

Supporting Information

A Computational Study of Cycloaddition Reactions of 16-Electron d^8 ML_4 Complexes with C_{60} .

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Cartesian coordinates for the B3LYP/LANL2DZ optimized structures.

Fe(CO)4-(singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.786507
6	1.301511	0.000000	-1.223820
6	-0.315643	-1.780389	-0.136561
6	-0.316103	1.780268	-0.136726
8	0.183884	-0.000045	2.950729
8	2.275510	-0.000021	-1.887536
8	-0.636484	-2.900713	-0.275339
8	-0.637278	2.900513	-0.275635

Fe(CO)4-(triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	-0.291846	-0.000039	-0.126365
6	0.259113	0.000090	1.639182
6	1.372073	0.000109	-0.933862
6	-0.780271	-1.787142	-0.337402
6	-0.780660	1.786941	-0.337546
8	0.606502	0.000173	2.761695
8	2.427534	0.000203	-1.450268
8	-1.058931	-2.920019	-0.457582
8	-1.059568	2.919747	-0.457820

Ru(CO)4-(singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.953699
6	1.938445	0.000000	-0.093853
6	-0.184334	-0.629229	-1.840334
6	-1.631157	1.047228	-0.094976
8	-0.039413	-0.135347	3.118952
8	3.096886	0.190895	-0.181511
8	-0.331698	-1.132008	-2.890680
8	-2.503001	1.833448	-0.183544

Ru(CO)4-(triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	-0.308640	-0.000039	-0.133442
6	0.272703	0.000099	1.714603
6	1.435926	0.000117	-0.975625
6	-0.699883	-1.938216	-0.302650
6	-0.700305	1.938039	-0.302806
8	0.655519	0.000186	2.827414
8	2.508678	0.000213	-1.459445
8	-0.853542	-3.103229	-0.369031
8	-0.854219	3.103014	-0.369281

Os(CO)4-(singlet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.936262
6	1.011843	0.000000	-1.650698
6	-0.514707	-1.860112	-0.145697
6	-0.512796	1.860686	-0.145199
8	0.201513	0.000017	3.097366
8	1.790330	-0.000005	-2.535529
8	-1.011730	-2.919575	-0.286412
8	-1.008650	2.920713	-0.285600

Os(CO)4-(triplet)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	-0.209708	-0.000026	-0.090638
6	0.354465	0.000109	1.735594
6	1.507160	0.000125	-0.930375
6	-0.631464	-1.901819	-0.273036
6	-0.631880	1.901660	-0.273188

8	0.727163	0.000196	2.854949
8	2.577718	0.000220	-1.426100
8	-0.884562	-3.049485	-0.382550
8	-0.885229	3.049262	-0.382794

 C60

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

PC-Fe

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	5.736731	0.015254	0.116579
6	2.118503	0.053118	0.678418
6	2.117401	0.066631	-0.730251
6	5.549677	1.825650	0.116468
8	5.351452	2.981447	0.115872
6	6.548314	-0.011601	1.699331
8	7.253785	-0.040539	2.645197
6	5.480243	-1.783830	0.114386
8	5.258259	-2.935869	0.112665
6	6.569578	-0.010176	-1.455115
8	7.286838	-0.038595	-2.392099
6	1.636913	1.249456	-1.449881
6	1.179570	2.368561	-0.736103
6	1.179283	2.354652	0.727529
6	1.636381	1.222087	1.420054
6	0.909804	0.744818	2.597666
6	0.935748	-0.717824	2.583578
6	1.678501	-1.146205	1.397546

6	1.262210	-2.280879	0.683067
6	1.262544	-2.266725	-0.780647
6	1.679043	-1.118438	-1.472720
6	0.937346	-0.667537	-2.651230
6	0.911299	0.795114	-2.637231
6	-0.237592	1.480522	-3.064210
6	-0.711352	2.649193	-2.321559
6	-0.017214	3.084010	-1.181645
6	-0.757446	3.511837	0.006010
6	-0.018028	3.061226	1.185795
6	-0.712856	2.604458	2.316632
6	-0.239466	1.421860	3.036994
6	-1.410485	0.665376	3.481958
6	-1.385438	-0.738248	3.468473
6	-0.188403	-1.443910	3.009423
6	-0.619448	-2.628617	2.266326
6	0.090942	-3.038253	1.127109
6	-0.632358	-3.492340	-0.061209
6	0.091601	-3.015558	-1.240100
6	-0.618004	-2.583867	-2.371677
6	-0.186408	-1.385223	-3.091764
6	-1.383242	-0.670875	-3.538025
6	-1.408288	0.732752	-3.524556
6	-2.605653	1.439103	-3.066375
6	-2.174874	2.623812	-2.322815
6	-2.885036	3.033715	-1.183240
6	-2.161346	3.487357	0.005298
6	-2.885749	3.010980	1.184450
6	-2.176347	2.579086	2.316342
6	-2.607647	1.380422	3.036749
6	-3.730699	0.662382	2.595924
6	-3.704585	-0.800988	2.581912
6	-2.556419	-1.486770	3.009184
6	-2.082954	-2.655481	2.266216
6	-2.776827	-3.090522	1.125982
6	-2.036219	-3.517922	-0.061931
6	-2.775954	-3.067758	-1.241946
6	-2.081427	-2.610698	-2.373142
6	-2.554547	-1.428064	-3.093973
6	-3.702992	-0.750673	-2.654257
6	-3.729013	0.712686	-2.640169
6	-4.469615	1.140344	-1.452221
6	-4.056509	2.276914	-0.738831
6	-4.056992	2.262857	0.724792
6	-4.470519	1.112769	1.415880
6	-4.901528	-0.072010	0.672361
6	-4.428257	-1.254773	1.393063
6	-3.973825	-2.375776	0.680205
6	-3.973374	-2.361758	-0.783312
6	-4.427348	-1.227233	-1.474740

