-0.673394	2.406474
6	5.010553	0.732261	2.388717
6	5.491069	1.448411	1.207062
6	5.951393	0.731371	0.090218
6	5.586753	1.167363	-1.259100
7	-5.998316	2.049619	0.015389
6	-6.436877	2.555973	1.193407
1	-6.202238	1.967415	2.075496
6	-7.149707	3.767258	1.267192
1	-7.486550	4.141955	2.229361
6	-7.409910	4.474792	0.078028
1	-7.950149	5.418676	0.102980
6	-6.957802	3.940706	-1.144287
1	-7.141069	4.453273	-2.083954
6	-6.255686	2.721768	-1.133259
1	-5.889875	2.258892	-2.045226

8	-5.165444	0.008607	-1.650606
7	-5.997682	-2.047774	-0.001338
6	-6.357868	-2.649070	-1.161285
1	-6.074994	-2.127738	-2.071228
6	-7.056840	-3.869958	-1.184255
1	-7.326115	-4.323745	-2.133427
6	-7.392253	-4.483078	0.038377
1	-7.925147	-5.431309	0.053662
6	-7.025119	-3.848811	1.240803
1	-7.270078	-4.285755	2.204448
6	-6.326224	-2.629181	1.178080
1	-6.016442	-2.093294	2.070556
8	-5.040678	-0.005833	1.599608

SCF Done: E(RB+HF-LYP) = -3176.87242291 A.U.

[6,6]-Ru-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.102457	0.706718	0.010868
6	1.099294	-0.724832	-0.006693
8	3.347230	-1.324923	-0.006918
44	4.526784	0.001694	-0.000299
8	3.343941	1.325774	0.008693
6	0.597677	1.441655	-1.164379
6	-0.134020	2.615747	-0.698027
6	-0.134848	2.597498	0.766022
6	0.596832	1.412280	1.203830
6	0.160067	0.699330	2.326303
6	0.156662	-0.771490	2.307956
6	0.590207	-1.457941	1.167955
6	-0.146773	-2.628628	0.700814
6	-0.145880	-2.610376	-0.763192
6	0.592021	-1.428543	-1.200123

6	0.159443	-0.713595	-2.323052
6	0.162835	0.757239	-2.304964
6	-1.017705	1.218399	-3.032421
6	-1.719002	2.353341	-2.588693
6	-1.266624	3.067876	-1.396107
6	-2.450117	3.514938	-0.658285
6	-2.450935	3.497377	0.746070
6	-1.268376	3.031921	1.473890
6	-1.722087	2.287919	2.647851
6	-1.021233	1.142224	3.063733
6	-1.756292	-0.046460	3.501263
6	-1.026823	-1.227240	3.034091
6	-1.732911	-2.358867	2.589558
6	-1.282394	-3.075444	1.397529
6	-2.467171	-3.517079	0.658416
6	-2.466306	-3.499537	-0.745899
6	-1.280703	-3.039517	-1.472303
6	-1.729689	-2.293473	-2.646747
6	-1.023018	-1.151079	-3.061854
6	-1.752069	0.040963	-3.500339
6	-3.156293	0.044271	-3.504070
6	-3.886329	1.225010	-3.037825
6	-3.182116	2.355186	-2.589712
6	-3.634313	3.073726	-1.396600
6	-4.771836	2.632863	-0.700396
6	-4.772640	2.614575	0.763293
6	-3.635923	3.037808	1.471716
6	-3.185292	2.289815	2.647221
6	-3.890101	1.148759	3.065876
6	-3.160521	-0.043222	3.503424
6	-3.895494	-1.220544	3.036285
6	-3.196044	-2.353999	2.588991
6	-3.650209	-3.070415	1.395352
6	-4.784886	-2.624211	0.697878
6	-4.783924	-2.605931	-0.765797
6	-3.648361	-3.034505	-1.472880
6	-3.192905	-2.288637	-2.647881
6	-3.891890	-1.144300	-3.067330
6	-5.074231	-0.698301	-2.330530
6	-5.070847	0.766222	-2.312273

6	-5.504756	1.455313	-1.167707
6	-5.958920	0.709359	0.006833
6	-5.506163	1.425826	1.200168
6	-5.073630	0.708279	2.327674
6	-5.077074	-0.756246	2.309438
6	-5.512885	-1.443291	1.164371
6	-5.962205	-0.695229	-0.010701
6	-5.511425	-1.413799	-1.203531
7	6.003062	-2.280493	0.003552
6	6.458745	-2.800741	1.169170
1	6.272158	-2.202787	2.057670
6	7.134801	-4.035584	1.230349
1	7.489727	-4.414863	2.184301
6	7.340726	-4.755659	0.037226
1	7.871257	-5.706198	0.048225
6	6.849558	-4.223506	-1.170949
1	6.979505	-4.752335	-2.111402
6	6.184410	-2.981703	-1.143737
1	5.788130	-2.527079	-2.047794
8	5.298355	0.004105	-1.565725
7	6.000704	2.290000	-0.006248
6	6.430980	2.825157	-1.174896
1	6.228692	2.236929	-2.066331
6	7.101308	4.062953	-1.235768
1	7.435387	4.454469	-2.192331
6	7.328931	4.770036	-0.038988
1	7.855857	5.722404	-0.049963
6	6.864236	4.222461	1.172744
1	7.011477	4.740837	2.116320
6	6.202974	2.978768	1.144874
1	5.826554	2.512197	2.051365
8	5.301958	0.003511	1.563376

