

SUPPORTING INFORMATION

Computing Redox Potentials in Solution: Density Functional Theory as A Tool for Rational Design of Redox Agents.

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Table S1. Optimized structures.

=====			
Anthracene - 1(0)			
=====			
C	0.000000000	1.224456584	0.722879770
C	0.000000000	2.480780837	1.408070163
H	0.000000000	2.477854074	2.495241909
C	0.000000000	3.662405496	0.713562397
H	0.000000000	4.608975252	1.246602525
C	0.000000000	3.662405496	-0.713562397
H	0.000000000	4.608975252	-1.246602525
C	0.000000000	2.480780837	-1.408070163
H	0.000000000	2.477854074	-2.495241909
C	0.000000000	1.224456584	-0.722879770
C	0.000000000	0.000000000	1.405029971
C	0.000000000	-1.224456584	0.722879770
C	0.000000000	-1.224456584	-0.722879770
C	0.000000000	0.000000000	-1.405029971
C	0.000000000	-2.480780837	1.408070163
C	0.000000000	-3.662405496	0.713562397
C	0.000000000	-3.662405496	-0.713562397
C	0.000000000	-2.480780837	-1.408070163
H	0.000000000	0.000000000	2.492949255
H	0.000000000	0.000000000	-2.492949255
H	0.000000000	-2.477854074	2.495241909
H	0.000000000	-4.608975252	1.246602525
H	0.000000000	-4.608975252	-1.246602525
H	0.000000000	-2.477854074	-2.495241909
=====			
Anthracene - 1(-)			
=====			
C	0.000000000	1.241221923	0.726443808
C	0.000000000	2.492529309	1.398910781
H	0.000000000	2.491142235	2.488640611
C	0.000000000	3.701618130	0.702100783
H	0.000000000	4.643673040	1.248769004
C	0.000000000	3.701618130	-0.702100783
H	0.000000000	4.643673040	-1.248769004
C	0.000000000	2.492529309	-1.398910781
H	0.000000000	2.491142235	-2.488640611
C	0.000000000	1.241221923	-0.726443808
C	0.000000000	0.000000000	1.404389454
C	0.000000000	-1.241221923	0.726443808
C	0.000000000	-1.241221923	-0.726443808
C	0.000000000	0.000000000	-1.404389454
C	0.000000000	-2.492529309	1.398910781
C	0.000000000	-3.701618130	0.702100783
C	0.000000000	-3.701618130	-0.702100783
C	0.000000000	-2.492529309	-1.398910781
H	0.000000000	0.000000000	2.494468205
H	0.000000000	0.000000000	-2.494468205
H	0.000000000	-2.491142235	2.488640611
H	0.000000000	-4.643673040	1.248769004
H	0.000000000	-4.643673040	-1.248769004
H	0.000000000	-2.491142235	-2.488640611
=====			
Azobenzene - 2(0)			
=====			
C	-2.430338137	0.781306136	0.000000000
H	-1.871174461	1.710198979	0.000000000
C	-3.820629358	0.767205206	0.000000000
H	-4.369696807	1.704914914	0.000000000
C	-4.518452704	-0.448811502	0.000000000
H	-5.604928099	-0.449920705	0.000000000
C	-3.817803080	-1.657303473	0.000000000
H	-4.356223432	-2.600595325	0.000000000
C	-2.423462949	-1.650496853	0.000000000
H	-1.850062348	-2.572481944	0.000000000
C	-1.724824471	-0.435205770	0.000000000
N	-0.309938391	-0.549362805	0.000000000
N	0.309938391	0.549362805	0.000000000
C	1.724824471	0.435205770	0.000000000
C	2.423462949	1.650496853	0.000000000
H	1.850062348	2.572481944	0.000000000
C	3.817803080	1.657303473	0.000000000
=====			
H	4.356223432	2.600595325	0.000000000
C	4.518452704	0.448811502	0.000000000
H	5.604928099	0.449920705	0.000000000
C	3.820629358	-0.767205206	0.000000000
H	4.369696807	-1.704914914	0.000000000
C	2.430338137	-0.781306136	0.000000000
H	1.871174461	-1.710198979	0.000000000
=====			
Azobenzene - 2(-)			
=====			
C	-2.419653758	0.754622790	0.000000000
H	-1.850182881	1.677220675	0.000000000
C	-3.808998407	0.752907372	0.000000000
H	-4.342351006	1.704211865	0.000000000
C	-4.539827265	-0.446034879	0.000000000
H	-5.627579037	-0.435017388	0.000000000
C	-3.832690615	-1.660807339	0.000000000
H	-4.378067381	-2.604324082	0.000000000
C	-2.444430126	-1.673641141	0.000000000
H	-1.888528909	-2.608415095	0.000000000
C	-1.687519210	-0.469552874	0.000000000
N	-0.319342821	-0.586504074	0.000000000
N	0.319342821	0.586504074	0.000000000
C	1.687519210	0.469552874	0.000000000
C	2.444430126	1.673641141	0.000000000
H	1.888528909	2.608415095	0.000000000
C	3.832690615	1.660807339	0.000000000
H	4.378067381	2.604324082	0.000000000
C	4.539827265	0.446034879	0.000000000
H	5.627579037	0.435017388	0.000000000
C	3.808998407	-0.752907372	0.000000000
H	4.342351006	-1.704211865	0.000000000
C	2.419653758	-0.754622790	0.000000000
H	1.850182881	-1.677220675	0.000000000
=====			
Benzophenone - 3(0)			
=====			
C	0.472714358	2.436491767	1.001301229
H	0.885544463	2.305991482	1.996438574
C	0.452777371	3.685871062	0.387545718
H	0.871022487	4.548093281	0.899212752
C	-0.111741246	3.831162970	-0.884522024
H	-0.132760380	4.807027249	-1.361835270
C	-0.656711512	2.722854779	-1.536387773
H	-1.112723828	2.836412910	-2.515740706
C	-0.618910730	1.465491948	-0.930641119
H	-1.058308223	0.611250555	-1.435076607
C	-0.046470425	1.309764900	0.341782523
C	-0.033967040	0.004031084	1.083564271
C	0.004047429	-1.302334476	0.343937100
C	-0.507758955	-2.434821790	0.999617631
H	-0.934187910	-2.307381326	1.989383416
C	-0.462600990	-3.685214971	0.389477462
H	-0.873883887	-4.552284438	0.898613260
C	0.118756133	-3.825383943	-0.875675180
H	0.159752135	-4.802057138	-1.350065016
C	0.655089687	-2.710824957	-1.524024364
H	1.123816757	-2.820015995	-2.497863857
C	0.593511749	-1.452951574	-0.921295830
H	1.026815543	-0.593980841	-1.422825024
O	-0.053199435	0.005181104	2.310021503
=====			
Benzophenone - 3(-)			
=====			
C	0.314126283	2.453544983	1.061355919
H	0.573166351	2.294779871	2.103276718
C	0.301990759	3.723880820	0.503529989
H	0.576411918	4.581327322	1.118309612
C	-0.060613690	3.919903323	-0.840362707
H	-0.070947661	4.915899995	-1.277745979
C	-0.431593463	2.797828520	-1.596146618
H	-0.754135542	2.924156011	-2.629569909
C	-0.411880389	1.519677488	-1.044738151
H	-0.758353346	0.688114577	-1.648744410

3

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C -0.013234129 1.293361968 0.302118081
C 0.002651209 -0.000327584 1.007403973
C 0.015191455 -1.293998340 0.301858513
C -0.311884388 -2.453959003 1.061499021
H -0.567747052 -2.295164622 2.104250833
C -0.301839867 -3.724142740 0.503325614
H -0.575429516 -4.581558152 1.118507499
C 0.058174353 -3.920027516 -0.841340956
H 0.067144167 -4.915924851 -1.278929424
C 0.428820769 -2.798178589 -1.597599612
H 0.750114777 -2.924655498 -2.631406127
C 0.411691218 -1.520228902 -1.045593428
H 0.757331293 -0.688543636 -1.649892831
O 0.004733742 -0.000561205 2.284799284

```

Nitrobenzene - 4(0)

```

C 0.000000000 0.000000000 -0.178872727
N 0.000000000 0.000000000 -1.652992492
C 0.000000000 1.221874877 0.491886249
H 0.000000000 2.142636758 -0.078469908
C 0.000000000 1.213529819 1.885392305
H 0.000000000 2.153562001 2.428489905
C 0.000000000 0.000000000 2.580725320
H 0.000000000 0.000000000 3.666950056
C 0.000000000 -1.213529819 1.885392305
H 0.000000000 -2.153562001 2.428489905
C 0.000000000 -1.221874877 0.491886249
H 0.000000000 -2.142636758 -0.078469908
O 0.000000000 1.090606965 -2.224532106
O 0.000000000 -1.090606965 -2.224532106

```

Nitrobenzene - 4(-)

```

C 0.000000000 0.000000000 -0.224487771
N 0.000000000 0.000000000 -1.618590641
C 0.000000000 1.224195913 0.499161391
H 0.000000000 2.144518909 -0.071979227
C 0.000000000 1.210148524 1.885870118
H 0.000000000 2.157332958 2.425977548
C 0.000000000 0.000000000 2.607752129
H 0.000000000 0.000000000 3.695492649
C 0.000000000 -1.210148524 1.885870118
H 0.000000000 -2.157332958 2.425977548
C 0.000000000 -1.224195913 0.499161391
H 0.000000000 -2.144518909 -0.071979227
O 0.000000000 1.127798805 -2.239584660
O 0.000000000 -1.127798805 -2.239584660

```

Tetracyano-quinodimethane - 5(0)

```

C 0.000000000 0.000000000 1.423088026
C 0.000000000 0.000000000 2.812729819
C 0.000000000 1.241238087 0.677843676
H 0.000000000 2.177944219 1.225524136
C 0.000000000 1.241238087 -0.677843676
H 0.000000000 2.177944219 -1.225524136
C 0.000000000 0.000000000 -1.423088026
C 0.000000000 0.000000000 -2.812729819
C 0.000000000 -1.241238087 -0.677843676
H 0.000000000 -2.177944219 -1.225524136
C 0.000000000 -1.241238087 0.677843676
H 0.000000000 -2.177944219 1.225524136
C 0.000000000 1.212216921 3.562327285
C 0.000000000 -1.212216921 3.562327285
C 0.000000000 1.212216921 -3.562327285
C 0.000000000 -1.212216921 -3.562327285
N 0.000000000 2.210347904 4.161705783
N 0.000000000 -2.210347904 4.161705783
N 0.000000000 -2.210347904 -4.161705783
N 0.000000000 2.210347904 -4.161705783

```

Tetracyano-quinodimethane - 5(-)

```

C 0.000000000 0.000000000 1.431631388

```

```

C 0.000000000 0.000000000 2.863204006
C 0.000000000 1.216039257 0.687315390
H 0.000000000 2.159339194 1.225862617
C 0.000000000 1.216039257 -0.687315390
H 0.000000000 2.159339194 -1.225862617
C 0.000000000 0.000000000 -1.431631388
C 0.000000000 0.000000000 -2.863204006
C 0.000000000 -1.216039257 -0.687315390
H 0.000000000 -2.159339194 -1.225862617
C 0.000000000 -1.216039257 0.687315390
H 0.000000000 -2.159339194 1.225862617
C 0.000000000 1.205060283 3.603337983
C 0.000000000 -1.205060283 3.603337983
C 0.000000000 1.205060283 -3.603337983
C 0.000000000 -1.205060283 -3.603337983
N 0.000000000 2.210088306 4.202084769
N 0.000000000 -2.210088306 4.202084769
N 0.000000000 -2.210088306 -4.202084769
N 0.000000000 2.210088306 -4.202084769

```

Tetracyano-quinodimethane - 5(-2)