6 -4.901155 -0.058516 -0.731839

PC-Ru

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	5.749217	0.008442	0.113432
6	2.112839	0.052524	0.679859
6	2.112340	0.066147	-0.728378
6	5.588401	1.961296	0.112700
8	5.399267	3.118418	0.112417
6	6.544195	-0.007246	1.865822
8	7.270634	-0.023284	2.797107
6	5.537397	-1.940417	0.113822
8	5.334675	-3.094790	0.114130
6	6.569141	-0.008718	-1.627436
8	7.307798	-0.025964	-2.548928
6	1.632887	1.248938	-1.448158
6	1.176228	2.368783	-0.734686
6	1.175358	2.354717	0.729019
6	1.631188	1.221310	1.421378
6	0.904628	0.744396	2.599143
6	0.930284	-0.718402	2.585000
6	1.672808	-1.146572	1.398719
6	1.257385	-2.281837	0.684224
6	1.258281	-2.267563	-0.779677
6	1.674468	-1.118549	-1.471218
6	0.933780	-0.667626	-2.650348
6	0.908047	0.795149	-2.636179
6	-0.240472	1.481067	-3.063757
6	-0.714182	2.649944	-2.321151
6	-0.020276	3.084548	-1.180659
6	-0.760870	3.512490	0.006879
6	-0.021980	3.061552	1.186996
6	-0.717386	2.604791	2.317843
6	-0.244585	1.421862	3.038330
6	-1.415993	0.665456	3.482888
6	-1.391262	-0.738451	3.469328
6	-0.194140	-1.444506	3.010576
6	-0.625124	-2.629271	2.267191
6	0.085700	-3.039067	1.127866
6	-0.637323	-3.492938	-0.060923
6	0.087237	-3.016148	-1.239687
6	-0.621989	-2.584092	-2.371794
6	-0.189916	-1.385263	-3.091608
6	-1.386500	-0.670444	-3.538281

6	-1.411227	0.733457	-3.524657
6	-2.608596	1.440082	-3.066694
6	-2.177779	2.624757	-2.322817
6	-2.888396	3.034828	-1.183281
6	-2.165031	3.488284	0.005662
6	-2.889964	3.011877	1.184617
6	-2.180945	2.579616	2.316919
6	-2.612823	1.380858	3.037136
6	-3.736009	0.662964	2.595713
6	-3.710239	-0.800493	2.581591
6	-2.562251	-1.486723	3.009370
6	-2.088741	-2.655645	2.266406
6	-2.782429	-3.090537	1.125660
6	-2.041500	-3.518130	-0.062151
6	-2.780699	-3.067563	-1.242514
6	-2.085522	-2.610436	-2.373624
6	-2.558151	-1.427468	-3.094568
6	-3.706734	-0.749713	-2.655063
6	-3.732411	0.713736	-2.640844
6	-4.473345	1.141480	-1.453036
6	-4.060215	2.278087	-0.739300
6	-4.061232	2.263901	0.724418
6	-4.475297	1.113653	1.415352
6	-4.906280	-0.071034	0.671525
6	-4.433574	-1.254041	1.392345
6	-3.979122	-2.375289	0.679451
6	-3.978138	-2.361139	-0.784169
6	-4.431617	-1.226241	-1.475755
6	-4.905392	-0.057414	-0.732865

PC-Os

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	5.740153	0.004959	0.108280
6	2.126967	0.053707	0.682283
6	2.126930	0.067353	-0.726780
6	5.492425	1.942224	0.106873
8	5.233974	3.088645	0.105552
6	6.497291	-0.009272	1.868431
8	7.184054	-0.024242	2.832619
6	5.436735	-1.923796	0.108450
8	5.154077	-3.064814	0.108091
6	6.527113	-0.011087	-1.639040
8	7.229905	-0.027118	-2.591354
6	1.646760	1.250044	-1.446554

6	1.189300	2.369690	-0.733051
6	1.187906	2.355604	0.730799
6	1.643992	1.222389	1.423494
6	0.917006	0.745229	2.600908
6	0.943038	-0.717605	2.586717
6	1.686152	-1.145579	1.400769
6	1.271102	-2.280797	0.685945
6	1.272522	-2.266518	-0.777989
6	1.688893	-1.117529	-1.469559
6	0.948435	-0.666783	-2.648922
6	0.922322	0.796027	-2.634790
6	-0.226360	1.481664	-3.062810
6	-0.700696	2.650441	-2.320309
6	-0.007238	3.085232	-1.179449
6	-0.748410	3.512993	0.007897
6	-0.009788	3.062214	1.188347
6	-0.705565	2.605244	2.319046
6	-0.232671	1.422405	3.039736
6	-1.404066	0.665665	3.483883
6	-1.378929	-0.738366	3.470288
6	-0.181427	-1.444063	3.011919
6	-0.611813	-2.628907	2.268283
6	0.099573	-3.038425	1.129131
6	-0.622872	-3.492509	-0.059913
6	0.101956	-3.015494	-1.238406
6	-0.607013	-2.583695	-2.370859
6	-0.175006	-1.384765	-3.090610
6	-1.371655	-0.670298	-3.537746
6	-1.396787	0.733730	-3.524149
6	-2.594574	1.440056	-3.066593
6	-2.164347	2.624886	-2.322512
6	-2.875526	3.034758	-1.183087
6	-2.152677	3.488423	0.006171
6	-2.877941	3.011785	1.184910
6	-2.169181	2.579702	2.317604
6	-2.600988	1.380773	3.037691
6	-3.723910	0.662497	2.595799
6	-3.697709	-0.801016	2.581668
6	-2.549578	-1.486987	3.009886
6	-2.075449	-2.655770	2.267034
6	-2.768618	-3.090853	1.125920
6	-2.027089	-3.518192	-0.061653
6	-2.766042	-3.067862	-1.242308
6	-2.070565	-2.610524	-2.373280
6	-2.543291	-1.427681	-3.094441
6	-3.692330	-0.750191	-2.655316
6	-3.718437	0.713317	-2.641101
6	-4.459926	1.140859	-1.453488
6	-4.047322	2.277679	-0.739517
6	-4.048864	2.263481	0.724262

6	-4.462907	1.113007	1.415111
6	-4.893302	-0.071844	0.671086
6	-4.420498	-1.254773	1.392095
6	-3.965387	-2.375968	0.679280
6	-3.963880	-2.361805	-0.784388
6	-4.417511	-1.226946	-1.476205
6	-4.891907	-0.058210	-0.733451