SCF Done: E(RB+HF-LYP) = -3176.87520407   A.U.

[6,5]-Os-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.188128	-0.754876	-0.080026
6	-1.191090	0.744118	-0.097917
8	-3.152119	1.313895	-0.082043
76	-4.388157	-0.001022	-0.044083
8	-3.160229	-1.323367	-0.079468
6	-0.620809	-1.450107	-1.201276
6	0.230767	-2.627673	-1.010907
6	0.579718	-3.051430	0.276471
6	0.099399	-2.293145	1.441124
6	-0.714527	-1.169602	1.266186
6	-0.478559	0.021957	2.068844
6	-0.716323	1.192620	1.237256
6	0.093783	2.322413	1.384182
6	0.572110	3.052691	0.200829
6	0.223724	2.596640	-1.075589
6	-0.625536	1.412867	-1.236918
6	-0.148574	0.677581	-2.372426
6	-0.146703	-0.742254	-2.355206
6	1.000376	-1.474490	-2.916757
6	1.229670	-2.648527	-2.079552
6	2.541339	-3.079944	-1.814414
6	2.906959	-3.515120	-0.467274
6	1.944546	-3.497142	0.557035
6	2.308873	-3.024577	1.892984
6	1.168940	-2.282908	2.436426
6	1.385478	-1.142418	3.227383
6	0.543223	0.035344	3.040618
6	1.382482	1.219515	3.198166
6	1.163231	2.339655	2.379336
6	2.301219	3.070393	1.817417
6	1.935745	3.508551	0.470171
6	2.898167	3.504428	-0.554326
6	2.533480	3.034819	-1.890200
6	1.222841	2.593491	-2.144365
6	0.996673	1.398579	-2.952111
6	2.086399	0.692046	-3.477325

6	2.088330	-0.778485	-3.459134
6	3.454044	-1.223433	-3.186758
6	3.677087	-2.352666	-2.379455
6	4.748416	-2.336712	-1.380655
6	4.271238	-3.055269	-0.196818
6	4.620549	-2.604773	1.086014
6	3.618616	-2.590650	2.154371
6	3.843944	-1.395874	2.970889
6	2.750659	-0.688309	3.497263
6	2.748800	0.775706	3.479018
6	3.840312	1.472838	2.935379
6	3.612018	2.646464	2.089451
6	4.613836	2.636688	1.021008
6	4.263612	3.054710	-0.272584
6	4.742323	2.307898	-1.438145
6	3.670995	2.296420	-2.436944
6	3.450956	1.147068	-3.216143
6	4.295534	-0.035040	-3.032747
6	5.323900	-0.021886	-2.076665
6	5.553524	-1.195951	-1.232212
6	5.919492	-0.725674	0.105822
6	5.461160	-1.415130	1.241073
6	4.981434	-0.670111	2.405087
6	4.979656	0.736192	2.387635
6	5.457485	1.453440	1.205483
6	5.917559	0.737214	0.087676
6	5.550377	1.173277	-1.261545
7	-5.896127	1.947277	0.008843
6	-6.328882	2.455886	1.189811
1	-6.068841	1.879211	2.071340
6	-7.062582	3.652375	1.258782
1	-7.396058	4.026808	2.221941
6	-7.349100	4.345518	0.068013
1	-7.916543	5.273057	0.090530
6	-6.886623	3.818177	-1.152636
1	-7.079175	4.325549	-2.093086
6	-6.163499	2.613765	-1.143099
1	-5.787676	2.156125	-2.052296
8	-5.043827	0.005974	-1.689122
7	-5.914213	-1.939017	-0.003235

6	-6.279871	-2.535618	-1.165960
1	-5.983452	-2.019084	-2.073092
6	-6.997011	-3.743873	-1.186779
1	-7.270820	-4.193526	-2.136431
6	-7.345091	-4.351150	0.034502
1	-7.901541	-5.285617	0.049174
6	-6.958299	-3.729068	1.236418
1	-7.202272	-4.166653	2.199812
6	-6.241160	-2.522124	1.177744
1	-5.912387	-1.996215	2.068055
8	-4.940363	-0.005312	1.639767

SCF Done: E(RB+HF-LYP) = -3174.14424100 A.U.