```

C 0.000000000 0.000000000 1.445309645
C 0.000000000 0.000000000 2.918625930
C 0.000000000 1.196481315 0.696373313
H 0.000000000 2.146929726 1.226631069
C 0.000000000 1.196481315 -0.696373313
H 0.000000000 2.146929726 -1.226631069
C 0.000000000 0.000000000 -1.445309645
C 0.000000000 0.000000000 -2.918625930
C 0.000000000 -1.196481315 -0.696373313
H 0.000000000 -2.146929726 -1.226631069
C 0.000000000 -1.196481315 0.696373313
H 0.000000000 -2.146929726 1.226631069
C 0.000000000 1.196489774 3.653784108
C 0.000000000 -1.196489774 3.653784108
C 0.000000000 1.196489774 -3.653784108
C 0.000000000 -1.196489774 -3.653784108
N 0.000000000 2.205563182 4.261434162
N 0.000000000 -2.205563182 4.261434162
N 0.000000000 -2.205563182 -4.261434162
N 0.000000000 2.205563182 -4.261434162

```

Tetrathiafulvalene - 6(+2)

```

C 0.373517955 0.570611017 -3.188946637
S 0.807550026 1.200720336 -1.648934513
C 0.000000000 0.000000000 -0.730177009
S -0.807550026 -1.200720336 -1.648934513
C -0.373517955 -0.570611017 -3.188946637
H 0.720387980 1.096660545 -4.074911127
H -0.720387980 -1.096660545 -4.074911127
S -0.084479908 1.444541105 1.648925347
C -0.031305260 0.681286062 3.188983149
C 0.031305260 -0.681286062 3.188983149
S 0.084479908 -1.444541105 1.648925347
C 0.000000000 0.000000000 0.730141927
H -0.062787495 1.310608678 4.074976006
H 0.062787495 -1.310608678 4.074976006

```

Tetrathiafulvalene - 6(+)

```

C 0.534734482 -0.217003481 -2.460641834
S 2.088994808 0.551736558 -2.623665325
C 3.020351394 -0.866140360 -2.204582852
S 2.065223762 -2.284358886 -1.844641625
C 0.523784166 -1.516226899 -2.104030366
H -0.343918805 0.386983113 -2.653950829
H -0.365009428 -2.120440397 -1.965637810
S 5.373203444 0.553622087 -2.516992189
C 6.914547580 -0.215047817 -2.258816265
C 6.903721821 -1.515118657 -1.905352628
S 5.349496471 -2.284568756 -1.745623230
C 4.418102780 -0.865658468 -2.161223178
H 7.803149796 0.389886455 -2.395341808
H 7.782478864 -2.119239866 -1.713003380

```

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Tetrathiafulvalene - 6(0)

=====			
C	0.522236837	-0.222107342	-2.461142025
S	2.081738605	0.579965245	-2.628535054
C	3.044428096	-0.865824953	-2.203126442
S	2.058012006	-2.311970314	-1.838058276
C	0.511602234	-1.512431028	-2.108569632
H	-0.361243005	0.374195561	-2.653489457
H	-0.381791925	-2.109934334	-1.974771980
S	5.380778130	0.580661284	-2.525686880
C	6.927106333	-0.220524007	-2.260075262
C	6.916166573	-1.510862721	-1.907583068
S	5.356265129	-2.311298357	-1.735344910
C	4.393990628	-0.865549915	-2.161702818
H	7.820508019	0.376398106	-2.396512157
H	7.799745768	-2.107818085	-1.717839784

(Cp-COCH₃)₂Fe - 7 (+)

=====			
Fe	0.002873441	0.000962900	-0.008683935
C	1.473265519	-1.453398292	-0.350869073
C	1.540876271	-1.006283660	1.004873698
C	1.807919902	0.401083513	0.996003980
C	1.895997039	0.825276858	-0.361477382
C	1.696566644	-0.322377677	-1.203114239
H	1.257241376	-2.463532514	-0.673316582
H	1.383788414	-1.617898361	1.883244934
H	1.889740877	1.034583512	1.869013171
H	2.061044799	1.828118098	-0.730978898
C	1.677067203	-0.233333932	-2.710656627
C	-1.889540856	-0.826779553	-0.318013117
C	-1.779863709	-0.401031370	1.037606520
C	-1.513306114	1.006444917	1.039179777
C	-1.474786604	1.453790702	-0.318631053
C	-1.708816435	0.320216598	-1.166288106
H	-2.054306446	-1.830779347	-0.684880392
H	-1.841858333	-1.033283057	1.913147527
H	-1.338550741	1.621822307	1.911622249
H	-1.257604521	2.461484620	-0.646574297
C	-1.706313349	0.233807902	-2.674228746
O	1.675239603	0.875324109	-3.213479578
C	1.666667241	-1.515682344	-3.497481193
H	1.750632135	-1.285832602	-4.559658750
H	0.726559169	-2.052393170	-3.321702139
H	2.491586935	-2.168573395	-3.191053965
O	-1.699202923	-0.874753707	-3.177847478
C	-1.695183015	1.515514271	-3.463249456
H	-1.920385080	1.294577945	-4.507009843
H	-0.692430914	1.958636767	-3.409715442
H	-2.413341397	2.241546292	-3.069612288

(Cp-COCH₃)₂Fe - 7 (0)

=====			
Fe	0.007224547	0.001204949	-0.012723992
C	1.499067628	-1.399985158	-0.366064768
C	1.550614865	-0.972395589	0.990485568
C	1.773815575	0.440286443	1.005149755
C	1.857933360	0.890744350	-0.339381934
C	1.696522393	-0.246472826	-1.200559976
H	1.316670386	-2.409272100	-0.706721927
H	1.403888625	-1.599882752	1.858845191
H	1.825801544	1.061914928	1.888433954
H	2.004317181	1.903339487	-0.685135983
C	1.701154319	-0.165182892	-2.682963551
C	-1.848598526	-0.890335820	-0.303174655
C	-1.739849480	-0.438280738	1.039053070
C	-1.517151510	0.974388482	1.018713183
C	-1.491278493	1.400851618	-0.339039928
C	-1.704659543	0.246323556	-1.168243574
H	-2.001710282	-1.903216767	-0.645078875
H	-1.775033325	-1.058611239	1.924051860
H	-1.354615216	1.603035341	1.883420271
H	-1.317546442	2.410053395	-0.684436835
C	-1.732807419	0.162926039	-2.650144761
O	1.829731408	0.918475041	-3.239681999
C	1.532373162	-1.448402404	-3.470977439
H	1.742494398	-1.249472959	-4.522791806

H	0.498033129	-1.799481572	-3.376208631
H	2.194209377	-2.237725046	-3.100168446
O	-1.870389157	-0.921498904	-3.203272553
C	-1.577316259	1.445176309	-3.442729388
H	-1.798056065	1.242631032	-4.491682751
H	-0.543946643	1.801839664	-3.360057790
H	-2.239307216	2.232007512	-3.066826196

FeCp₂ (Ferrocene) - 8 (+)

=====			
Fe	0.000000000	0.000000000	0.000000000
C	1.713968522	-1.214320399	0.000000000
C	1.713127940	-0.373951524	1.156829722
C	1.711053493	0.985921636	0.714925072
C	1.711053493	0.985921636	-0.714925072
C	1.713127940	-0.373951524	-1.156829722
H	1.682676955	-2.295444286	0.000000000
H	1.683959782	-0.708220343	2.185030210
H	1.681637060	1.860660905	1.350322764
H	1.681637060	1.860660905	-1.350322764
H	1.683959782	-0.708220343	-2.185030210
C	-1.711053493	-0.985921636	-0.714925072
C	-1.711053493	-0.985921636	0.714925072
C	-1.713127940	0.373951524	1.156829722
C	-1.713968522	1.214320399	0.000000000
C	-1.713127940	0.373951524	-1.156829722
H	-1.681637060	-1.860660905	-1.350322764
H	-1.681637060	-1.860660905	1.350322764
H	-1.683959782	0.708220343	2.185030210
H	-1.682676955	2.295444286	0.000000000
H	-1.683959782	0.708220343	-2.185030210

FeCp₂ (Ferrocene) - 8 (0)

=====			
Fe	0.000000000	0.000000000	0.000000000
C	1.690212303	-1.211881370	0.000000000
C	1.688782192	-0.372719513	1.155116329
C	1.686699546	0.985152677	0.713868575
C	1.686699546	0.985152677	-0.713868575
C	1.688782192	-0.372719513	-1.155116329
H	1.658693118	-2.292747141	0.000000000
H	1.659481811	-0.706811274	2.183103176
H	1.658670941	1.859690738	1.349180037
H	1.658670941	1.859690738	-1.349180037
H	1.659481811	-0.706811274	-2.183103176
C	-1.686699546	-0.985152677	-0.713868575
C	-1.686699546	-0.985152677	0.713868575
C	-1.688782192	0.372719513	1.155116329
C	-1.690212303	1.211881370	0.000000000
C	-1.688782192	0.372719513	-1.155116329
H	-1.658670941	-1.859690738	-1.349180037
H	-1.658670941	-1.859690738	1.349180037
H	-1.659481811	0.706811274	2.183103176
H	-1.658693118	2.292747141	0.000000000
H	-1.659481811	0.706811274	-2.183103176

Fe(Cp*)₂ - 9 (+)

=====			
Fe	0.000741423	0.000198697	-0.000258795
C	1.722828571	-1.223758902	0.003928538
C	1.720382165	-0.378206731	1.167752711
C	1.720887612	0.990085917	0.722988535
C	1.725580859	0.990183912	-0.715789405
C	1.726895757	-0.378127446	-1.160075558
C	1.785901222	-2.722061640	0.004012468
C	1.779767834	-0.841357601	2.592689668
C	1.781841107	2.202235343	1.603824267
C	1.791182204	2.202946861	-1.595168992
C	1.793658511	-0.843084959	-2.584057062
C	-1.720975350	-0.989309099	-0.721321244
C	-1.715601891	-0.991183512	0.717856892
C	-1.716975538	0.377558677	1.162511164
C	-1.722904021	1.222347971	-0.002701740
C	-1.734205830	0.377721464	-1.165629374
C	-1.779510917	-2.197674868	-1.607707679
C	-1.775695366	-2.204488399	1.597284952
C	-1.778192052	0.841863825	2.587181293

5

```

C -1.783554564 2.720868630 -0.009383273
C -1.823376216 0.841904638 -2.594303452
H 2.831553546 -3.053845464 0.004256971
H 1.309042288 -3.149485214 -0.881125490
H 1.308620780 -3.149460113 0.888967711
H 2.840097178 -0.942026061 -2.898057300
H 1.315955258 -0.136999310 -3.267544842
H 1.319763344 -1.818449419 -2.716352649
H 2.837332096 2.467846985 -1.792254870
H 1.317399887 3.069810643 -1.128823554
H 1.312473397 2.032781350 -2.562548804
H 2.827121563 2.471973845 1.799093393
H 1.304772895 2.027017004 2.570928759
H 1.303714469 3.067575515 1.138951084
H 2.824578701 -0.945838867 2.910273732
H 1.300620681 -1.814335825 2.724595770
H 1.302700715 -0.130753340 3.271725511
H -1.295246289 0.135497196 3.266570071
H -2.823353767 0.939395976 2.905802928
H -1.305642377 1.818329272 2.717326876
H -1.298567367 -3.069310193 1.130166937
H -2.820594689 -2.474358325 1.794242906
H -1.296592132 -2.030668039 2.563717268
H -1.299953526 3.141531383 -0.894219956
H -1.308915877 3.150892839 0.875731929
H -2.828389020 3.055692985 -0.013628124
H -0.843412874 0.987164622 -3.059814533
H -2.359017277 1.792545194 -2.656783313
H -2.368674035 0.114506141 -3.201069756
H -1.299761579 -3.064079029 -1.146341839
H -1.300189940 -2.015504803 -2.572489712
H -2.823987157 -2.470186805 -1.804283629

```

Fe(Cp*)₂ - 9(0)