[6,5]-TS-Fe

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.332563
6	1.422116	0.000000	1.877472
6	-1.770614	-0.027920	-0.334029
8	-2.900509	-0.046584	-0.670358
6	-0.068172	1.810265	-0.124792
8	-0.142338	2.969513	-0.277539
6	1.212221	0.011140	-1.319936
8	1.920180	0.020181	-2.263060
6	0.005084	-1.808376	-0.090226
8	0.003096	-2.974377	-0.198830
6	-0.254659	1.319040	2.961478
6	0.956612	2.126295	2.862479
6	1.997344	1.319191	2.235131
6	3.321786	1.439437	2.670024
6	4.154887	0.243412	2.843381
6	3.611924	-1.021776	2.587596
6	2.226045	-1.153219	2.133318
6	1.663487	-2.328533	2.757897
6	0.317244	-2.329373	3.191338
6	-0.502768	-1.153133	3.013226
6	-1.362432	-1.020588	4.191177
6	-1.649971	0.245399	4.716378
6	-1.075075	1.440630	4.087990
6	-0.735386	2.384286	5.151740
6	0.420236	3.174340	5.049409
6	1.285269	3.039575	3.880391
6	2.670390	3.173498	4.323355
6	3.668242	2.382859	3.731406
6	4.708921	1.774660	4.561562
6	5.008844	0.452065	4.013158
6	5.291755	-0.618769	4.877895
6	4.728580	-1.941615	4.607656
6	3.909059	-2.139146	3.483390

6	2.699029	-2.949486	3.593965
6	2.356915	-3.534805	4.820172
6	0.959718	-3.533897	5.271188
6	-0.034005	-2.948667	4.475869
6	-1.079937	-2.137317	5.092715
6	-1.087563	-1.939588	6.483862
6	-1.385273	-0.616271	7.032000
6	-1.660209	0.454451	6.164580
6	-1.095405	1.776690	6.433602
6	-0.279444	1.978249	7.558747
6	0.929720	2.796988	7.449831
6	1.271365	3.384880	6.221245
6	2.664790	3.383494	5.771580
6	3.659794	2.795833	6.569032
6	4.704018	1.975988	5.951353
6	4.995851	0.859893	6.852782
6	5.282030	-0.410000	6.327370
6	4.714220	-1.606221	6.952295
6	4.371948	-2.551665	5.887826
6	3.208793	-3.333472	5.991449
6	2.342089	-3.206086	7.164326
6	0.953366	-3.332940	6.719436
6	-0.050795	-2.550118	7.314765
6	0.294186	-1.604826	8.378400
6	-0.530934	-0.407743	8.202879
6	0.010095	0.861701	8.460294
6	1.399198	0.990108	8.906140
6	1.966572	2.185141	8.282175
6	3.304586	2.184772	7.850717
6	4.129023	0.989213	8.026379
6	3.582937	-0.158516	8.624808
6	3.881298	-1.482753	8.075760
6	2.671738	-2.300150	8.185269
6	1.626771	-1.482011	8.803251
6	2.190961	-0.157929	9.074300

[6,6]-TS-Fe

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.626734
6	1.396704	0.000000	2.425530
6	0.679343	-1.662141	-0.089331
8	1.091167	-2.766012	-0.156090
6	-1.769340	0.096760	0.365135

8	-2.935569	0.161158	0.514835
6	0.832441	1.581615	-0.188003
8	1.349498	2.632204	-0.332012
6	-0.238971	-0.028126	-1.777099
8	-0.394147	-0.045489	-2.939627
6	2.192784	-1.181534	2.783739
6	1.565222	-2.303106	3.335987
6	0.118222	-2.305947	3.556811
6	-0.644340	-1.182639	3.224314
6	-1.695133	-0.720012	4.123413
6	-1.696684	0.741804	4.111113
6	-0.646446	1.191411	3.204596
6	0.112320	2.322864	3.517534
6	1.559241	2.319717	3.296974
6	2.189855	1.190169	2.765047
6	3.467155	0.742177	3.310605
6	3.469124	-0.720573	3.323127
6	4.073213	-1.410645	4.383423
6	3.420654	-2.588883	4.952854
6	2.193581	-3.028951	4.438281
6	1.136175	-3.475802	5.344948
6	-0.146594	-3.029689	4.799764
6	-1.160025	-2.590868	5.662423
6	-1.952656	-1.411642	5.317260
6	-2.220135	-0.669644	6.548220
6	-2.222211	0.732250	6.536585
6	-1.956531	1.453224	5.292545
6	-1.167026	2.640004	5.617479
6	-0.154143	3.067251	4.748299
6	1.127150	3.525843	5.285195
6	2.185889	3.066437	4.386143
6	3.413824	2.638654	4.908844
6	4.069597	1.452476	4.359763
6	4.699509	0.731799	5.465887
6	4.701299	-0.669643	5.478219
6	4.436891	-1.391249	6.723023
6	3.645882	-2.578183	6.398565
6	2.632167	-3.004563	7.267995
6	1.350618	-3.464395	6.730352
6	0.291815	-3.006145	7.630505
6	-0.937301	-2.578812	7.108720
6	-1.592249	-1.391412	7.656437
6	-0.992292	-0.680621	8.705159
6	-0.993955	0.782768	8.692383
6	-1.596150	1.474339	7.632179
6	-0.944201	2.653926	7.063734
6	0.283520	3.093273	7.578814
6	1.341225	3.538992	6.670669
6	2.623832	3.092140	7.216063
6	3.639127	2.653184	6.354576

6	4.432805	1.473825	6.699111
6	4.179073	0.783005	7.892268
6	4.180918	-0.680138	7.905025
6	3.123106	-1.125904	8.811885
6	2.365310	-2.263767	8.500675
6	0.919022	-2.263930	8.724241
6	0.290703	-1.126344	9.250767
6	1.081231	0.061483	9.574979
6	0.287426	1.241178	9.230419
6	0.912740	2.371674	8.685114
6	2.358967	2.371601	8.461433
6	3.119840	1.241332	8.792187
6	2.467757	0.061699	9.361221