[6,6]-Os-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.097347	0.702792	0.011007
6	1.094059	-0.721503	-0.006196
8	3.307174	-1.328514	0.001212
76	4.496290	-0.004309	0.000514
8	3.303940	1.316989	0.002392
6	0.601533	1.439385	-1.163731
6	-0.126426	2.615261	-0.698120
6	-0.127266	2.597198	0.766124
6	0.600779	1.410330	1.203487
6	0.168500	0.699292	2.328843
6	0.164644	-0.770895	2.310721
6	0.593170	-1.455860	1.168007
6	-0.140863	-2.627819	0.701458
6	-0.139825	-2.609729	-0.762793
6	0.595292	-1.426753	-1.199255
6	0.167729	-0.713396	-2.325077
6	0.171460	0.756790	-2.307075

6	-1.008938	1.218791	-3.033902
6	-1.709571	2.354589	-2.590001
6	-1.257614	3.068984	-1.397115
6	-2.440684	3.516498	-0.658724
6	-2.441565	3.499052	0.746096
6	-1.259495	3.033291	1.474711
6	-1.712931	2.289670	2.649080
6	-1.012787	1.143206	3.065427
6	-1.748043	-0.045359	3.502865
6	-1.019145	-1.226628	3.036054
6	-1.725259	-2.358651	2.591254
6	-1.275503	-3.075384	1.398966
6	-2.460059	-3.516624	0.659122
6	-2.459091	-3.499194	-0.745665
6	-1.273612	-3.039697	-1.472758
6	-1.721703	-2.293732	-2.647645
6	-1.014954	-1.151033	-3.063124
6	-1.743410	0.041381	-3.501574
6	-3.147883	0.045147	-3.504532
6	-3.877245	1.226211	-3.038426
6	-3.172634	2.356334	-2.590274
6	-3.624709	3.075221	-1.397088
6	-4.762426	2.634583	-0.700655
6	-4.763305	2.616441	0.763045
6	-3.626466	3.039564	1.471742
6	-3.176104	2.291476	2.647527
6	-3.881375	1.150562	3.066350
6	-3.152527	-0.041654	3.504083
6	-3.887537	-1.218825	3.037009
6	-3.188345	-2.352664	2.589743
6	-3.642717	-3.069115	1.395970
6	-4.777225	-2.622413	0.698142
6	-4.776168	-2.604279	-0.765540
6	-3.640679	-3.033464	-1.472766
6	-3.184884	-2.287806	-2.647996
6	-3.883569	-1.143178	-3.067704
6	-5.065684	-0.696604	-2.330599
6	-5.061837	0.767761	-2.312492
6	-5.495585	1.457181	-1.167934
6	-5.950058	0.711503	0.006704

6	-5.497130	1.427936	1.200044
6	-5.064897	0.710281	2.327720
6	-5.068804	-0.754088	2.309634
6	-5.504760	-1.441182	1.164525
6	-5.953774	-0.693098	-0.010695
6	-5.503159	-1.411928	-1.203477
7	5.974245	-2.101899	0.012132
6	6.421834	-2.625009	1.180977
1	6.205767	-2.042162	2.070767
6	7.124630	-3.843928	1.234743
1	7.475220	-4.225959	2.189195
6	7.364113	-4.545200	0.037465
1	7.915698	-5.483552	0.045652
6	6.876864	-4.009926	-1.170970
1	7.031749	-4.524948	-2.114824
6	6.184317	-2.784368	-1.142648
1	5.791075	-2.326522	-2.045099
8	5.199078	-0.011850	-1.619949
7	5.967236	2.104392	-0.014025
6	6.392252	2.640370	-1.185493
1	6.167910	2.062685	-2.076604
6	7.083223	3.866011	-1.240682
1	7.415401	4.258715	-2.197380
6	7.334980	4.560279	-0.041816
1	7.877884	5.503650	-0.051192
6	6.871354	4.011420	1.169775
1	7.036277	4.520542	2.115141
6	6.189189	2.780002	1.142515
1	5.813512	2.311703	2.047118
8	5.203259	0.008360	1.619434

SCF Done: E(RB+HF-LYP) = -3174.15083445 A.U.