```

Fe 0.001542965 -0.000125195 0.000426651
C 1.694283376 -1.220463370 0.004193734
C 1.691941230 -0.376924772 1.164721388
C 1.692300078 0.987613424 0.721325892
C 1.696071833 0.987537656 -0.713701451
C 1.697331289 -0.377317069 -1.156891111
C 1.759138715 -2.721043723 0.004467206
C 1.753128079 -0.840788747 2.591950187
C 1.755156897 2.201726356 1.603321450
C 1.763602256 2.202389326 -1.594320141
C 1.766480433 -0.843373850 -2.583019311
C -1.691257079 -0.986862717 -0.720086076
C -1.687171398 -0.988422147 0.715014330
C -1.688420853 0.376696827 1.158697302
C -1.693220818 1.219263007 -0.002907539
C -1.702015768 0.376772807 -1.162984794
C -1.753863495 -2.196953242 -1.607977198
C -1.751017180 -2.202898515 1.596482258
C -1.753674328 0.840939977 2.585647855
C -1.757794728 2.720028431 -0.009194862
C -1.792733465 0.841926587 -2.594215515
H 2.799483517 -3.074004048 0.002900279
H 1.270455376 -3.145958779 -0.877265895
H 1.273246600 -3.145463415 0.887876677
H 2.807884041 -0.951891108 -2.915642699
H 1.281200476 -0.137730620 -3.263968186
H 1.279928689 -1.814409894 -2.713557131
H 2.804658544 2.486057966 -1.800939116
H 1.277172510 3.064710282 -1.12907805
H 1.277313426 2.030968701 -2.559344608
H 2.795107509 2.489403916 1.809901928
H 1.269071411 2.025460643 2.567314505
H 1.265731950 3.063073716 1.139266712
H 2.792656207 -0.951249734 2.929613372
H 1.264401602 -1.810764113 2.722108812
H 1.265554450 -0.132067742 3.267680991
H -1.262951761 0.135158299 3.262249963
H -2.794027253 0.946257787 2.922400947
H -1.269972697 1.813574978 2.715650538
H -1.266158004 -3.065557391 1.129981649
H -2.791072726 -2.487361542 1.806762394
H -1.260758714 -2.029002500 2.558841234

```

```

H -1.265043592 3.139505821 -0.891269788
H -1.273649728 3.147658081 0.873676018
H -2.797951733 3.074158784 -0.013455074
H -0.813570627 0.988882216 -3.062696121
H -2.330685686 1.792996172 -2.661162404
H -2.339399662 0.116568123 -3.205363529
H -1.268442900 -3.061416767 -1.145572265
H -1.261536169 -2.016422618 -2.568113449
H -2.793623155 -2.482356114 -1.819718823

```

CoCp₂ - 10(+)

```

Co 0.000000000 0.000000000 0.000000000
C 1.689288743 -1.213354243 0.000000000
C 1.688135439 -0.373884690 1.155457499
C 1.686563105 0.984517147 0.714145631
C 1.686563105 0.984517147 -0.714145631
C 1.688135439 -0.373884690 -1.155457499
H 1.660545607 -2.294476840 0.000000000
H 1.659038118 -0.707983818 2.183649252
H 1.656861044 1.859109487 1.349655378
H 1.656861044 1.859109487 -1.349655378
H 1.659038118 -0.707983818 -2.183649252
C -1.686563105 -0.984517147 -0.714145631
C -1.686563105 -0.984517147 0.714145631
C -1.688135439 0.373884690 1.155457499
C -1.689288743 1.213354243 0.000000000
C -1.688135439 0.373884690 -1.155457499
H -1.656861044 -1.859109487 -1.349655378
H -1.656861044 -1.859109487 1.349655378
H -1.659038118 0.707983818 2.183649252
H -1.660545607 2.294476840 0.000000000
H -1.659038118 0.707983818 -2.183649252

```

CoCp₂ - 10(0)

```

Co 0.000000000 0.000000000 0.000000000
C 1.754644375 -1.197189447 0.000000000
C 1.823689968 -0.364420729 1.164533084
C 1.785679352 0.973932857 0.723224627
C 1.785679352 0.973932857 -0.723224627
C 1.823689968 -0.364420729 -1.164533084
H 1.738820557 -2.279229787 0.000000000
H 1.806908173 -0.703713942 2.190793796
H 1.771395808 1.855304364 1.350210051
H 1.771395808 1.855304364 -1.350210051
H 1.806908173 -0.703713942 -2.190793796
C -1.785679352 -0.973932857 -0.723224627
C -1.785679352 -0.973932857 0.723224627
C -1.823689968 0.364420729 1.164533084
C -1.754644375 1.197189447 0.000000000
C -1.823689968 0.364420729 -1.164533084
H -1.771395808 -1.855304364 -1.350210051
H -1.771395808 -1.855304364 1.350210051
H -1.806908173 0.703713942 2.190793796
H -1.738820557 2.279229787 0.000000000
H -1.806908173 0.703713942 -2.190793796

```

[Me₃(Ph)]₂Cr - 11(+)

```

Cr 0.008020336 0.000160168 -0.010285112
C -1.572831865 0.074852099 -1.513570828
C -1.656145800 1.255704574 -0.728213014
C -1.746855581 1.118313669 0.682300054
C 1.642956813 -1.257051859 0.733730936
C 1.757162409 -1.119061595 -0.677131810
C 1.779637712 0.155381544 -1.304255265
C 1.684999199 1.310616073 -0.482076167
H -1.747719001 2.009803612 1.300957990
C -1.657298676 2.617008751 -1.368695615
H -1.453799812 0.163988827 -2.588269889
H 1.763377201 -2.011131157 -1.294397867
C 1.911572670 0.281781060 -2.797983445
H 1.635570500 2.288126020 -0.950105116
C 1.633604764 -2.617841331 1.376594483
C -1.745471867 -0.155662592 1.310363456
C -1.682232656 -1.312831824 0.486983901

```

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```

C -1.859756212 -0.278620113 2.805904109
C -1.598240389 -1.219707804 -0.925318072
H -1.637020783 -2.290041182 0.956029830
C -1.532959174 -2.447503140 -1.792747563
C 1.559881124 -0.077769323 1.521440450
H 1.418200847 -0.167606166 2.593182019
C 1.570682308 1.215262692 0.931769863
C 1.483293780 2.453602129 1.782675761
H 2.490714861 2.789603418 2.058454705
H 0.935467159 2.270629950 2.710696610
H 1.000545026 3.277925046 1.251166197
H 2.659243966 -2.925108603 1.616094671
H 1.212677691 -3.376873427 0.712100281
H 1.066549680 -2.621054438 2.311083659
H 2.970909510 0.352641193 -3.074764072
H 1.416478769 1.181070652 -3.173594393
H 1.497111072 -0.586083269 -3.317461144
H -0.859202161 -2.308031796 -2.642758736
H -2.526705699 -2.669383918 -2.200047999
H -1.203402502 -3.325427988 -1.231099662
H -1.377391064 -1.186609769 3.176975997
H -2.916748546 -0.328644329 3.095907877
H -1.421995805 0.581903734 3.318426818
H -1.221989366 2.592914543 -2.370970285
H -1.108252175 3.348871736 -0.769309785
H -2.686463731 2.983164818 -1.466501282

```

=====

[Me3(Ph)]2Cr - 11(0)

=====

```

Cr -0.000146733 0.000226969 -0.003137127
C -1.545278429 0.084544381 -1.520887760
C -1.625997861 1.261785027 -0.730707896
C -1.723103018 1.125968922 0.679706931
C 1.625785641 -1.260408382 0.728963689
C 1.725499671 -1.123194175 -0.681139025
C 1.747469889 0.153484003 -1.302701184
C 1.660493844 1.308682140 -0.481486254
H -1.733602915 2.018786434 1.298522676
C -1.633344776 2.626375995 -1.375525758
H -1.423659117 0.175034577 -2.596665041
H 1.742383328 -2.015244897 -1.300929989
C 1.880503017 0.279748240 -2.800682278
H 1.626864845 2.289394987 -0.947551958
C 1.632725648 -2.624960837 1.373692047
C -1.740386688 -0.149829281 1.303405024
C -1.660677570 -1.305868672 0.482325627
C -1.868204304 -0.275033140 2.801945941
C -1.562343648 -1.207061478 -0.931262291
H -1.624036094 -2.286213982 0.948985181
C -1.502222084 -2.449126055 -1.786237405
C 1.542715760 -0.083963710 1.519731049
H 1.415915096 -0.175784391 2.594780033
C 1.557560540 1.208526811 0.931539556
C 1.492404124 2.447870597 1.790365935
H 2.499193109 2.780118302 2.076603839
H 0.931144447 2.263978816 2.711516025
H 1.010400398 3.274437949 1.259543156
H 2.657998411 -2.945935342 1.601114414
H 1.189662851 -3.378222305 0.715137845
H 1.070995566 -2.623959413 2.312735154
H 2.936449397 0.331020949 -3.097695714
H 1.389520671 1.185850966 -3.168358203
H 1.434810028 -0.578449749 -3.312697392
H -0.954826576 -2.266077924 -2.715907024
H -2.511118144 -2.787726580 -2.058102493
H -1.009309920 -3.270823838 -1.258204643
H -1.375404421 -1.180672656 3.168448794
H -2.923115063 -0.326983179 3.102492923
H -1.421387080 0.583641257 3.312217089
H -1.069363235 2.626330106 -2.313249954
H -1.193457530 3.380056074 -0.715468664
H -2.658545875 2.945524591 -1.606014583

```

=====

CpFePh - 12(+)

=====

```

Fe -0.071283184 -0.005096483 -0.033831053
C 1.591229803 -1.356564043 -0.122868100

```

```

C 1.538147509 -0.762879977 1.160125564
C 1.482945810 0.645162795 1.287693108
C 1.481762341 1.459933337 0.130859507
C 1.589361754 -0.542266088 -1.279440022
H 1.375281604 1.095347239 2.267659147
H 1.374130479 2.534269436 0.224652268
C -1.712086761 -1.040064966 -0.791099148
C -1.744998960 -1.049121702 0.635148553
C -1.803781225 0.304000905 1.083080208
C -1.806842846 1.149177894 -0.066027170
C -1.749952317 0.318630700 -1.224413887
H -1.638461449 -1.909166306 -1.430513603
H -1.700481794 -1.926170376 1.266297961
H -1.812350215 0.632474370 2.113405129
H -1.818208267 2.230530934 -0.059397302
H -1.710160111 0.659824039 -2.249859255
C 1.534829332 0.865625535 -1.152216917
H 1.562179741 -2.435706562 -0.220222055
H 1.471287361 -1.388849780 2.042455682
H 1.559730106 -0.997738484 -2.262537690
H 1.465089826 1.485964350 -2.038289461

```

=====

CpFePh - 12(0)

=====

```

Fe -0.031782661 -0.006212777 -0.034857882
C 1.694089185 -1.363990535 -0.137531802
C 1.558989748 -0.761000972 1.144769739
C 1.560290237 0.653060931 1.293210339
C 1.553995110 1.465490492 0.143066480
C 1.697263361 -0.553103222 -1.285036193
H 1.476757878 1.095478340 2.279662818
H 1.464862884 2.542565046 0.231868127
C -1.859897454 -1.047288652 -0.792146855
C -1.823812985 -1.037723821 0.628215203
C -1.935192835 0.324559172 1.081755376
C -1.936431913 1.153627114 -0.053602205
C -1.830808767 0.307663305 -1.214904042
H -1.810384688 -1.919628587 -1.429174199
H -1.806260677 -1.910937082 1.267920702
H -1.966387793 0.646076636 2.114183708
H -1.970353395 2.234924801 -0.061290587
H -1.817315991 0.652273102 -2.241119004
C 1.555272339 0.855447172 -1.142347504
H 1.708653945 -2.444547870 -0.228932407
H 1.467257802 -1.390088405 2.023457978
H 1.713418331 -0.999441097 -2.273285718
H 1.462238930 1.475255658 -2.027503774