[6,5]-TS-Ru

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.690226
6	1.336597	0.000000	2.038519
6	-1.896391	0.311300	0.323354
8	-3.054232	0.510706	0.408456
6	0.135619	1.885577	-0.484866
8	0.179541	3.000810	-0.850153
6	1.572317	-0.314610	-1.107746
8	2.464957	-0.509601	-1.849596
6	-0.404660	-1.907884	-0.111493
8	-0.687374	-3.047681	-0.213858
6	-0.228638	1.337144	3.262016
6	0.957776	2.150501	3.011088
6	1.933162	1.333071	2.296959
6	3.298677	1.468221	2.582593
6	4.150656	0.279444	2.688774
6	3.587735	-0.996813	2.516350
6	2.164926	-1.141070	2.220595
6	1.675845	-2.315128	2.923738
6	0.386931	-2.315091	3.495057
6	-0.461844	-1.138377	3.379220
6	-1.194027	-0.984907	4.639118
6	-1.432763	0.292651	5.171606
6	-0.935719	1.477450	4.465243
6	-0.490658	2.445917	5.468396
6	0.648341	3.234573	5.226057
6	1.385217	3.084425	3.971779
6	2.810758	3.232062	4.264351

6	3.748151	2.434769	3.584599
6	4.873454	1.845140	4.311813
6	5.121301	0.512876	3.757709
6	5.498143	-0.542643	4.609319
6	4.915754	-1.873681	4.424890
6	3.981742	-2.096865	3.397487
6	2.795851	-2.913490	3.650231
6	2.590790	-3.479002	4.920124
6	1.251444	-3.475233	5.514895
6	0.172140	-2.907637	4.815079
6	-0.806306	-2.083324	5.524273
6	-0.668627	-1.859188	6.907336
6	-0.915255	-0.526749	7.461187
6	-1.287897	0.528313	6.607296
6	-0.707261	1.859688	6.791797
6	0.225876	2.083854	7.820402
6	1.412493	2.905139	7.567388
6	1.618188	3.471538	6.296297
6	2.956406	3.468278	5.701487
6	4.035545	2.898983	6.400939
6	5.013342	2.071101	5.690652
6	5.405282	0.973228	6.576888
6	5.642646	-0.307749	6.046631
6	5.150486	-1.494409	6.751435
6	4.702366	-2.462161	5.747294
6	3.561851	-3.249200	5.990066
6	2.823722	-3.101323	7.246279
6	1.395991	-3.243370	6.951989
6	0.455017	-2.450774	7.635011
6	0.905074	-1.483307	8.638917
6	0.057412	-0.292974	8.529789
6	0.616235	0.985573	8.705284
6	2.044672	1.126754	8.997761
6	2.535488	2.313342	8.295257
6	3.821943	2.311082	7.724015
6	4.667810	1.121049	7.832707
6	4.194076	-0.018575	8.508098
6	4.440836	-1.352494	7.954979
6	3.253909	-2.173145	8.208102
6	2.274825	-1.346479	8.917835
6	2.856688	-0.014622	9.102028

[6,6]-TS-Ru

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

44	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.751042
6	1.394702	0.000000	2.655663
6	0.701016	-1.781429	-0.044325
8	1.130406	-2.871383	-0.060126
6	-1.880631	0.227286	0.357947
8	-3.030531	0.372464	0.468016
6	1.057437	1.579431	-0.219283
8	1.712729	2.536126	-0.382505
6	-0.210124	-0.056136	-1.914299
8	-0.331374	-0.089158	-3.072139
6	2.167024	-1.174868	3.054154
6	1.509939	-2.287026	3.573346
6	0.055400	-2.289974	3.701985
6	-0.681671	-1.175679	3.312827
6	-1.788307	-0.706716	4.136159
6	-1.790338	0.752604	4.108961
6	-0.684227	1.193554	3.269388
6	0.047321	2.325930	3.614904
6	1.501633	2.322025	3.487418
6	2.163250	1.193482	3.011163
6	3.404576	0.753698	3.638011
6	3.407017	-0.706874	3.665872
6	3.940352	-1.381759	4.762764
6	3.253603	-2.553556	5.301914
6	2.068697	-3.000352	4.719182
6	0.958199	-3.438329	5.560199
6	-0.286158	-2.999815	4.931768
6	-1.347160	-2.556732	5.719695
6	-2.115961	-1.383092	5.313907
6	-2.460139	-0.630014	6.515536
6	-2.463127	0.764746	6.489531
6	-2.121431	1.472443	5.259408
6	-1.356368	2.662582	5.621125
6	-0.296352	3.080418	4.818135
6	0.946165	3.546612	5.428584
6	2.058144	3.081223	4.604094
6	3.244425	2.661521	5.203938
6	3.935130	1.471947	4.710477
6	4.493111	0.764702	5.859676
6	4.495768	-0.629604	5.886289
6	4.154373	-1.337811	7.117247
6	3.387405	-2.527458	6.756751
6	2.326715	-2.944036	7.560679
6	1.084277	-3.411437	6.949606
6	-0.027932	-2.946444	7.774701
6	-1.215887	-2.528904	7.175312
6	-1.904140	-1.338489	7.667273
6	-1.374636	-0.619538	8.738266
6	-1.376822	0.841158	8.710313

6	-1.909219	1.517753	7.613537
6	-1.225137	2.691204	7.076538
6	-0.039076	3.135386	7.660420
6	1.071623	3.573045	6.817976
6	2.315572	3.134025	7.446024
6	3.378253	2.690762	6.659024
6	4.148735	1.517827	7.064088
6	3.823274	0.842174	8.239962
6	3.825700	-0.618466	8.267889
6	2.714596	-1.056028	9.109178
6	1.982821	-2.192439	8.765103
6	0.527702	-2.192670	8.896655
6	-0.130294	-1.056927	9.367983
6	0.635652	0.133668	9.728605
6	-0.134601	1.306653	9.323173
6	0.519236	2.426743	8.809999
6	1.974229	2.426895	8.678265
6	2.710019	1.307036	9.065105
6	2.026082	0.134158	9.603738