[6,5]-Fe-Pro

Atomic Coordinates (Angstroms)

Number	X	Y	Z
6	1.780597	0.114380	-0.125531
6	1.605797	-1.385195	-0.258583
6	1.044343	0.815741	-1.285591
6	0.159110	1.842680	-0.793230
6	0.062269	1.750559	0.642682
6	1.100005	0.759782	1.205699
6	0.401817	-0.237524	2.106526
6	0.517124	-1.619345	1.955184
6	1.121427	-2.195616	0.768238
6	0.523765	-3.421265	0.181130
6	0.646551	-3.315285	-1.264644
6	1.301935	-2.038221	-1.541349
6	0.899410	-1.281846	-2.640949
6	0.754577	0.187249	-2.494847
6	-0.400119	0.588619	-3.281564
6	-1.237143	1.627804	-2.836751
6	-0.953050	2.270022	-1.565758
6	-2.216044	2.561494	-0.911409
6	-2.314985	2.415476	0.484141
6	-1.157264	2.010474	1.263965
6	-1.646954	1.147582	2.366576
6	-0.885124	0.048029	2.758603
6	-1.546465	-1.222720	3.048794
6	-0.677638	-2.274694	2.544163
6	-1.225879	-3.414892	1.958958
6	-0.609717	-4.002764	0.747110
6	-1.683981	-4.501201	-0.103022
6	-1.578204	-4.389447	-1.502487
6	-0.388780	-3.784115	-2.094804
6	-0.810084	-2.990074	-3.245734
6	-0.180318	-1.757994	-3.504587
6	-0.980320	-0.602741	-3.906633
6	-2.373056	-0.716302	-4.039475
6	-3.245654	0.357961	-3.557379
6	-2.687986	1.507623	-2.973511
6	-3.297396	2.089059	-1.774548
6	-4.439362	1.497549	-1.209129
6	-4.551624	1.362790	0.246034

6	-3.513143	1.814235	1.075203
6	-3.097792	1.025868	2.233900
6	-3.740186	-0.194153	2.517722
6	-2.943510	-1.346337	2.930191
6	-3.518229	-2.538346	2.313043
6	-2.671775	-3.558757	1.839404
6	-2.956602	-4.218835	0.563782
6	-4.072654	-3.828438	-0.193036
6	-3.959712	-3.698424	-1.647560
6	-2.741665	-3.975229	-2.288452
6	-2.266224	-3.104416	-3.367908
6	-3.030081	-1.994637	-3.758896
6	-4.303780	-1.707135	-3.092888
6	-4.434219	-0.256925	-2.971011
6	-5.020543	0.302938	-1.817315
6	-5.497111	-0.568089	-0.745515
6	-5.212548	0.087961	0.533877
6	-4.813405	-0.673884	1.642090
6	-4.677355	-2.128367	1.518414
6	-4.945920	-2.757215	0.292258
6	-5.367666	-1.962598	-0.863651
6	-4.759888	-2.542584	-2.058945
26	3.726338	1.667353	1.114747
8	2.133354	1.447208	1.973662
8	3.205517	0.423593	-0.123949
8	4.640331	0.692213	2.047781
8	3.345521	3.000297	0.250558
7	4.203234	3.142835	2.680385
6	3.990868	4.461581	2.466866
6	4.601050	2.708696	3.899209
6	4.185134	5.412381	3.481910
1	3.654258	4.727011	1.469974
6	4.809934	3.598771	4.964878
1	4.743809	1.637452	3.996291
6	4.601619	4.974713	4.753197
1	4.006848	6.463068	3.276170
1	5.121595	3.216283	5.931640
1	4.754471	5.686806	5.559809
7	5.675512	1.927943	0.036341
6	6.762632	1.211099	0.406472

6	5.755670	2.785173	-1.008372
6	7.992927	1.339294	-0.260323
1	6.617133	0.535877	1.243728
6	6.950737	2.966615	-1.724702
1	4.841707	3.317665	-1.250603
6	8.090726	2.234468	-1.342614
1	8.844465	0.749193	0.063832
1	6.978606	3.661071	-2.558937
1	9.030054	2.355777	-1.876764

SCF Done: E(RB+HF-LYP) = -3206.41605840 A.U.

[6,6]-Fe-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.549765	0.883389	0.079467
6	1.594464	-0.711200	-0.037678
6	0.781628	1.591354	-1.057622
6	0.005057	2.686920	-0.523117
6	0.000795	2.577480	0.938021
6	0.776615	1.414536	1.309038
6	0.355821	0.623175	2.365250
6	0.397711	-0.861484	2.254754
6	0.854806	-1.460558	1.093187
6	0.147490	-2.598312	0.550055
6	0.153640	-2.489859	-0.911227
6	0.867091	-1.285480	-1.273948
6	0.415432	-0.517701	-2.334799
6	0.372786	0.966905	-2.224049
6	-0.819051	1.426195	-2.923894
6	-1.559739	2.515986	-2.427614
6	-1.137056	3.161902	-1.195127
6	-2.335299	3.530231	-0.437541
6	-2.340127	3.424931	0.961440