```

=====

Cp*2Co - 13(+)

=====

```

Co 0.000000000 0.000000000 0.000000000
C 1.696387320 -1.221323108 0.000000000
C 1.695801408 -0.376510652 1.162777447
C 1.694494281 0.990488202 0.718674389
C 1.694494281 0.990488202 -0.718674389
C 1.695801408 -0.376510652 -1.162777447
C 1.762979219 -2.718520697 0.000000000
C 1.762205796 -0.839241407 2.586643249
C 1.760501902 2.201776749 1.598757704
C 1.760501902 2.201776749 -1.598757704
C 1.762205796 -0.839241407 -2.586643249
C -1.694494281 -0.990488202 -0.718674389
C -1.694494281 -0.990488202 0.718674389
C -1.695801408 0.376510652 1.162777447
C -1.696387320 1.221323108 0.000000000
C -1.695801408 0.376510652 -1.162777447
C -1.760501902 -2.201776749 -1.598757704
C -1.760501902 -2.201776749 1.598757704
C -1.762205796 0.839241407 2.586643249
C -1.762979219 2.718520697 0.000000000
C -1.762205796 0.839241407 -2.586643249
H 2.807281376 2.468847797 -1.792328856
H 1.284887226 3.069447739 -1.134871309
H 1.285577723 2.028460390 -2.567622582
H -2.809026317 0.939719508 -2.900631091
H -1.285714546 0.130521713 -3.268520920
H -1.288279586 1.814748790 -2.721058894

```

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```

H 2.809026317 -0.939719508 -2.900631091
H 1.285714546 -0.130521713 -3.268520920
H 1.288279586 -1.814748790 -2.721058894
H -2.807281376 -2.468847797 -1.792328856
H -1.284887226 -3.069447739 -1.134871309
H -1.285577723 -2.028460390 -2.567622582
H 2.809793485 -3.048204395 0.000000000
H 1.287739334 -3.147908026 -0.885471781
H 1.287739334 -3.147908026 0.885471781
H -2.807281376 -2.468847797 1.792328856
H -1.285577723 -2.028460390 2.567622582
H -1.284887226 -3.069447739 1.134871309
H 2.809026317 -0.939719508 2.900631091
H 1.288279586 -1.814748790 2.721058894
H 1.285714546 -0.130521713 3.268520920
H -2.809026317 0.939719508 2.900631091
H -1.288279586 1.814748790 2.721058894
H -1.285714546 0.130521713 3.268520920
H 2.807281376 2.468847797 1.792328856
H 1.285577723 2.028460390 2.567622582
H 1.284887226 3.069447739 1.134871309
H -2.809793485 3.048204395 0.000000000
H -1.287739334 3.147908026 -0.885471781
H -1.287739334 3.147908026 0.885471781

```

Cp*2Co - 13(0)

```

Co 0.000000000 0.000000000 0.000000000
C 1.743911238 -1.201975371 0.000000000
C 1.816031055 -0.364148149 1.171975592
C 1.776223120 0.980455949 0.728404612
C 1.776223120 0.980455949 -0.728404612
C 1.816031055 -0.364148149 -1.171975592
C 1.795424505 -2.703501171 0.000000000
C 1.873064721 -0.841601154 2.594641084
C 1.829736819 2.210024253 1.589336322
C 1.829736819 2.210024253 -1.589336322
C 1.873064721 -0.841601154 -2.594641084
C -1.776223120 -0.980455949 -0.728404612
C -1.776223120 -0.980455949 0.728404612
C -1.816031055 0.364148149 1.171975592
C -1.743911238 1.201975371 0.000000000
C -1.816031055 0.364148149 -1.171975592
C -1.829736819 -2.210024253 -1.589336322
C -1.829736819 -2.210024253 1.589336322
C -1.873064721 0.841601154 2.594641084
C -1.795424505 2.703501171 0.000000000
C -1.873064721 0.841601154 -2.594641084
H 2.861259650 2.566626810 -1.716854172
H 1.256819901 3.033520791 -1.151683270
H 1.424928204 2.020590391 -2.588193472
H -2.906136748 1.029904783 -2.919107440
H -1.446091421 0.106340681 -3.283822775
H -1.318781336 1.776137061 -2.728978264
H 2.906136748 -1.029904783 -2.919107440
H 1.446091421 -0.106340681 -3.283822775
H 1.318781336 -1.776137061 -2.728978264
H -2.861259650 -2.566626810 -1.716854172
H -1.256819901 -3.033520791 -1.151683270
H -1.424928204 -2.020590391 -2.588193472
H 2.832309196 -3.067138060 0.000000000
H 1.304997929 -3.123918386 -0.883356844
H 1.304997929 -3.123918386 0.883356844
H -2.861259650 -2.566626810 1.716854172
H -1.424928204 -2.020590391 2.588193472
H -1.256819901 -3.033520791 1.151683270
H 2.906136748 -1.029904783 2.919107440
H 1.318781336 -1.776137061 2.728978264
H 1.446091421 -0.106340681 3.283822775
H -2.906136748 1.029904783 2.919107440
H -1.318781336 1.776137061 2.728978264
H -1.446091421 0.106340681 3.283822775
H 2.861259650 2.566626810 1.716854172
H 1.424928204 2.020590391 2.588193472
H 1.256819901 3.033520791 1.151683270
H -2.832309196 3.067138060 0.000000000
H -1.304997929 3.123918386 -0.883356844

```

H -1.304997929 3.123918386 0.883356844

CpFeAr* - 14(+)

```

Fe -0.062760894 0.021746942 -0.020143517
C 1.585681033 -1.375214085 -0.106378262
C 1.534131511 -0.774616826 1.189571291
C 1.531370223 0.647868723 1.317512050
C 1.517264934 1.469529829 0.149233257
C 1.611466081 -0.552510577 -1.273061269
C 1.546614291 1.270655167 2.698325738
C 1.466053462 2.975624252 0.286572800
C -1.713035126 -0.989789717 -0.783502711
C -1.756902140 -0.989431112 0.642322743
C -1.793542672 0.367283815 1.081775207
C -1.774462161 1.205695569 -0.072608905
C -1.724364925 0.366794562 -1.225292981
H -1.650025567 -1.863269177 -1.417734582
H -1.734660204 -1.863222994 1.278753797
H -1.804051353 0.701618824 2.110052524
H -1.764960125 2.286931494 -0.072249351
H -1.670154638 0.700705824 -2.252364500
C 1.567999667 0.869393529 -1.146983462
C 1.626883399 -2.881713643 -0.252677224
C 1.485774302 -1.645709658 2.426515217
C 1.665374128 -1.177553278 -2.650684821
C 1.584187915 1.750062790 -2.378020165
H 1.651879863 2.352333165 2.661139307
H 2.396091364 0.882101175 3.268575135
H 0.640164633 1.042614184 3.266303401
H 1.206482616 3.465704923 -0.649358512
H 2.447141331 3.356784190 0.594476914
H 0.739286747 3.292029374 1.036558812
H 2.576863685 -3.182824688 -0.708239219
H 0.824166261 -3.255386843 -0.892698064
H 1.552784055 -3.393322961 0.703691615
H 2.459054037 -2.122687392 2.591036044
H 0.742486763 -2.439814181 2.334467719
H 1.244022178 -1.076385415 3.321253283
H 2.601545856 -0.902990769 -3.148538518
H 0.843434796 -0.834916511 -3.284328861
H 1.623308993 -2.263444297 -2.614705647
H 2.477404425 2.384197488 -2.369792748
H 0.715062350 2.411363355 -2.418700986
H 1.602134608 1.173032303 -3.299309924

```

CpFeAr* - 14(0)