[6,5]-TS-Os

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.427397
6	1.479082	0.000000	2.202379
6	-1.881257	-0.019456	-0.399915
8	-2.998466	-0.028517	-0.791926
6	-0.044943	1.957070	-0.072310
8	-0.081796	3.126641	-0.152718
6	1.558532	0.026805	-1.153177
8	2.417091	0.043410	-1.964852
6	0.000767	-1.959470	-0.079938
8	-0.002061	-3.130026	-0.154034
6	-0.328585	1.310603	3.054131
6	0.885329	2.113711	3.129275
6	2.000191	1.311856	2.636360
6	3.257231	1.421075	3.245680
6	4.059350	0.220927	3.509757
6	3.554645	-1.038837	3.162120
6	2.240415	-1.158728	2.525925
6	1.597251	-2.340952	3.055086
6	0.205529	-2.344986	3.303331
6	-0.580453	-1.162861	3.039632
6	-1.592958	-1.047229	4.087066

6	-1.946310	0.212953	4.588999
6	-1.292444	1.416609	4.061995
6	-1.096317	2.342305	5.176702
6	0.063803	3.129845	5.241646
6	1.076977	3.010879	4.196375
6	2.390528	3.132139	4.823380
6	3.458167	2.347424	4.358287
6	4.377878	1.723125	5.311065
6	4.747689	0.407962	4.787181
6	4.910745	-0.676849	5.665148
6	4.387566	-1.993386	5.300995
6	3.725378	-2.170117	4.074200
6	2.510904	-2.978660	4.009928
6	2.006311	-3.582470	5.170152
6	0.561526	-3.586470	5.429512
6	-0.315738	-2.984055	4.517882
6	-1.434241	-2.179290	5.001579
6	-1.627868	-2.002546	6.381311
6	-1.993916	-0.685708	6.904491
6	-2.149879	0.399360	6.025590
6	-1.625724	1.715733	6.389018
6	-0.966707	1.895888	7.615910
6	0.246528	2.712372	7.682653
6	0.750452	3.318154	6.520366
6	2.191191	3.320041	6.261532
6	3.069240	2.715486	7.175541
6	4.186227	1.902590	6.690461
6	4.354020	0.772068	7.605510
6	4.707256	-0.490537	7.103433
6	4.058592	-1.694178	7.627360
6	3.860603	-2.621782	6.512260
6	2.693583	-3.402310	6.447823
6	1.678004	-3.290654	7.496438
6	0.361201	-3.406942	6.867235
6	-0.712565	-2.629861	7.334397
6	-0.511800	-1.700773	8.448009
6	-1.304613	-0.498821	8.182445
6	-0.802490	0.765113	8.531259
6	0.514439	0.881889	9.161629
6	1.161613	2.084473	8.636855
6	2.544824	2.085693	8.387819
6	3.337286	0.885293	8.653561
6	2.715523	-0.269422	9.156769
6	3.083336	-1.585740	8.631847
6	1.869055	-2.401063	8.565853
6	0.751404	-1.589159	9.050682
6	1.275444	-0.271233	9.415408

[6,6]-TS-Os

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.734978
6	1.397354	0.000000	2.621778
6	0.702385	-1.781882	-0.035287
8	1.137009	-2.870863	-0.051070
6	-1.874990	0.240930	0.366303
8	-3.021059	0.394353	0.503944
6	1.078280	1.567267	-0.214086
8	1.749559	2.513500	-0.381035
6	-0.230368	-0.051557	-1.917680
8	-0.360773	-0.079685	-3.074873
6	2.174389	-1.176443	3.011398
6	1.524278	-2.288334	3.537673
6	0.070878	-2.292171	3.686700
6	-0.670918	-1.177462	3.311772
6	-1.764274	-0.710984	4.152347
6	-1.766316	0.748115	4.130349
6	-0.673611	1.192010	3.276636
6	0.062539	2.322109	3.615676
6	1.515719	2.317913	3.467744
6	2.170190	1.192115	2.977980
6	3.419423	0.749880	3.585429
6	3.421937	-0.710653	3.607910
6	3.970757	-1.389112	4.694550
6	3.291711	-2.562153	5.239230
6	2.098633	-3.006062	4.671906
6	1.000179	-3.446763	5.526990
6	-0.252853	-3.005799	4.918069
6	-1.302451	-2.566013	5.722495
6	-2.076270	-1.391406	5.331857
6	-2.403309	-0.642390	6.540686
6	-2.406240	0.751975	6.519578
6	-2.081721	1.463966	5.287500
6	-1.311808	2.652246	5.642229
6	-0.263370	3.072099	4.825617
6	0.987828	3.535826	5.419912
6	2.087822	3.073110	4.578290
6	3.282247	2.651449	5.159663
6	3.965553	1.464067	4.652355
6	4.539803	0.752807	5.790942
6	4.542378	-0.641018	5.812555
6	4.218273	-1.353359	7.045623
6	3.446087	-2.541401	6.691813
6	2.396980	-2.960415	7.508922

6	1.145868	-3.425258	6.913968
6	0.045651	-2.963198	7.756559
6	-1.150314	-2.543459	7.175845
6	-1.831157	-1.354909	7.681784
6	-1.286402	-0.640039	8.747294
6	-1.288656	0.820668	8.724474
6	-1.836323	1.500898	7.638072
6	-1.159743	2.675855	7.095429
6	0.034331	3.117618	7.663633
6	1.132969	3.557786	6.806889
6	2.385585	3.116444	7.415669
6	3.436706	2.675886	6.612456
6	4.212560	1.501663	7.002555
6	3.903570	0.822253	8.180160
6	3.906085	-0.638300	8.202928
6	2.807037	-1.078535	9.058217
6	2.070422	-2.213228	8.720513
6	0.617361	-2.213621	8.872752
6	-0.033398	-1.079756	9.357399
6	0.737879	0.109262	9.711111
6	-0.037791	1.283639	9.320897
6	0.608742	2.405028	8.802361
6	2.061665	2.405379	8.649961
6	2.802367	1.284388	9.022431
6	2.125949	0.109901	9.566599

[6,5]-Pro-Fe

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	-4.450304	-0.001270	0.003477
6	-2.268317	0.748115	-0.021329
6	-2.267916	-0.750551	-0.022803
6	-4.522570	-0.008190	1.820962
8	-4.624880	-0.012484	2.987265
6	-5.320007	1.567125	0.022497
8	-5.974944	2.546155	0.035514
6	-4.595815	0.005917	-1.811350
8	-4.765823	0.010657	-2.970237
6	-5.319381	-1.570058	0.010921
8	-5.973578	-2.549567	0.017079
6	-1.742772	-1.435367	1.122592
6	-1.302898	-0.711516	2.288375
6	-1.303299	0.705509	2.289716
6	-1.743467	1.431167	1.125200
6	-0.887370	2.611546	0.979725