6	-1.147291	2.947049	1.664439
6	-1.578888	2.125541	2.784314
6	-0.840979	0.973462	3.117302
6	-1.539557	-0.261053	3.473612
6	-0.774410	-1.387329	2.940573
6	-1.446828	-2.516919	2.435935
6	-0.973840	-3.137614	1.208557
6	-2.140741	-3.572231	0.437211
6	-2.135381	-3.467161	-0.961834
6	-0.963293	-2.922807	-1.651051
6	-1.426863	-2.126240	-2.776288
6	-0.751149	-0.934351	-3.100648
6	-1.513578	0.258999	-3.465165
6	-2.916574	0.220891	-3.490169
6	-3.686534	1.348870	-2.960536
6	-3.020887	2.472739	-2.440593
6	-3.502606	3.102089	-1.208817
6	-4.628829	2.581658	-0.548176
6	-4.633761	2.472245	0.911941
6	-3.512484	2.886758	1.651391
6	-3.040421	2.081357	2.780037
6	-3.709693	0.892683	3.120491
6	-2.942692	-0.301793	3.481347
6	-3.642051	-1.471034	2.943695
6	-2.908104	-2.555475	2.431922
6	-3.339058	-3.210372	1.194831
6	-4.484913	-2.754400	0.520676
6	-4.479181	-2.644749	-0.939507
6	-3.327926	-2.995430	-1.665665
6	-2.888542	-2.164312	-2.788791
6	-3.619543	-1.015056	-3.137734
6	-4.815979	-0.651631	-2.383322
6	-4.857872	0.809941	-2.274193
6	-5.320357	1.412683	-1.091631
6	-5.754313	0.580892	0.031758
6	-5.328890	1.236002	1.269666
6	-4.875154	0.463017	2.352322
6	-4.833771	-0.998679	2.243242
6	-5.247374	-1.626206	1.055424
6	-5.714134	-0.819559	-0.073049

6	-5.238256	-1.449186	-1.305690
26	4.239085	0.150347	0.161975
8	2.986553	-1.150058	-0.062033
8	2.915859	1.398385	0.103136
8	4.715219	0.245814	-1.400874
8	4.380576	0.066297	1.791023
7	5.779866	-1.413881	0.224851
6	6.296739	-1.826182	1.406047
6	6.168017	-2.009612	-0.927953
6	7.248989	-2.856175	1.474309
1	5.918356	-1.317186	2.286360
6	7.110163	-3.051032	-0.937918
1	5.707109	-1.631377	-1.834239
6	7.664736	-3.479658	0.282677
1	7.644700	-3.158753	2.438632
1	7.392883	-3.510618	-1.879904
1	8.397833	-4.281957	0.305018
7	5.701262	1.778993	0.401531
6	6.344590	2.285348	-0.676932
6	5.902657	2.323576	1.625507
6	7.235391	3.365133	-0.563622
1	6.120931	1.806224	-1.624747
6	6.776944	3.405660	1.816520
1	5.345434	1.871998	2.439703
6	7.458162	3.935177	0.704328
1	7.732845	3.745555	-1.450300
1	6.910915	3.819197	2.811627
1	8.140511	4.773017	0.821889

SCF Done: E(RB+HF-LYP) = -3206.44415032 A.U.

[6,5]-Ru-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	1.323271	1.017173	0.307669
6	1.129694	-0.483600	0.186096
6	0.566109	1.715558	-0.841762
6	-0.300452	2.753016	-0.339079
6	-0.375544	2.665088	1.096309
6	0.662298	1.672243	1.647578
6	-0.026199	0.683600	2.563531
6	0.072274	-0.697741	2.419136
6	0.649282	-1.283126	1.222028
6	0.026104	-2.504863	0.652734
6	0.123597	-2.407256	-0.794643
6	0.790622	-1.139585	-1.089288
6	0.374183	-0.385430	-2.185082
6	0.247518	1.085808	-2.042532
6	-0.918275	1.497084	-2.808465
6	-1.735645	2.548011	-2.354052
6	-1.420748	3.192654	-1.092036
6	-2.667549	3.501750	-0.414499
6	-2.742497	3.362795	0.983543
6	-1.575911	2.945900	1.742376
6	-2.052625	2.094532	2.859488
6	-1.295543	0.988361	3.242079
6	-1.965003	-0.273425	3.551624
6	-1.117675	-1.337488	3.034989
6	-1.689451	-2.473163	2.464722
6	-1.102468	-3.072008	1.243215
6	-2.198278	-3.562324	0.416635
6	-2.117822	-3.457861	-0.985045
6	-0.933194	-2.868595	-1.602619
6	-1.367645	-2.075989	-2.749233
6	-0.728620	-0.852492	-3.024728
6	-1.523498	0.309776	-3.416518
6	-2.919921	0.211704	-3.523178
6	-3.771238	1.297955	-3.029698
6	-3.190062	2.444043	-2.462273
6	-3.770309	3.037889	-1.254510
6	-4.907828	2.461583	-0.664418
6	-4.994135	2.334627	0.793298
6	-3.935573	2.778176	1.600956
6	-3.506922	1.989698	2.755416