```

Fe -0.038632468 -0.006063426 -0.040308957
C 1.675738305 -1.360931046 -0.105302005
C 1.511244466 -0.745292936 1.179635431
C 1.617256803 0.683541454 1.326461332
C 1.645573161 1.498234716 0.178390853
C 1.666017794 -0.541256729 -1.263177326
C 1.622039831 1.284586202 2.716300022
C 1.710771709 3.006913785 0.312375007
C -1.905694656 -1.025027479 -0.810906044
C -1.858021969 -1.024248097 0.606778297
C -1.902638692 0.338328944 1.068952772
C -1.893854154 1.177379175 -0.065571754
C -1.826319584 0.332721007 -1.227240929
H -1.894565351 -1.894461708 -1.454153403
H -1.864020919 -1.899445892 1.244232406
H -1.930801910 0.652778761 2.103983864
H -1.906656780 2.259257779 -0.069484060
H -1.806257537 0.681654298 -2.252212185
C 1.534454099 0.881791576 -1.117334092
C 1.786256675 -2.867599794 -0.235337363
C 1.350209049 -1.600602743 2.420107669
C 1.730508803 -1.146484874 -2.651061033
C 1.409720136 1.752427017 -2.351822250
H 1.863378615 2.347018319 2.700342756
H 2.356584145 0.788201256 3.358841689
H 0.644104266 1.182426629 3.200034085
H 1.837479952 3.497312734 -0.651846699
H 2.561285448 3.304509506 0.934472732
H 0.806706944 3.416015430 0.776888899

```

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H	2.661901561	-3.139644790	-0.833643772
H	0.906681870	-3.303313859	-0.720963273
H	1.904487109	-3.352436108	0.733095460
H	2.320628962	-1.914886838	2.828110126
H	0.769210294	-2.500369621	2.210713951
H	0.823325226	-1.060133979	3.207378012
H	2.554813694	-0.716717383	-3.231032156
H	0.806770490	-0.964618396	-3.209570593
H	1.878212799	-2.225228971	-2.620023116
H	2.375571993	2.190093174	-2.638594242
H	0.708216082	2.573554836	-2.188582881
H	1.041918532	1.185822081	-3.206739893

Cp*FeAr* - 15(+)

Fe	-0.054549806	-0.014244572	-0.039391230
C	1.580761599	-1.385631669	-0.139545913
C	1.545178312	-0.789344154	1.143044204
C	1.508455782	0.619774635	1.269208821
C	1.507772621	1.432914168	0.111173096
C	1.579608274	-0.572880274	-1.297545197
H	1.410705012	1.072123416	2.249357332
H	1.410063475	2.508443310	0.203761017
C	-1.713635622	-1.039222815	-0.784325311
C	-1.735581625	-1.041972779	0.651724608
C	-1.774802403	0.322958817	1.097303872
C	-1.776474109	1.169128823	-0.063356430
C	-1.738586351	0.327171548	-1.226427136
C	-1.723643557	-2.250921662	-1.667532907
C	-1.771483634	-2.256854767	1.530027037
C	-1.862069040	0.782480941	2.522235643
C	-1.865977460	2.666255869	-0.062628096
C	-1.779422996	0.790662584	-2.652061568
C	1.543486682	0.836014150	-1.171670889
H	1.537459507	-2.464428329	-0.235000423
H	1.478205457	-1.413199653	2.026906874
H	1.536571047	-1.029223348	-2.279715318
H	1.474116143	1.455796960	-2.058236629
H	-2.756739628	-2.550041826	-1.883167191
H	-1.230348014	-3.104139965	-1.195335080
H	-1.233676728	-2.061353569	-2.625806263
H	-2.809942742	-2.564446978	1.704027742
H	-1.320898815	-2.066611371	2.507265792
H	-1.253458257	-3.104861133	1.075168294
H	-2.912524782	0.853020175	2.830326866
H	-1.416092164	1.770590459	2.660139681
H	-1.368969467	0.087555645	3.206611825
H	-2.917027109	2.979561957	-0.085479386
H	-1.377310822	3.104978313	-0.936200331
H	-1.416838201	3.101701734	0.833462720
H	-2.819011968	0.858943486	-2.995429255
H	-1.261157420	0.099272319	-3.321227634
H	-1.332076804	1.780472944	-2.771940704

Cp*FeAr* - 15(0)

Fe	0.010915215	-0.028430613	-0.048518548
C	1.702439209	-1.377373417	-0.138648053
C	1.588711497	-0.769558310	1.143554953
C	1.595286471	0.645590976	1.286725359
C	1.588278273	1.454197903	0.134573886
C	1.707307398	-0.567304844	-1.291399066
H	1.514014231	1.091186524	2.271940037
H	1.501732058	2.531770014	0.220059307
C	-1.836636712	-1.049672354	-0.793851711
C	-1.777063172	-1.037563331	0.633129804
C	-1.862010154	0.336304448	1.090273600
C	-1.859954123	1.166236225	-0.050177373
C	-1.783862988	0.309628620	-1.219924434
C	-1.870740613	-2.264817445	-1.675159356
C	-1.809155509	-2.246703576	1.525919048
C	-1.948593305	0.773671000	2.524464433
C	-1.947267515	2.665417970	-0.075306345
C	-1.821905913	0.791184138	-2.643402785
C	1.588794330	0.843110225	-1.151119935
H	1.703365831	-2.458340300	-0.227174652
H	1.507738367	-1.396177826	2.025266462

H	1.714369266	-1.015843741	-2.278853341
H	1.506874658	1.463142203	-2.037348035
H	-2.899015920	-2.591466542	-1.886485606
H	-1.353367784	-3.112711516	-1.213571665
H	-1.389119008	-2.076516858	-2.640544180
H	-2.839201602	-2.536494006	1.775926057
H	-1.286996985	-2.063919326	2.470491894
H	-1.335638625	-3.110894371	1.049308122
H	-2.983836850	0.761192324	2.893320591
H	-1.569454111	1.791999664	2.658804489
H	-1.366804786	0.118859116	3.181909427
H	-2.982802500	3.011420731	-0.201211637
H	-1.365548254	3.089594307	-0.900554454
H	-1.569009018	3.106969714	0.852420383
H	-2.853299224	0.947248547	-2.988985184
H	-1.357052148	0.071055383	-3.324209398
H	-1.294891834	1.743396640	-2.761055428

Rh(Cp)2 - 16(+)

Rh	0.000000000	0.000000000	0.000000000
C	1.875074623	-1.216694214	0.000000000
C	1.873733850	-0.374795637	1.158732379
C	1.872419558	0.987421555	0.716143568
C	1.872419558	0.987421555	-0.716143568
C	1.873733850	-0.374795637	-1.158732379
H	1.877184867	-2.298118385	0.000000000
H	1.875736531	-0.708903681	2.187248060
H	1.873112982	1.862316018	1.351786386
H	1.873112982	1.862316018	-1.351786386
H	1.875736531	-0.708903681	-2.187248060
C	-1.872419558	-0.987421555	-0.716143568
C	-1.872419558	-0.987421555	0.716143568
C	-1.873733850	0.374795637	1.158732379
C	-1.875074623	1.216694214	0.000000000
C	-1.873733850	0.374795637	-1.158732379
H	-1.873112982	-1.862316018	-1.351786386
H	-1.873112982	-1.862316018	1.351786386
H	-1.875736531	0.708903681	2.187248060
H	-1.877184867	2.298118385	0.000000000
H	-1.875736531	0.708903681	-2.187248060

Rh(Cp)2 - 16(0)

Rh	0.000000000	0.000000000	0.000000000
C	1.938343568	-1.199876509	0.000000000
C	2.016430474	-0.366685955	1.166695418
C	1.969235788	0.973928965	0.724179738
C	1.969235788	0.973928965	-0.724179738
C	2.016430474	-0.366685955	-1.166695418
H	1.944206903	-2.281911463	0.000000000
H	2.018661445	-0.706382174	2.192717632
H	1.975512841	1.855732829	1.350353780
H	1.975512841	1.855732829	-1.350353780
H	2.018661445	-0.706382174	-2.192717632
C	-1.969235788	-0.973928965	-0.724179738
C	-1.969235788	-0.973928965	0.724179738
C	-2.016430474	0.366685955	1.166695418
C	-1.938343568	1.199876509	0.000000000
C	-2.016430474	0.366685955	-1.166695418
H	-1.975512841	-1.855732829	-1.350353780
H	-1.975512841	-1.855732829	1.350353780
H	-2.018661445	0.706382174	2.192717632
H	-1.944206903	2.281911463	0.000000000
H	-2.018661445	0.706382174	-2.192717632

Rh(Cp)2 - 16(-1)

Rh	0.000000000	0.000000000	0.000000000
C	2.057892663	-1.193423680	0.000000000
C	2.185642958	-0.367298138	1.169215622
C	2.102284383	0.964743302	0.725741877
C	2.102284383	0.964743302	-0.725741877
C	2.185642958	-0.367298138	-1.169215622
H	2.084489520	-2.278258583	0.000000000
H	2.168390332	-0.707585349	2.196960686
H	2.115553834	1.851965378	1.348462402

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```

H 2.115553834 1.851965378 -1.348462402
H 2.168390332 -0.707585349 -2.196960686
C -2.102284383 -0.964743302 -0.725741877
C -2.102284383 -0.964743302 0.725741877
C -2.185642958 0.367298138 1.169215622
C -2.057892663 1.193423680 0.000000000
C -2.185642958 0.367298138 -1.169215622
H -2.115553834 -1.851965378 -1.348462402
H -2.115553834 -1.851965378 1.348462402
H -2.168390332 0.707585349 2.196960686
H -2.084489520 2.278258583 0.000000000
H -2.168390332 0.707585349 -2.196960686

```

=====
Cr(Cp*)₂ - 17(+)
=====

```

Cr -0.001650834 -0.003046276 0.002309563
C 1.812437219 -1.167348478 -0.022714153
C 1.821302602 -0.338532769 1.158228685
C 1.866544485 1.032798005 0.734156901
C 1.883252061 1.058553227 -0.695394629
C 1.845076355 -0.293767398 -1.168658090
C 1.903594135 -2.668110725 -0.050306649
C 1.891818235 -0.826049787 2.578354157
C 1.923140850 2.231317231 1.636137605
C 1.947246955 2.288529519 -1.552708691
C 1.921073591 -0.727768352 -2.605050750
C -1.867550180 -1.047790035 -0.690241928
C -1.900213668 -1.022377888 0.738891510
C -1.857268947 0.344719354 1.163980351
C -1.809449281 1.177278422 -0.010221244
C -1.811617220 0.308914241 -1.162465319
C -1.927271047 -2.275811870 -1.552078722
C -1.975043862 -2.219811748 1.640143423
C -1.935218544 0.830606607 2.583331290
C -1.889934421 2.678482931 -0.033276807
C -1.877354302 0.747249806 -2.598919485
H 2.953178764 -2.986368603 -0.050274865
H 1.436459537 -3.088531025 -0.944540648
H 1.426817979 -3.120785800 0.822868373
H 2.968302970 -0.815661185 -2.919541435
H 1.439884595 -0.010932434 -3.275608537
H 1.453720461 -1.703380999 -2.760563114
H 2.992868874 2.567035653 -1.734386024
H 1.462630120 3.145049972 -1.077072082
H 1.480994780 2.130341574 -2.528447779
H 2.966582913 2.483768337 1.862853873
H 1.420871859 2.049092081 2.589641412
H 1.469846229 3.112245730 1.174431780
H 2.937427848 -0.942417589 2.888556488
H 1.407862029 -1.798427825 2.699870346
H 1.422449964 -0.125702461 3.274068354
H -1.487802239 0.120769319 3.283795431
H -2.982605392 0.965034859 2.880422120
H -1.436548157 1.794584711 2.712303379
H -1.523440490 -3.104089962 1.183677515
H -3.022810844 -2.464475359 1.855101208
H -1.482466046 -2.040885714 2.599351471
H -1.402728230 3.098880717 -0.916766559
H -1.427982371 3.125080621 0.850961705
H -2.937367624 3.003187888 -0.053216753
H -1.409004680 0.021587723 -3.268962030
H -1.388986062 1.712874644 -2.752627903
H -2.921727657 0.856832619 -2.915737958
H -1.470934540 -3.141127431 -1.064599000
H -1.428754049 -2.124164478 -2.512796757
H -2.971289337 -2.536283311 -1.766299003

```

=====
Cr(Cp*)₂ - 17(0)
=====

```

Cr 0.001250646 0.007384082 -0.013636342
C 1.765785079 -1.227070622 0.000570678
C 1.755889147 -0.376092363 1.160660094
C 1.763584788 0.997842919 0.725267266
C 1.775364645 0.995475778 -0.712891891
C 1.777982081 -0.374285956 -1.157717459
C 1.859460377 -2.726649373 0.011580973
C 1.786527839 -0.846343912 2.588115781

```

```

C 1.856323606 2.202870830 1.613372619
C 1.837117828 2.202183936 -1.599347074
C 1.845229472 -0.826668221 -2.586342899
C -1.766724102 -0.994621731 -0.724717073
C -1.751304614 -0.991089419 0.712230108
C -1.754060014 0.383189114 1.156291257
C -1.772537001 1.231165766 -0.004737874
C -1.788302257 0.376693204 -1.162274734
C -1.856309849 -2.207330009 -1.603422318
C -1.806837526 -2.203985349 1.598392767
C -1.810847090 0.842519507 2.585418341
C -1.866396417 2.728663588 -0.002615899
C -1.843096550 0.829354248 -2.598431754
H 2.904558610 -3.066069334 0.014083364
H 1.377261663 -3.167694093 -0.865868071
H 1.378289917 -3.155725985 0.897549812
H 2.885510952 -0.940082981 -2.919864690
H 1.368011890 -0.112219664 -3.263745211
H 1.349851787 -1.791691419 -2.728479265
H 2.874592320 2.490689728 -1.805253195
H 1.344744026 3.064080315 -1.143251762
H 1.356328442 2.024617616 -2.564756544
H 2.901570190 2.474190714 1.814736476
H 1.374580468 2.028986053 2.581413908
H 1.375197945 3.074709681 1.160930268
H 2.819090471 -0.960931892 2.945443735
H 1.293046714 -1.816885530 2.707658387
H 1.288245406 -0.140357599 3.260089946
H -1.319102190 0.133289543 3.259973932
H -2.849955302 0.948762549 2.927731421
H -1.321953236 1.813010649 2.715496515
H -1.317202541 -3.065356849 1.132136208
H -2.845699924 -2.493489814 1.812796443
H -1.315791689 -2.026727175 2.561470926
H -1.382525514 3.163340616 -0.882568084
H -1.385482760 3.158959806 0.881649558
H -2.912563311 3.066648195 -0.002387605
H -0.860116871 0.884087793 -3.079198137
H -2.293146261 1.823591864 -2.673365025
H -2.456846041 0.145862349 -3.194641649
H -1.373918822 -3.075239948 -1.141566807
H -1.372743464 -2.038887339 -2.570437963
H -2.901967935 -2.483266736 -1.802286295