6	-0.497280	3.049547	-0.291192
6	-0.937785	2.308822	-1.480472
6	-1.756799	1.183275	-1.346855
6	-1.490358	0.000869	-2.158302
6	-1.756181	-1.183120	-1.349013
6	-0.936590	-2.308036	-1.484610
6	-0.495698	-3.050624	-0.296619
6	-0.885991	-2.615015	0.975057
6	0.076549	-2.623899	2.076014
6	-0.177040	-1.439351	2.890729
6	0.893503	-0.738002	3.459352
6	0.893125	0.731079	3.460684
6	-0.177799	1.432863	2.893327
6	0.075180	2.618987	2.080690
6	1.393522	3.054147	1.862455
6	1.801964	3.507693	0.533379
6	0.874402	3.503357	-0.522163
6	1.282339	3.049697	-1.851355
6	0.163203	2.314129	-2.441819
6	0.408079	1.184137	-3.237975
6	-0.435847	0.001963	-3.089485
6	0.408701	-1.179518	-3.240098
6	0.164430	-2.311031	-2.445920
6	1.283957	-3.047079	-1.856765
6	0.876235	-3.503306	-0.528367
6	1.803810	-3.508972	0.527176
6	1.395130	-3.057981	1.857033
6	2.513514	-2.326591	2.450308
6	2.266530	-1.187972	3.236753
6	3.113935	-0.002561	3.096726
6	2.265911	1.182158	3.238859
6	2.512296	2.322297	2.454426
6	3.614784	2.321112	1.490563
6	3.175344	3.054631	0.301744
6	3.566322	2.621058	-0.974903
6	2.600372	2.619888	-2.075198
6	2.854825	1.436971	-2.899951
6	1.781202	0.734979	-3.470942
6	1.781586	-0.729217	-3.472248
6	2.855582	-1.431659	-2.902493
6	2.601760	-2.616154	-2.079821
6	3.567738	-2.618782	-0.979540
6	3.176942	-3.054762	0.296338
6	3.616014	-2.323135	1.486455
6	4.427156	-1.185221	1.351190
6	4.172228	-0.001466	2.173934
6	4.426530	1.183869	1.353281
6	4.836554	0.731994	0.021877
6	4.414569	1.435561	-1.118580
6	3.975273	0.705417	-2.307342

6	3.975644	-0.700564	-2.308593
6	4.415331	-1.432562	-1.121110
6	4.836956	-0.730787	0.020588

[6,6]-Pro-Fe

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
26	-4.521102	0.000110	0.000223
6	-2.501811	0.739280	-0.001828
6	-2.501836	-0.739250	0.002094
6	-4.598155	0.004254	1.823998
8	-4.722814	0.006671	2.985108
6	-5.504859	1.508722	-0.003255
8	-6.174968	2.472125	-0.005432
6	-4.598295	-0.004265	-1.823537
8	-4.723057	-0.007038	-2.984636
6	-5.505352	-1.508167	0.003712
8	-6.175862	-2.471277	0.005827
6	-1.916771	-1.437221	1.186108
6	-1.475817	-0.732546	2.309680
6	-1.475817	0.744837	2.305773
6	-1.916723	1.443507	1.178448
6	-1.172595	2.607508	0.723350
6	-1.172652	2.603627	-0.737075
6	-1.916834	1.437232	-1.185896
6	-1.476001	0.732548	-2.309512
6	-1.476043	-0.744837	-2.305604
6	-1.916871	-1.443492	-1.178237
6	-1.172733	-2.607516	-0.723206
6	-1.172661	-2.603634	0.737220
6	-0.038736	-3.047814	1.442661
6	0.410629	-2.318815	2.621428
6	-0.294720	-1.175944	3.039730
6	0.436075	0.009266	3.488892
6	-0.294665	1.192094	3.033423
6	0.410699	2.332699	2.608996
6	-0.038670	3.055443	1.426394
6	1.144392	3.509517	0.692355
6	1.144329	3.505777	-0.711120
6	-0.038780	3.047780	-1.442618
6	0.410461	2.318765	-2.621421
6	-0.294954	1.175914	-3.039662
6	0.435768	-0.009315	-3.488887
6	-0.294963	-1.192123	-3.033356
6	0.410407	-2.332745	-2.608988

6	-0.038876	-3.055473	-1.426345
6	1.144238	-3.509582	-0.692414
6	1.144297	-3.505845	0.711061
6	2.328221	-3.052436	1.442625
6	1.873680	-2.316954	2.624325
6	2.574356	-1.177191	3.053103
6	1.839718	0.009271	3.497649
6	2.574362	1.193340	3.046787
6	1.873733	2.330809	2.611891
6	2.328322	3.059999	1.426325
6	3.464106	2.622210	0.725043
6	3.464026	2.618308	-0.739269
6	2.328177	3.052339	-1.442790
6	1.873511	2.316869	-2.624453
6	2.574118	1.177084	-3.053286
6	1.839409	-0.009358	-3.497770
6	2.574061	-1.193444	-3.046968
6	1.873443	-2.330900	-2.612019
6	2.328116	-3.060098	-1.426489
6	3.463975	-2.622342	-0.725306
6	3.464020	-2.618436	0.739006
6	4.193582	-1.431878	1.187648
6	3.757358	-0.726482	2.321699
6	3.757382	0.738707	2.317803
6	4.193622	1.438020	1.180001
6	4.645353	0.702264	-0.002056
6	4.193518	1.431730	-1.187976
6	3.757175	0.726344	-2.321990
6	3.757161	-0.738844	-2.318094
6	4.193478	-1.438168	-1.180329
6	4.645338	-0.702425	0.001687

[6,5]-Pro-Ru

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	-4.701716	-0.004838	-0.000039
6	-2.192012	0.741799	-0.015364
6	-2.192860	-0.739793	-0.017663
6	-4.753093	0.004241	1.960881
8	-4.791976	0.009939	3.131462
6	-5.492439	1.769810	-0.001421
8	-6.138704	2.759288	-0.001585
6	-4.815939	-0.013738	-1.957454
8	-4.906754	-0.018830	-3.125143
6	-5.488562	-1.780706	0.015308