6	-4.157034	0.778001	3.057062
6	-3.365551	-0.381321	3.459544
6	-3.965220	-1.569416	2.858873
6	-3.138904	-2.601060	2.373456
6	-3.455049	-3.263106	1.106458
6	-4.580888	-2.863540	0.369260
6	-4.494204	-2.741196	-1.087754
6	-3.291701	-3.034362	-1.750424
6	-2.827317	-2.174119	-2.842926
6	-3.586296	-1.057774	-3.224563
6	-4.843531	-0.752627	-2.535374
6	-4.955315	0.699329	-2.417961
6	-5.513561	1.270800	-1.255848
6	-5.979488	0.410156	-0.171052
6	-5.663500	1.068597	1.099871
6	-5.251941	0.306973	2.203742
6	-5.134581	-1.149630	2.084270
6	-5.432918	-1.780564	0.866112
6	-5.867502	-0.986203	-0.285134
6	-5.289326	-1.578292	-1.489096
44	3.389108	2.656357	1.538359
8	1.679598	2.398415	2.419870
8	2.762048	1.333588	0.241958
8	4.358100	1.600370	2.570293
8	3.003902	4.116689	0.619963
7	3.885648	4.174175	3.144047
6	3.676293	5.497462	2.928890
6	4.250966	3.740370	4.377415
6	3.840474	6.444464	3.950458
1	3.360559	5.763362	1.925657
6	4.425698	4.631105	5.447304
1	4.394784	2.670216	4.477534
6	4.219968	6.006696	5.233020
1	3.664265	7.494509	3.739818
1	4.708424	4.247073	6.422265
1	4.344917	6.717772	6.045196
7	5.412473	2.970931	0.533237
6	6.492354	2.247007	0.926311
6	5.554478	3.915108	-0.433041
6	7.765770	2.462943	0.375331

1	6.304927	1.507293	1.697006
6	6.798012	4.184074	-1.026672
1	4.649933	4.449921	-0.701200
6	7.926473	3.451973	-0.613091
1	8.605484	1.868667	0.721502
1	6.871634	4.952581	-1.790022
1	8.903656	3.646810	-1.048968

SCF Done: E(RB+HF-LYP) = -3176.94920089 A.U.

[6,6]-Ru-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.490116	0.876495	0.147114
6	1.534208	-0.721185	0.034045
6	0.741411	1.581294	-1.003676
6	-0.041223	2.679998	-0.484379
6	-0.069690	2.573545	0.976478
6	0.696907	1.409302	1.361655
6	0.258255	0.621221	2.412402
6	0.299103	-0.863450	2.305436
6	0.772945	-1.464727	1.152483
6	0.074125	-2.603078	0.600248
6	0.104731	-2.497087	-0.860589
6	0.825774	-1.294157	-1.213186
6	0.392978	-0.528412	-2.282828
6	0.350967	0.956434	-2.175533
6	-0.828126	1.416663	-2.895926
6	-1.574762	2.508779	-2.413905
6	-1.171088	3.156025	-1.175883
6	-2.380838	3.527969	-0.438415
6	-2.408795	3.425246	0.960493
6	-1.228500	2.946499	1.683827
6	-1.679629	2.127913	2.798003

6	-0.949517	0.975052	3.144721
6	-1.655834	-0.257599	3.492178
6	-0.884377	-1.386250	2.973544
6	-1.550162	-2.515738	2.460153
6	-1.058391	-3.139409	1.241756
6	-2.213241	-3.573474	0.452182
6	-2.184673	-3.470755	-0.946747
6	-1.000500	-2.929722	-1.617853
6	-1.444345	-2.134579	-2.751864
6	-0.761472	-0.944432	-3.067199
6	-1.515600	0.249635	-3.446355
6	-2.918099	0.213974	-3.494214
6	-3.694552	1.344284	-2.979197
6	-3.035583	2.468041	-2.450538
6	-3.536182	3.100459	-1.227817
6	-4.673999	2.583188	-0.584701
6	-4.702957	2.476361	0.875336
6	-3.593189	2.890398	1.632234
6	-3.141023	2.086184	2.769872
6	-3.817859	0.899281	3.101563
6	-3.059009	-0.295897	3.476950
6	-3.751566	-1.464894	2.930049
6	-3.011284	-2.551633	2.432331
6	-3.423068	-3.208030	1.189522
6	-4.556955	-2.751289	0.495938
6	-4.527170	-2.644404	-0.964208
6	-3.364747	-2.998280	-1.670799
6	-2.905715	-2.170013	-2.788152
6	-3.628883	-1.020088	-3.150925
6	-4.836760	-0.653222	-2.416791
6	-4.877787	0.808618	-2.311042
6	-5.358520	1.414329	-1.137295
6	-5.812288	0.585370	-0.019643
6	-5.405960	1.242008	1.223879
6	-4.971510	0.470236	2.315316
6	-4.930924	-0.991788	2.209447
6	-5.326063	-1.620797	1.016104
6	-5.772749	-0.815373	-0.121274
6	-5.278104	-1.448112	-1.344843
44	4.309380	0.145100	0.214339