```

=====
Cr(Cp*)₂ - 17(-)
=====

```

Cr 0.001060973 0.007241393 -0.009957617
C 1.860960996 -1.214750598 0.026503988
C 1.873639521 -0.379289500 1.180992756
C 1.820750310 0.982295485 0.753211199
C 1.777409393 0.997982658 -0.686501723
C 1.800995856 -0.374942606 -1.137288132
C 1.952737980 -2.715832451 0.022130315
C 1.948262596 -0.849453996 2.607326183
C 1.898037017 2.191747389 1.643874329
C 1.899279875 2.216735377 -1.560351560
C 1.929959093 -0.834070516 -2.564212118
C -1.821057333 -0.984233099 -0.752436077
C -1.765818666 -0.987956508 0.686503472
C -1.791221261 0.387992778 1.127115340
C -1.864137344 1.218578068 -0.042845147
C -1.883094657 0.373457661 -1.190620451
C -1.900528602 -2.201498503 -1.632210502
C -1.867895102 -2.200865742 1.571159501
C -1.909454728 0.858339164 2.551329291
C -1.967733698 2.718851357 -0.048159537
C -1.976496570 0.832134011 -2.619594968
H 2.994361992 -3.075957299 -0.031266379
H 1.420774725 -3.144116466 -0.835069051
H 1.506744417 -3.148096048 0.925117084
H 2.980205104 -0.903296505 -2.900463666
H 1.419058179 -0.148552009 -3.250266274
H 1.480389550 -1.823483645 -2.708623347
H 2.948405301 2.494005485 -1.769421645
H 1.422991100 3.089365528 -1.098291089
H 1.410078438 2.062560349 -2.529182809
H 2.935701344 2.524462860 1.821163677

```

10

H	1.448920786	1.997624282	2.624704544	Mn	0.000850402	0.000231315	-0.000382071
H	1.359837819	3.041200268	1.207768296	C	1.723047049	-1.223189442	0.004249667
H	2.987123223	-0.941432492	2.965716037	C	1.720082242	-0.378007240	1.167359766
H	1.474978103	-1.830063323	2.730648683	C	1.721153311	0.989501511	0.723056088
H	1.433377821	-0.156953456	3.282754425	C	1.726417929	0.989417730	-0.714868151
H	-1.390861257	0.180291736	3.239071851	C	1.727700925	-0.378047331	-1.158972279
H	-2.957039795	0.927033187	2.895844658	C	1.788851471	-2.723744086	0.004541679
H	-1.462081944	1.850424713	2.683473294	C	1.781554038	-0.842008637	2.594543027
H	-1.391975678	-3.073932024	1.109356952	C	1.784685679	2.203439897	1.605350851
H	-2.912291182	-2.483450604	1.795918372	C	1.795079051	2.203875884	-1.595889004
H	-1.367281738	-2.036157859	2.532467897	C	1.797681063	-0.843318710	-2.585272429
H	-1.551186547	3.146358625	-0.966993768	C	-1.721808035	-0.988799284	-0.721183811
H	-1.415164677	3.158989194	0.789651675	C	-1.716530007	-0.990526568	0.716836716
H	-3.010180263	3.071386318	0.031965939	C	-1.717846431	0.377629825	1.161364435
H	-1.467169290	0.136404905	-3.295607962	C	-1.723757020	1.221709324	-0.002828027
H	-1.507660851	1.813173455	-2.756317292	C	-1.733752877	0.377376334	-1.164898761
H	-3.019699731	0.918217747	-2.965934353	C	-1.782888477	-2.198797870	-1.609352794
H	-1.353178377	-3.044458553	-1.194928816	C	-1.778961624	-2.205150782	1.598268961
H	-1.462638038	-2.012944530	-2.619133591	C	-1.781499857	0.842042116	2.588354124
H	-2.938146078	-2.541205894	-1.795869819	C	-1.787247931	2.722566816	-0.009786558
=====				C	-1.822600028	0.842355119	-2.596634674
Mn(Cp*)2 - 18(+)				H	2.829386649	-3.077115499	0.004498200
=====				H	1.301253160	-3.148716250	-0.877851798
Mn	-0.000387578	0.001937020	0.003052714	H	1.301513271	-3.148237581	0.887272046
C	1.786798680	-1.198363553	0.040012854	H	2.839209899	-0.948830897	-2.919382106
C	1.829827240	-0.355047648	1.199457756	H	1.309799328	-0.138672218	-3.265536259
C	1.817783862	1.006113619	0.762830674	H	1.313697793	-1.815682267	-2.715940477
C	1.768538244	1.016662646	-0.671274698	H	2.836293191	2.485769551	-1.805614128
C	1.754740241	-0.351300265	-1.124656440	H	1.311537517	3.067419814	-1.129753460
C	1.870859047	-2.697443795	0.039221757	H	1.305911254	2.033152443	-2.559678273
C	1.909361227	-0.820479582	2.622693410	H	2.824739786	2.490886287	1.813335484
C	1.885127731	2.213797956	1.649497482	H	1.297335189	2.027221282	2.568857123
C	1.833620702	2.236178942	-1.544930074	H	1.295961414	3.065172084	1.141068795
C	1.835437385	-0.809251375	-2.553256042	H	2.821130673	-0.952912493	2.932994918
C	-1.815016789	-1.013098661	-0.753613245	H	1.292258436	-1.811888011	2.724403539
C	-1.768728016	-1.015501271	0.680398225	H	1.293698575	-0.133160077	3.270147498
C	-1.758132849	0.354576764	1.126451893	H	-1.288583457	0.136673732	3.264020923
C	-1.790885991	1.195679247	-0.043255345	H	-2.821347117	0.946916567	2.927731258
C	-1.829332675	0.346051338	-1.198034110	H	-1.297771268	1.814931215	2.717121647
C	-1.876298518	-2.225995865	-1.633507104	H	-1.291990993	-3.066709208	1.131695534
C	-1.828130005	-2.230288788	1.561179346	H	-2.818542057	-2.492205660	1.808904469
C	-1.841852211	0.820618802	2.552456992	H	-1.288631528	-2.030236027	2.560557876
C	-1.876980574	2.694554510	-0.050690874	H	-1.293223445	3.140839907	-0.891824155
C	-1.906985815	0.804032327	-2.623779863	H	-1.302717118	3.150017514	0.873042627
H	2.919753385	-3.018246147	0.025703315	H	-2.826961802	3.078752551	-0.014885521
H	1.387192817	-3.131200294	-0.839376784	H	-0.844360169	0.987559780	-3.068063526
H	1.409556586	-3.132012334	0.929627483	H	-2.358952415	1.794390333	-2.662817019
H	2.883114893	-0.904913912	-2.863294358	H	-2.371888539	0.117776996	-3.206380500
H	1.357578168	-0.100642076	-3.234377271	H	-1.294605748	-3.062171016	-1.147724915
H	1.363499053	-1.784809705	-2.694858593	H	-1.291526855	-2.016491515	-2.569741638
H	2.878238525	2.499367098	-1.751595193	H	-2.822098902	-2.487308610	-1.820845881
H	1.367790590	3.103081910	-1.069472285	=====			
H	1.342976377	2.073332244	-2.507678049	Mn(Cp*)2 - 18(-)			
H	2.931464998	2.487449326	1.834978147	=====			
H	1.420694406	2.032891220	2.622132903	Mn	0.002612710	-0.000052202	0.000521445
H	1.399649660	3.080793467	1.194927023	C	1.709177512	-1.223927823	0.005564211
H	2.958480054	-0.925437671	2.926835801	C	1.705776843	-0.378325707	1.169192637
H	1.433666064	-1.794498152	2.760309517	C	1.706927364	0.989737525	0.724489168
H	1.442410690	-0.111496904	3.310922430	C	1.711886886	0.989489758	-0.714232751
H	-1.364806561	0.116216250	3.238347380	C	1.713494806	-0.378599213	-1.158446570
H	-2.889981567	0.918075258	2.860540813	C	1.796838447	-2.724018978	0.006301497
H	-1.370060562	1.796847499	2.689223689	C	1.788441005	-0.841941548	2.596195718
H	-1.349324167	-3.095153186	1.095053935	C	1.791524019	2.203354727	1.606528073
H	-2.871486134	-2.503611061	1.761229373	C	1.800688004	2.203485882	-1.595264037
H	-1.347107804	-2.055801044	2.526587241	C	1.805227529	-0.844211563	-2.584147823
H	-1.408076469	3.125241779	-0.939144164	C	-1.705950073	-0.988666415	-0.723437959
H	-1.401719659	3.132944089	0.830155360	C	-1.702068585	-0.990543255	0.715227309
H	-2.926295677	3.014202283	-0.048318903	C	-1.703564181	0.378149941	1.160195938
H	-1.424745054	0.099808898	-3.306464470	C	-1.708140399	1.222734937	-0.004387215
H	-1.445453685	1.784778112	-2.762034111	C	-1.717045271	0.378169395	-1.167045283
H	-2.955644124	0.891858513	-2.934777440	C	-1.791783869	-2.198254507	-1.611074995
H	-1.387902624	-3.088350900	-1.173347467	C	-1.787268274	-2.204741214	1.596495623
H	-1.411715790	-2.048712004	-2.606710353	C	-1.790822210	0.841885728	2.586853023
H	-2.921273989	-2.505147890	-1.818475079	C	-1.797059540	2.722871177	-0.009898128
=====				C	-1.829543449	0.843061424	-2.599210562
Mn(Cp*)2 - 18(0)				H	2.838285590	-3.090209486	0.005544942
=====				H	1.305234235	-3.154491890	-0.873909849

11

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H 1.306998896 -3.153192179 0.888086218
H 2.847589687 -0.950886202 -2.931634123
H 1.311334217 -0.144621421 -3.268820939
H 1.321013882 -1.818392623 -2.718640560
H 2.842301598 2.494895736 -1.816153705
H 1.316538474 3.070562071 -1.131230874
H 1.304753557 2.038388179 -2.559091372
H 2.832247854 2.501924735 1.822136110
H 1.300981516 2.031711653 2.571725955
H 1.298959393 3.067953008 1.146509947
H 2.828718195 -0.955808866 2.947732984
H 1.296601924 -1.812287780 2.731110976
H 1.296054828 -0.136458964 3.275561035
H -1.295801943 0.139071079 3.267120257
H -2.832034684 0.950958587 2.937123824
H -1.303710261 1.814675407 2.721963338
H -1.298891137 -3.070218356 1.133579243
H -2.827985999 -2.500585959 1.815847572
H -1.292394469 -2.035597899 2.559953700
H -1.303011266 3.148776650 -0.890836468
H -1.309194320 3.155544351 0.871086090
H -2.838818905 3.088875193 -0.013060580
H -0.859224330 0.976148236 -3.094598453
H -2.355883097 1.804284313 -2.663269478
H -2.401913564 0.127768112 -3.204767499
H -1.302553678 -3.065812262 -1.153475844
H -1.297665199 -2.022582172 -2.573651072
H -2.832829951 -2.494292408 -1.829894125

```

Ru(Cp*)₂ - 19(+)

```

Ru 0.000048561 0.002725226 -0.002255312
C 1.912708297 -1.227157370 0.001890369
C 1.907763198 -0.381586730 1.169919856
C 1.912260266 0.990641506 0.726969990
C 1.920196821 0.992619513 -0.714327896
C 1.920089510 -0.377473245 -1.162268331
C 1.992021331 -2.725652438 -0.000067296
C 1.983167572 -0.847735982 2.594221696
C 1.990915889 2.200823787 1.610766743
C 2.000509373 2.206009037 -1.593421880
C 2.001433789 -0.837608815 -2.588125123
C -1.914360475 -0.994024819 -0.719845695
C -1.905767669 -0.993046972 0.722044410
C -1.907981665 0.379477775 1.165372719
C -1.917722391 1.223627468 -0.003647414
C -1.929428185 0.374723669 -1.167060106
C -1.986403612 -2.203675196 -1.605313898
C -1.977249728 -2.204766404 1.604441545
C -1.982398949 0.846094003 2.589659537
C -1.993549048 2.722577845 -0.013402636
C -2.026044569 0.835527438 -2.598163249
H 3.040677900 -3.048176088 0.004677476
H 1.521853039 -3.155744102 -0.887759479
H 1.513079892 -3.158226552 0.881680104
H 3.050472868 -0.932013130 -2.895360616
H 1.524858890 -0.130319705 -3.271648700
H 1.530636214 -1.813780239 -2.727246742
H 3.049331206 2.463679483 -1.786823252
H 1.530273095 3.075917130 -1.128623846
H 1.522796893 2.038913891 -2.562148899
H 3.039401455 2.458309750 1.806034105
H 1.511142802 2.028937546 2.577339439
H 1.521141494 3.072313311 1.148312904
H 3.031032304 -0.949166131 2.903101802
H 1.507323239 -1.822287571 2.727792933
H 1.507756089 -0.140533663 3.278204589
H -1.500977771 0.141962398 3.272688940
H -3.029779018 0.942233312 2.901688304
H -1.511150557 1.823254046 2.721057568
H -1.503209007 -3.072830739 1.139762745
H -3.023969132 -2.468299400 1.800768918
H -1.496934537 -2.031651139 2.570575265