8	-6.132311	-2.771698	0.025241
6	-1.712063	-1.434373	1.124253
6	-1.270350	-0.707769	2.301229
6	-1.270045	0.702161	2.303391
6	-1.711644	1.432710	1.128773
6	-0.861305	2.614749	0.985454
6	-0.470804	3.052402	-0.288438
6	-0.912010	2.317003	-1.477365
6	-1.727896	1.186108	-1.343905
6	-1.468941	0.004238	-2.160986
6	-1.728306	-1.180063	-1.347601
6	-0.912920	-2.310842	-1.484658
6	-0.472024	-3.050143	-0.298044
6	-0.862319	-2.616328	0.977238
6	0.102647	-2.622475	2.077562
6	-0.148472	-1.439228	2.897887
6	0.925012	-0.738204	3.466303
6	0.925310	0.728039	3.468602
6	-0.147910	1.431289	2.902384
6	0.103682	2.617009	2.085786
6	1.421367	3.050878	1.865203
6	1.828801	3.505526	0.535569
6	0.901266	3.505150	-0.519584
6	1.308349	3.053455	-1.850314
6	0.187963	2.320721	-2.441814
6	0.430537	1.188639	-3.236240
6	-0.415303	0.005501	-3.091027
6	0.430061	-1.177516	-3.239994
6	0.187056	-2.311963	-2.449106
6	1.307126	-3.047068	-1.859957
6	0.899839	-3.502795	-0.530638
6	1.827374	-3.506754	0.524521
6	1.420137	-3.056163	1.855601
6	2.540727	-2.326145	2.448768
6	2.297670	-1.189686	3.238525
6	3.145936	-0.004958	3.097703
6	2.298143	1.179671	3.242259
6	2.541636	2.318495	2.456050
6	3.642507	2.318632	1.490664
6	3.201735	3.052888	0.303150
6	3.592074	2.620508	-0.974544
6	2.625662	2.621511	-2.074272
6	2.878111	1.438744	-2.899645
6	1.803347	0.737619	-3.469543
6	1.803054	-0.726308	-3.471878
6	2.877533	-1.429667	-2.904180
6	2.624614	-2.614921	-2.082533
6	3.591048	-2.617791	-0.982812
6	3.200479	-3.053964	0.293524
6	3.641583	-2.323683	1.483358

6	4.454577	-1.186834	1.348056
6	4.201949	-0.003714	2.172268
6	4.455043	1.181883	1.351779
6	4.863170	0.731184	0.019754
6	4.439970	1.435607	-1.119541
6	3.998943	0.705958	-2.308779
6	3.998669	-0.699205	-2.311007
6	4.439399	-1.432758	-1.124065
6	4.862888	-0.732115	0.017450

[6,6]-Pro-Ru

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
44	4.447755	0.000130	0.000683
6	2.285960	-0.003019	0.744186
6	2.286144	0.004503	-0.741924
6	4.485621	1.965843	0.001496
8	4.557379	3.131132	-0.000946
6	5.550737	-0.002271	1.620746
8	6.248401	-0.004221	2.565246
6	4.484146	-1.965628	-0.002900
8	4.555027	-3.130981	-0.007054
6	5.552306	0.001377	-1.618266
8	6.251009	0.002493	-2.562041
6	1.694862	1.190389	-1.433041
6	1.254616	2.312337	-0.725854
6	1.254319	2.304739	0.751929
6	1.694168	1.175381	1.447484
6	0.950092	0.717062	2.610136
6	0.950343	-0.743288	2.602431
6	1.694539	-1.189064	1.435050
6	1.255065	-2.311151	0.727621
6	1.255548	-2.303543	-0.750150
6	1.695149	-1.173995	-1.445446
6	0.951901	-0.715991	-2.608653
6	0.951614	0.744376	-2.600931
6	-0.182188	1.451099	-3.043986
6	-0.631765	2.627791	-2.312079
6	0.073446	3.042840	-1.167523
6	-0.657943	3.488564	0.018615
6	0.072707	3.030442	1.200491
6	-0.633268	2.603312	2.340127
6	-0.184097	1.419000	3.059852
6	-1.367255	0.683365	3.511583
6	-1.366958	-0.720082	3.504213

6	-0.183523	-1.450418	3.044771
6	-0.632163	-2.627337	2.312671
6	0.073952	-3.042134	1.168592
6	-0.656481	-3.488240	-0.018031
6	0.074687	-3.029822	-1.199478
6	-0.630677	-2.602978	-2.339632
6	-0.181589	-1.418456	-3.059135
6	-1.364694	-0.683267	-3.511633
6	-1.364980	0.720222	-3.504230
6	-2.549138	1.450404	-3.049134
6	-2.094761	2.630292	-2.310369
6	-2.796018	3.055950	-1.169707
6	-2.061718	3.497326	0.018181
6	-2.796777	3.043477	1.200863
6	-2.096264	2.605793	2.337435
6	-2.551169	1.418250	3.063448
6	-3.686752	0.717936	2.623369
6	-3.686414	-0.746393	2.615674
6	-2.550523	-1.450779	3.048373
6	-2.095164	-2.630485	2.309961
6	-2.795485	-3.056487	1.168832
6	-2.060237	-3.497590	-0.018560
6	-2.794680	-3.044077	-1.201775
6	-2.093642	-2.606088	-2.337908
6	-2.548547	-1.418712	-3.064252
6	-3.684688	-0.718875	-2.624930
6	-3.684984	0.745461	-2.617230
6	-4.414991	1.190855	-1.429749
6	-3.979062	2.323175	-0.721302
6	-3.979557	2.315488	0.743941
6	-4.415969	1.175774	1.440109
6	-4.867202	-0.004432	0.701147
6	-4.415441	-1.192124	1.427695
6	-3.978538	-2.324257	0.719566
6	-3.978051	-2.316576	-0.745683
6	-4.414474	-1.177060	-1.442174
6	-4.866722	0.002945	-0.703536

[6,5]-Pro-Os

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	4.221127	-0.000415	-0.000125
6	1.981649	0.010326	-0.765965
6	1.982746	0.019587	0.760232
6	4.225643	-1.962811	-0.003251