8	2.926737	-1.202534	0.040915
8	2.855535	1.427835	0.203067
8	4.785198	0.245722	-1.485173
8	4.568308	0.061429	1.961252
7	5.930615	-1.447936	0.230261
6	6.407580	-1.933692	1.404923
6	6.372095	-1.971328	-0.942343
6	7.362210	-2.961666	1.444369
1	5.996188	-1.478351	2.299138
6	7.322370	-3.003609	-0.977115
1	5.945979	-1.538197	-1.840606
6	7.830131	-3.507750	0.234793
1	7.720339	-3.322674	2.403359
1	7.647333	-3.399302	-1.934103
1	8.566561	-4.307413	0.236635
7	5.837313	1.817821	0.399437
6	6.400444	2.357195	-0.711932
6	6.127579	2.337549	1.620045
6	7.291721	3.438454	-0.635478
1	6.112178	1.898451	-1.651634
6	7.008507	3.419423	1.770072
1	5.635503	1.862303	2.461485
6	7.604110	3.980468	0.625270
1	7.721371	3.842470	-1.546595
1	7.213156	3.809087	2.762362
1	8.288767	4.820146	0.712811

SCF Done: E(RB+HF-LYP) = -3176.97950395 A.U.

[6,5]-Os-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.294297	1.095669	0.313335
6	1.130760	-0.407336	0.198203

6	0.531858	1.777684	-0.839825
6	-0.355868	2.800062	-0.343465
6	-0.434256	2.716860	1.092624
6	0.620452	1.745542	1.650547
6	-0.052239	0.746278	2.567492
6	0.070677	-0.633639	2.426596
6	0.663533	-1.213130	1.234340
6	0.066853	-2.448484	0.665808
6	0.169079	-2.353165	-0.781612
6	0.811480	-1.073093	-1.076466
6	0.387333	-0.330390	-2.177110
6	0.230916	1.138427	-2.039607
6	-0.937887	1.525282	-2.813015
6	-1.777113	2.561527	-2.365205
6	-1.480534	3.216104	-1.103574
6	-2.736454	3.502948	-0.433122
6	-2.814900	3.366579	0.964719
6	-1.643882	2.974991	1.730498
6	-2.109322	2.118094	2.848089
6	-1.332567	1.027864	3.236803
6	-1.979985	-0.245425	3.546990
6	-1.110230	-1.294396	3.037781
6	-1.657419	-2.443162	2.469145
6	-1.053497	-3.034980	1.252506
6	-2.135673	-3.548532	0.421918
6	-2.050598	-3.446935	-0.979754
6	-0.874592	-2.836817	-1.593416
6	-1.318529	-2.055962	-2.744591
6	-0.701834	-0.821129	-3.021018
6	-1.516996	0.324658	-3.420359
6	-2.910777	0.199379	-3.533135
6	-3.785144	1.270548	-3.046997
6	-3.228699	2.429278	-2.480247
6	-3.825856	3.015316	-1.277035
6	-4.954977	2.419269	-0.690689
6	-5.045714	2.295011	0.766948
6	-3.999265	2.760895	1.578076
6	-3.560970	1.984510	2.736941
6	-4.189717	0.761783	3.039227
6	-3.377853	-0.380769	3.448824

6	-3.951837	-1.582015	2.849331
6	-3.103635	-2.599099	2.371103
6	-3.401139	-3.271181	1.104683
6	-4.530975	-2.895517	0.360836
6	-4.439666	-2.775936	-1.096085
6	-3.228601	-3.048183	-1.752041
6	-2.775519	-2.182295	-2.844959
6	-3.553832	-1.081801	-3.233711
6	-4.820217	-0.798810	-2.551697
6	-4.960564	0.651139	-2.439209
6	-5.535232	1.215401	-1.281499
6	-5.989463	0.349127	-0.196300
6	-5.692169	1.017262	1.074026
6	-5.271261	0.267149	2.182181
6	-5.125263	-1.187248	2.067779
6	-5.405922	-1.827562	0.850323
6	-5.850341	-1.045244	-0.305534
6	-5.254877	-1.629659	-1.504830
76	3.375897	2.731223	1.571247
8	1.631039	2.501519	2.411896
8	2.729582	1.441776	0.245822
8	4.276729	1.597740	2.600915
8	2.998828	4.207768	0.654133
7	3.923171	4.191663	3.162395
6	3.706960	5.522589	2.979221
6	4.341357	3.741708	4.377301
6	3.914137	6.450671	4.008624
1	3.351879	5.805262	1.994535
6	4.562136	4.617285	5.449543
1	4.485347	2.670452	4.455845
6	4.346972	5.995707	5.267854
1	3.728084	7.503224	3.820770
1	4.886971	4.217079	6.404720
1	4.504729	6.694062	6.085417
7	5.366751	2.984926	0.590465
6	6.427448	2.220507	0.970945
6	5.524151	3.893513	-0.411336
6	7.688316	2.358861	0.371986
1	6.227643	1.507118	1.762237
6	6.757792	4.079112	-1.052084

1	4.637360	4.460619	-0.670132
6	7.863581	3.305144	-0.654542
1	8.508534	1.732767	0.708695
1	6.839743	4.816125	-1.844716
1	8.831925	3.433492	-1.132599

SCF Done: E(RB+HF-LYP) = -3174.19316302 A.U.