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H -1.508959541 3.145620869 -0.896853257
H -1.524539629 3.157976910 0.872302275
H -3.041180303 3.048914532 -0.022357763
H -1.047766123 0.972010398 -3.070749241
H -2.555645003 1.789624578 -2.660744120
H -2.580443818 0.109828188 -3.198960421
H -1.514952563 -3.073882307 -1.142188749
H -1.502115447 -2.027581363 -2.569023353
H -3.033149122 -2.466146035 -1.804151467

```

Ru(Cp*)₂ - 19(0)

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Ru 0.001615294 -0.000199420 0.001614305
C 1.869271535 -1.225700395 0.002908808
C 1.864907644 -0.380038332 1.169631282
C 1.867649059 0.990911214 0.725931724
C 1.874162867 0.992037636 -0.714605793
C 1.875148746 -0.377317686 -1.161266816
C 1.960006118 -2.724894640 0.001549154
C 1.951530502 -0.845312215 2.595048728
C 1.956885176 2.202756277 1.608894839
C 1.966112412 2.205206545 -1.595159414
C 1.968592767 -0.838815495 -2.587284053
C -1.867973738 -0.991369973 -0.722621838
C -1.863407585 -0.991538802 0.718163392
C -1.864988642 0.379616860 1.161954125
C -1.870877741 1.223990720 -0.005596465
C -1.880397132 0.376772444 -1.168812916
C -1.953619057 -2.200728131 -1.609285792
C -1.948113933 -2.204146544 1.600091978
C -1.952089206 0.845779652 2.586931683
C -1.961022469 2.723443948 -0.013902331
C -1.995706134 0.839490106 -2.600149665
H 3.005668841 -3.063039686 0.004314523
H 1.479553456 -3.153874791 -0.882650767
H 1.474368466 -3.155423101 0.882138742
H 3.014787379 -0.939214451 -2.908394422
H 1.484577370 -0.133659206 -3.269719326
H 1.488711389 -1.812156078 -2.724727184
H 3.011996537 2.476409005 -1.795959801
H 1.485598282 3.072374398 -1.132848457
H 1.481825989 2.036696829 -2.561740485
H 3.002232905 2.474650586 1.811646330
H 1.470230595 2.031219917 2.573473704
H 1.476696341 3.070437755 1.147058304
H 2.996294260 -0.950942667 2.919188629
H 1.467471320 -1.817204750 2.728369304
H 1.467157204 -0.139517244 3.276180569
H -1.464685450 0.142059360 3.268078294
H -2.996599193 0.948899277 2.912451520
H -1.470402530 1.819166046 2.718663193
H -1.465274292 -3.069477301 1.136563228
H -2.992088425 -2.480024956 1.804098481
H -1.460508375 -2.031855317 2.564093351
H -1.467118946 3.147195023 -0.893184828
H -1.486379256 3.157046125 0.871128477
H -3.006284422 3.063237877 -0.024834016
H -1.022716612 0.972550728 -3.084798725
H -2.524111622 1.796381442 -2.659576312
H -2.562828754 0.118962549 -3.198519428
H -1.478126906 -3.070252107 -1.146296751
H -1.458340924 -2.026295273 -2.568917529
H -2.997873885 -2.471601357 -1.819799198

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Os(Cp*)₂ - 20(+)

```

Os 0.000873770 0.002066636 -0.002960191
C 1.888931026 -1.231773351 0.003199029
C 1.883548531 -0.382625497 1.175115280
C 1.888926461 0.994539117 0.730353109
C 1.897973724 0.995897747 -0.716253220
C 1.898304466 -0.379080034 -1.165365764
C 1.984355860 -2.730280284 0.002620106
C 1.972851373 -0.848201192 2.600055544
C 1.984212969 2.204378858 1.614567397
C 1.995283805 2.209977739 -1.594208382
C 1.997001807 -0.840621541 -2.590554973

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C	-1.891617892	-0.997633458	-0.722026404
C	-1.882060953	-0.997179748	0.724588798
C	-1.883335878	0.380334125	1.170025883
C	-1.893014899	1.228014412	-0.002866197
C	-1.904995561	0.376247663	-1.170436853
C	-1.982429037	-2.207812329	-1.606428634
C	-1.971107256	-2.208935667	1.607177597
C	-1.975335682	0.844682207	2.595105664
C	-1.987270234	2.726633673	-0.011167748
C	-2.023997423	0.836265679	-2.602114543
H	3.036348089	-3.040438126	0.009393708
H	1.518518196	-3.164662294	-0.884931558
H	1.507176649	-3.165426284	0.883784679
H	3.049781800	-0.936041970	-2.882962669
H	1.528344548	-0.133497018	-3.279141228
H	1.525502838	-1.815670090	-2.733284591
H	3.047701614	2.460320281	-1.774918914
H	1.523768159	3.080841415	-1.133080640
H	1.525527684	2.045784403	-2.566916389
H	3.036121105	2.450811996	1.803345519
H	1.506741467	2.035517343	2.582538414
H	1.518342014	3.078974885	1.154720655
H	3.023668218	-0.945519495	2.898728551
H	1.500035006	-1.823510907	2.736955873
H	1.499460651	-0.142198856	3.286265463
H	-1.496667693	0.141356638	3.280517701
H	-3.026430748	0.934882010	2.894795187
H	-1.508408584	1.822838747	2.732218903
H	-1.502908445	-3.080813661	1.144256222
H	-3.021515906	-2.459871211	1.797928592
H	-1.491903635	-2.040261374	2.574389944
H	-1.509080603	3.154767578	-0.895316077
H	-1.519427975	3.165283426	0.873243087
H	-3.038853498	3.038656549	-0.016533297
H	-1.055542060	0.975295611	-3.091571070
H	-2.559453445	1.787600405	-2.654631186
H	-2.588301726	0.108067929	-3.190386305
H	-1.512704150	-3.080279385	-1.146335084
H	-1.504043272	-2.035741314	-2.573503459
H	-3.033208229	-2.460352353	-1.794441294

Os(Cp*)2 - 20(0)

Os	0.002276754	0.000137900	0.000532544
C	1.864023798	-1.229130441	0.002605023
C	1.860132528	-0.381789651	1.172898922
C	1.860814982	0.993129619	0.728776637
C	1.865434417	0.995351358	-0.716175113
C	1.867449886	-0.377886047	-1.164769957
C	1.971015676	-2.727149710	0.001726049
C	1.963217591	-0.847410634	2.596990401
C	1.965592558	2.202556172	1.612882072
C	1.972770102	2.209227919	-1.593608815
C	1.976994330	-0.839703816	-2.589402442
C	-1.860301924	-0.994719601	-0.724610151
C	-1.859666740	-0.993838779	0.720186130
C	-1.860218605	0.381151943	1.164592176
C	-1.860567383	1.227663824	-0.006590969
C	-1.868286737	0.377380995	-1.173465878
C	-1.963331204	-2.204562363	-1.608268654
C	-1.963839178	-2.204147342	1.603317508
C	-1.966429907	0.846433165	2.588566358
C	-1.966792531	2.725680698	-0.013990380
C	-2.008234005	0.838346537	-2.603877058
H	3.020700156	-3.052381477	0.003882883
H	1.493189164	-3.160193998	-0.881586690
H	1.489659377	-3.160760399	0.882864321
H	3.027222136	-0.938659211	-2.897205930
H	1.498195890	-0.135168005	-3.275569343
H	1.498532785	-1.813063570	-2.729845625
H	3.022463139	2.472281960	-1.784567990
H	1.493453475	3.077021596	-1.131925056
H	1.493279615	2.044851680	-2.562882070
H	3.014826202	2.465033799	1.807320238
H	1.483890742	2.031325113	2.579687234
H	1.486937221	3.073083870	1.155612321
H	3.012116234	-0.948861435	2.908697090

H	1.483046624	-1.820507059	2.733449886
H	1.482150028	-0.143498430	3.281887398
H	-1.485353542	0.142842216	3.273927740
H	-3.015779314	0.946594478	2.899041828
H	-1.487265027	1.819950602	2.725915706
H	-1.485648814	-3.074142436	1.144317636
H	-3.012705780	-2.467048128	1.799066238
H	-1.480549072	-2.034064596	2.569583507
H	-1.477502120	3.153213980	-0.893701338
H	-1.494255989	3.161835314	0.870619055
H	-3.016122581	3.052589429	-0.022992933
H	-1.045052337	0.979244004	-3.103534261
H	-2.547334161	1.789831862	-2.653678834
H	-2.580162334	0.112150825	-3.190687497
H	-1.490474717	-3.075844241	-1.146374636
H	-1.473083975	-2.034673853	-2.571022489
H	-3.012058439	-2.465471910	-1.808736336

Fe(bpy)3 - 21(+3)

Fe	0.000000000	0.000000000	0.005908671
N	-1.721890419	1.027819353	0.066764309
N	-0.918780413	-1.027378521	1.462286730
C	-2.628834861	0.568600610	0.976157516
C	-3.887718801	1.163414882	1.096103002
C	-4.219520394	2.242979088	0.275245482
C	-3.281123628	2.705979949	-0.650005528
C	-2.045172664	2.069554413	-0.726683209
C	-2.164996297	-0.573962503	1.782444185
C	-2.905829993	-1.175242689	2.803447694
C	-2.363375793	-2.255103786	3.502776764
C	-1.087411912	-2.711572822	3.164030836
C	-0.395459661	-2.068916574	2.140942004
H	-4.606554781	0.792172636	1.816921606
H	-5.194712053	2.713118545	0.358444559
H	-3.495640128	3.543814791	-1.304872643
H	-1.291467035	2.399318594	-1.430075579
H	-3.893667533	-0.809034867	3.056848953
H	-2.929360194	-2.730671492	4.298034663
H	-0.629342123	-3.549382326	3.678838119
H	0.594650745	-2.393824292	1.848109502
N	0.918780413	1.027378521	1.462286730
N	1.721890419	-1.027819353	0.066764309
C	2.164996297	0.573962503	1.782444185
C	0.395459661	2.068916574	2.140942004
C	2.628834861	-0.568600610	0.976157516
C	2.045172664	-2.069554413	-0.726683209
C	2.905829993	1.175242689	2.803447694
C	1.087411912	2.711572822	3.164030836
H	-0.594650745	2.393824292	1.848109502
C	3.887718801	-1.163414882	1.096103002
C	3.281123628	-2.705979949	-0.650005528
H	1.291467035	-2.399318594	-1.430075579
C	2.363375793	2.255103786	3.502776764
H	3.893667533	0.809034867	3.056848953
H	0.629342123	3.549382326	3.678838119
C	4.219520394	-2.242979088	0.275245482
H	4.606554781	-0.792172636	1.816921606
H	3.495640128	-3.543814791	-1.304872643
H	2.929360194	2.730671492	4.298034663
H	5.194712053	-2.713118545	0.358444559
N	-0.806993930	-1.026833940	-1.520068013
N	0.806993930	1.026833940	-1.520068013
C	-0.466618248	-0.569963372	-2.759543070
C	-0.988080232	-1.165174881	-3.911524460
C	-1.866991489	-2.243242726	-3.791453796
C	-2.205528623	-2.704095945	-2.517068919
C	-1.658111592	-2.067176941	-1.406516368
C	0.466618248	0.569963372	-2.759543070
C	0.988080232	1.165174881	-3.911524460
C	1.866991489	2.243242726	-3.791453796
C	2.205528623	2.704095945	-2.517068919
C	1.658111592	2.067176941	-1.406516368
H	-0.718257333	-0.795386968	-4.893659774
H	-2.278962510	-2.713834088	-4.679054917
H	-2.881621713	-3.540899926	-2.377553628
H	-1.895520704	-2.396008408	-0.403004264