8	4.254513	-3.133040	-0.007311
6	5.249964	-0.008615	-1.638407
8	5.955549	-0.006640	-2.584264
6	4.295854	1.963354	0.003100
8	4.389000	3.130629	0.003221
6	5.243623	-0.014403	1.641818
8	5.945190	-0.021757	2.590748
6	1.411255	-1.125115	1.439968
6	0.969966	-2.282808	0.724946
6	0.968910	-2.291532	-0.700343
6	1.409530	-1.143022	-1.430576
6	0.549011	-0.999032	-2.609890
6	0.162830	0.268913	-3.054946
6	0.608291	1.462610	-2.317571
6	1.427979	1.332173	-1.194600
6	1.161426	2.145272	-0.015761
6	1.429429	1.346901	1.172788
6	0.611641	1.491618	2.295251
6	0.167467	0.307322	3.048474
6	0.552862	-0.966254	2.618825
6	-0.412208	-2.063854	2.635941
6	-0.160921	-2.881379	1.454152
6	-1.232140	-3.450395	0.757116
6	-1.233222	-3.459556	-0.714524
6	-0.163085	-2.899219	-1.420229
6	-0.416174	-2.096661	-2.611685
6	-1.735031	-1.877779	-3.046845
6	-2.139990	-0.550582	-3.506888
6	-1.208143	0.502077	-3.507504
6	-1.611613	1.834200	-3.059061
6	-0.490620	2.424490	-2.326418
6	-0.732700	3.229962	-1.202279
6	0.110270	3.083179	-0.020941
6	-0.730883	3.244890	1.159734
6	-0.487108	2.453696	2.293657
6	-1.606920	1.872759	3.035563
6	-1.202772	0.546292	3.500292
6	-2.134561	-0.506376	3.514143
6	-1.730360	-1.839378	3.070289
6	-2.849867	-2.432934	2.342564
6	-2.603831	-3.224302	1.206389
6	-3.451633	-3.088774	0.020722
6	-2.605628	-3.239180	-1.164461
6	-2.853421	-2.462141	-2.310065
6	-3.953531	-1.495573	-2.311772
6	-3.511817	-0.311666	-3.052530
6	-3.898282	0.968113	-2.625198
6	-2.928639	2.065171	-2.630137
6	-3.180032	2.897497	-1.451613
6	-2.104305	3.470055	-0.753992

6	-2.103186	3.479340	0.710555
6	-3.177786	2.915642	1.417066
6	-2.924590	2.098281	2.605661
6	-3.894197	1.001212	2.616103
6	-3.507047	-0.273125	3.058888
6	-3.949919	-1.466314	2.333826
6	-4.760498	-1.334770	1.195406
6	-4.508367	-2.164308	0.015753
6	-4.762345	-1.349700	-1.173850
6	-5.168293	-0.014645	-0.728393
6	-4.744329	1.120962	-1.438806
6	-4.301083	2.312042	-0.716052
6	-4.299984	2.320937	0.690730
6	-4.742074	1.139079	1.429165
6	-5.167152	-0.005418	0.733822

[6,6]-Pro-Os

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
76	-4.631798	0.000134	0.000314
6	-2.518679	0.758412	-0.001799
6	-2.518715	-0.758335	0.001910
6	-4.641369	0.011098	1.968105
8	-4.694370	0.017770	3.134980
6	-5.803711	1.556729	-0.008632
8	-6.519696	2.488967	-0.014845
6	-4.641693	-0.010894	-1.967455
8	-4.694697	-0.017728	-3.134325
6	-5.803855	-1.556317	0.009661
8	-6.519901	-2.488502	0.016281
6	-1.893284	-1.441022	1.185426
6	-1.452710	-0.735717	2.306545
6	-1.452646	0.746313	2.303056
6	-1.893195	1.446472	1.178677
6	-1.145312	2.605697	0.723992
6	-1.145370	2.602377	-0.736023
6	-1.893327	1.441075	-1.185373
6	-1.452819	0.735733	-2.306497
6	-1.452822	-0.746294	-2.303017
6	-1.893343	-1.446427	-1.178612
6	-1.145466	-2.605688	-0.723988
6	-1.145442	-2.602376	0.736040
6	-0.011915	-3.049324	1.441831
6	0.435915	-2.321248	2.619406
6	-0.271002	-1.177083	3.034652

6	0.459754	0.007987	3.483503
6	-0.270907	1.190965	3.029091
6	0.436013	2.333209	2.608632
6	-0.011815	3.055895	1.427747
6	1.171108	3.510620	0.693460
6	1.171063	3.507426	-0.709778
6	-0.011891	3.049283	-1.441883
6	0.435848	2.321213	-2.619492
6	-0.271151	1.177068	-3.034680
6	0.459543	-0.008031	-3.483594
6	-0.271149	-1.191000	-3.029148
6	0.435759	-2.333264	-2.608714
6	-0.012017	-3.055914	-1.427793
6	1.170936	-3.510700	-0.693600
6	1.170979	-3.507486	0.709637
6	2.354457	-3.054014	1.441575
6	1.898703	-2.318675	2.623226
6	2.598951	-1.178454	3.051838
6	1.863407	0.007977	3.495247
6	2.598989	1.192369	3.046422
6	1.898784	2.330587	2.612445
6	2.354592	3.060542	1.427500
6	3.490314	2.622368	0.726092
6	3.490248	2.619001	-0.738423
6	2.354483	3.053916	-1.441795
6	1.898628	2.318562	-2.623389
6	2.598813	1.178335	-3.052059
6	1.863206	-0.008077	-3.495437
6	2.598745	-1.192488	-3.046609
6	1.898540	-2.330699	-2.612638
6	2.354391	-3.060631	-1.427699
6	3.490174	-2.622527	-0.726353
6	3.490207	-2.619159	0.738150
6	4.218968	-1.432436	1.187102
6	3.781845	-0.727508	2.321320
6	3.781884	0.738005	2.317955
6	4.219012	1.437682	1.180502
6	4.670583	0.702274	-0.001785
6	4.218941	1.432258	-1.187417
6	3.781726	0.727338	-2.321596
6	3.781703	-0.738174	-2.318241
6	4.218898	-1.437880	-1.180822
6	4.670576	-0.702473	0.001442