[6,6]-Os-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.481016	0.873559	0.156020
6	1.524384	-0.724677	0.043295
6	0.737091	1.578399	-0.996542
6	-0.046314	2.677548	-0.479323
6	-0.077971	2.571529	0.981487
6	0.687287	1.407131	1.368379
6	0.245708	0.619683	2.418286
6	0.285614	-0.865097	2.311720
6	0.761851	-1.467119	1.160161
6	0.062656	-2.604603	0.606876
6	0.096351	-2.498907	-0.853868
6	0.819533	-1.296937	-1.205118
6	0.389218	-0.531242	-2.275716
6	0.348147	0.953629	-2.168849
6	-0.829000	1.414628	-2.891796
6	-1.575868	2.507615	-2.411920
6	-1.174307	3.154772	-1.173325
6	-2.385273	3.527850	-0.438310
6	-2.416194	3.425497	0.960595
6	-1.237805	2.945980	1.686531
6	-1.691739	2.128166	2.799940
6	-0.963179	0.974689	3.148157
6	-1.671199	-0.257365	3.494542

6	-0.899540	-1.386809	2.977689
6	-1.565224	-2.516020	2.463411
6	-1.071521	-3.140218	1.246232
6	-2.225081	-3.573505	0.454357
6	-2.193573	-3.471134	-0.944533
6	-1.007591	-2.931228	-1.613417
6	-1.448415	-2.136113	-2.748443
6	-0.763865	-0.946503	-3.062369
6	-1.516327	0.248050	-3.443419
6	-2.918769	0.213519	-3.494319
6	-3.695469	1.344596	-2.981267
6	-3.036707	2.467980	-2.451549
6	-3.539374	3.101091	-1.229981
6	-4.678949	2.584882	-0.589044
6	-4.710987	2.478429	0.871010
6	-3.602408	2.891784	1.630076
6	-3.153152	2.087489	2.768838
6	-3.831595	0.901191	3.099473
6	-3.074398	-0.294546	3.476632
6	-3.766825	-1.463160	2.928616
6	-3.026374	-2.550630	2.432661
6	-3.436159	-3.206953	1.189146
6	-4.568316	-2.749491	0.493152
6	-4.535470	-2.642988	-0.967003
6	-3.371836	-2.997933	-1.671127
6	-2.909803	-2.170310	-2.787751
6	-3.631324	-1.019895	-3.152265
6	-4.840395	-0.651897	-2.420669
6	-4.880466	0.810030	-2.315366
6	-5.363210	1.416405	-1.142742
6	-5.819941	0.588076	-0.025803
6	-5.415644	1.244702	1.218422
6	-4.983974	0.472847	2.310962
6	-4.944324	-0.989263	2.205498
6	-5.337590	-1.618259	1.011481
6	-5.781277	-0.812735	-0.127020
6	-5.284668	-1.446180	-1.349441
76	4.323033	0.141802	0.216221
8	2.920832	-1.201718	0.054218
8	2.851039	1.418780	0.216767

8	4.741099	0.242329	-1.508744
8	4.541968	0.056028	1.979072
7	5.937652	-1.397393	0.232239
6	6.407841	-1.893401	1.409680
6	6.407260	-1.903211	-0.941327
6	7.377723	-2.905054	1.448305
1	5.975147	-1.457737	2.302935
6	7.374485	-2.917784	-0.971338
1	5.984596	-1.469020	-1.840133
6	7.873624	-3.429451	0.240701
1	7.726133	-3.271263	2.408911
1	7.718991	-3.295412	-1.928620
1	8.622670	-4.217214	0.244184
7	5.842495	1.764951	0.390367
6	6.397757	2.312013	-0.725633
6	6.159043	2.273793	1.612922
6	7.302015	3.380487	-0.650101
1	6.087241	1.869243	-1.665152
6	7.054862	3.342422	1.756549
1	5.672151	1.798917	2.456868
6	7.640944	3.907982	0.609488
1	7.721448	3.787350	-1.564576
1	7.277613	3.719514	2.749608
1	8.336333	4.738946	0.694275

SCF Done: E(RB+HF-LYP) = -3174.22288909   A.U.