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H	0.718257333	0.795386968	-4.893659774
H	2.278962510	2.713834088	-4.679054917
H	2.881621713	3.540899926	-2.377553628
H	1.895520704	2.396008408	-0.403004264

Fe(bpy)3 - 21(+2)

Fe	0.000000000	0.000000000	0.002713920
N	-1.730882853	1.047735108	0.098245428
N	-0.949185024	-1.050455086	1.450891078
C	-2.638186332	0.579531706	0.996257422
C	-3.897780525	1.172429985	1.135798844
C	-4.231288569	2.268157543	0.341065395
C	-3.294831002	2.746845695	-0.575964975
C	-2.060723446	2.106837202	-0.664179132
C	-2.181163154	-0.582644208	1.787250287
C	-2.933025563	-1.176941985	2.806574191
C	-2.412907332	-2.274280061	3.491214995
C	-1.150362447	-2.752871325	3.138986354
C	-0.455274577	-2.111094388	2.116378034
H	-4.614367604	0.785907234	1.850452105
H	-5.205165453	2.737600456	0.437483181
H	-3.509757267	3.597366203	-1.213571150
H	-1.306272687	2.446789006	-1.362617592
H	-3.910476949	-0.790475333	3.069084762
H	-2.984679266	-2.745166975	4.284563497
H	-0.706818112	-3.604930689	3.642332328
H	0.526618937	-2.451573489	1.812320418
N	0.949185024	1.050455086	1.450891078
N	1.730882853	-1.047735108	0.098245428
C	2.181163154	0.582644208	1.787250287
C	0.455274577	2.111094388	2.116378034
C	2.638186332	-0.579531706	0.996257422
C	2.060723446	-2.106837202	-0.664179132
C	2.933025563	1.176941985	2.806574191
C	1.150362447	2.752871325	3.138986354
H	-0.526618937	2.451573489	1.812320418
C	3.897780525	-1.172429985	1.135798844
C	3.294831002	-2.746845695	-0.575964975
H	1.306272687	-2.446789006	-1.362617592
C	2.412907332	2.274280061	3.491214995
H	3.910476949	0.790475333	3.069084762
H	0.706818112	3.604930689	3.642332328
C	4.231288569	-2.268157543	0.341065395
H	4.614367604	-0.785907234	1.850452105
H	3.509757267	-3.597366203	-1.213571150
H	2.984679266	2.745166975	4.284563497
H	5.205165453	-2.737600456	0.437483181
N	-0.780841131	-1.049818930	-1.547156579
N	0.780841131	1.049818930	-1.547156579
C	-0.457853699	-0.580106391	-2.781760570
C	-0.968567701	-1.170324418	-3.943077765
C	-1.824086375	-2.265645352	-3.835899578
C	2.148721595	2.746434001	-2.566857911
C	1.606554919	2.108775333	-1.453172950
C	0.457853699	0.580106391	-2.781760570
C	0.968567701	1.170324418	-3.943077765
C	1.824086375	2.265645352	-3.835899578
C	2.148721595	2.746434001	-2.566857911
C	1.606554919	2.108775333	-1.453172950
H	-0.708700894	-0.781813964	-4.920454780
H	-2.228732957	-2.733042806	-4.728070356
H	-2.808524019	-3.596970557	-2.435234385
H	-1.833258415	-2.450955491	-0.451149956
H	0.708700894	0.781813964	-4.920454780
H	2.228732957	2.733042806	-4.728070356
H	2.808524019	3.596970557	-2.435234385
H	1.833258415	2.450955491	-0.451149956

Ru(bpy)3 - 22(+3)

Ru	0.000000000	0.000000000	-0.000137844
N	-1.854745209	1.025391467	0.093542414
N	-1.008493292	-1.025486430	1.559109947
C	-2.735778212	0.566809743	1.033225603
C	-3.997732452	1.154771628	1.166534343
C	-4.359003526	2.216155942	0.334582927

C	-3.449437207	2.670784305	-0.623717340
C	-2.209963699	2.045506312	-0.716396074
C	-2.261011664	-0.564063315	1.855595547
C	-3.006266114	-1.150283295	2.883555901
C	-2.467876323	-2.213728064	3.610070508
C	-1.185502859	-2.672188009	3.297481318
C	-0.485963126	-2.047884419	2.269368363
H	-4.699342198	0.792072741	1.907915046
H	-5.336653287	2.677644741	0.433437195
H	-3.690020461	3.492568245	-1.289526861
H	-1.473585465	2.363252245	-1.444777782
H	-3.997469583	-0.785038060	3.123163300
H	-3.041730437	-2.674341771	4.408283129
H	-0.730630807	-3.496259907	3.836428429
H	0.511384442	-2.368261517	1.992936810
N	1.008493292	1.025486430	1.559109947
N	1.854745209	-1.025391467	0.093542414
C	2.261011664	0.564063315	1.855595547
C	0.485963126	2.047884419	2.269368363
C	2.735778212	-0.566809743	1.033225603
C	2.209963699	-2.045506312	-0.716396074
C	3.006266114	1.150283295	2.883555901
C	1.185502859	2.672188009	3.297481318
H	-0.511384442	2.368261517	1.992936810
C	3.997732452	-1.154771628	1.166534343
C	3.449437207	-2.670784305	-0.623717340
H	1.473585465	-2.363252245	-1.444777782
C	2.467876323	2.213728064	3.610070508
H	3.997469583	0.785038060	3.123163300
H	0.730630807	3.496259907	3.836428429
C	4.359003526	-2.216155942	0.334582927
H	4.699342198	-0.792072741	1.907915046
H	3.690020461	-3.492568245	-1.289526861
H	3.041730437	2.674341771	4.408283129
H	5.336653287	-2.677644741	0.433437195
N	-0.845239055	-1.026089733	-1.653630001
N	0.845239055	1.026089733	-1.653630001
C	-0.474323488	-0.565791771	-2.886665854
C	-0.990639384	-1.153037344	-4.046190765
C	-1.889683831	-2.215901963	-3.943082755
C	-2.262024050	-2.672709565	-2.676206639
C	-1.722239395	-2.047865300	-1.556277018
C	0.474323488	0.565791771	-2.886665854
C	0.990639384	1.153037344	-4.046190765
C	1.889683831	2.215901963	-3.943082755
C	2.262024050	2.672709565	-2.676206639
C	1.722239395	2.047865300	-1.556277018
H	-0.701250636	-0.788845473	-5.024438812
H	-2.293399121	-2.676997823	-4.839140445
H	-2.957150519	-3.495942862	-2.551724029
H	-1.982778672	-2.367307373	-0.554365181
H	0.701250636	0.788845473	-5.024438812
H	2.293399121	2.676997823	-4.839140445
H	2.957150519	3.495942862	-2.551724029
H	1.982778672	2.367307373	-0.554365181

Ru(bpy)3 - 22(+2)

Ru	0.000000000	0.000000000	-0.001604596
N	-1.835921373	1.051635694	0.124901323
N	-1.024010100	-1.052839018	1.526487171
C	-2.726979747	0.576856568	1.042772977
C	-3.988526310	1.166227340	1.189917765
C	-4.343256689	2.252247622	0.391561618
C	-3.423570320	2.730882903	-0.543250073
C	-2.186031030	2.102184921	-0.643746744
C	-2.262186412	-0.575584677	1.845137015
C	-3.015759305	-1.162132022	2.868697314
C	-2.499794324	-2.248166511	3.573442770
C	-1.233135879	-2.729978793	3.237862477
C	-0.531613982	-2.103891271	2.212076782
H	-4.693127959	0.781940458	1.917302587
H	-5.319525086	2.713954686	0.498510874
H	-3.653870533	3.573617663	-1.185821102
H	-1.440529256	2.438695877	-1.354585990
H	-3.995970407	-0.775844543	3.120053547
H	-3.077011068	-2.707740017	4.369198334

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H	-0.790540023	-3.572903437	3.757177031	H	1.408624780	-2.470143103	-1.318009700
H	0.454533968	-2.442629370	1.917180469	C	2.562537574	2.338925270	3.462218156
N	1.024010100	1.052839018	1.526487171	H	4.045921970	0.854197288	3.034306743
N	1.835921373	-1.051635694	0.124901323	H	0.846618370	3.670714729	3.638031142
C	2.262186412	0.575584677	1.845137015	C	4.280506839	-2.340659864	0.492186566
C	0.531613982	2.103891271	2.212076782	H	4.647133423	-0.860061085	1.995929446
C	2.726979747	-0.576856568	1.042772977	H	3.580873296	-3.667206309	-1.089079479
C	2.186031030	-2.102184921	-0.643746744	H	3.160528657	2.833826952	4.220474765
C	3.015759305	1.162132022	2.868697314	H	5.235579512	-2.836251417	0.632777467
C	1.233135879	2.729978793	3.237862477	N	-0.784291306	-1.067713678	-1.641110648
H	-0.454533968	2.442629370	1.917180469	N	0.784291306	1.067713678	-1.641110648
C	3.988526310	-1.166227340	1.189917765	C	-0.430205971	-0.588562874	-2.880362368
C	3.423570320	-2.730882903	-0.543250073	C	-0.889782767	-1.231077104	-4.047024117
H	1.440529256	-2.438695877	-1.354585990	C	-1.715369251	-2.340047202	-3.951644253
C	2.499794324	2.248166511	3.573442770	C	-2.081464214	-2.809396848	-2.678307828
H	3.995970407	0.775844543	3.120053547	C	-1.592836527	-2.145131646	-1.562535105
H	0.790540023	3.572903437	3.757177031	C	0.430205971	0.588562874	-2.880362368
C	4.343256689	-2.252247622	0.391561618	C	0.889782767	1.231077104	-4.047024117
H	4.693127959	-0.781940458	1.917302587	C	1.715369251	2.340047202	-3.951644253
H	3.653870533	-3.573617663	-1.185821102	C	2.081464214	2.809396848	-2.678307828
H	3.077011068	2.707740017	4.369198334	C	1.592836527	2.145131646	-1.562535105
H	5.319525086	-2.713954686	0.498510874	H	-0.599324613	-0.857819582	-5.021760312
N	-0.809165689	-1.052723054	-1.655342638	H	-2.072350396	-2.835230119	-4.848791579
N	0.809165689	1.052723054	-1.655342638	H	-2.731064262	-3.668323200	-2.554070176
C	-0.463476851	-0.576284869	-2.886308886	H	-1.841149240	-2.471704707	-0.559169566
C	-0.970372199	-1.163463921	-4.051707489	H	0.599324613	0.857819582	-5.021760312
C	-1.838785397	-2.249410811	-3.958666413	H	2.072350396	2.835230119	-4.848791579
C	-2.184841678	-2.730045876	-2.694453581	H	2.731064262	3.668323200	-2.554070176
C	-1.649734992	-2.103245765	-1.572943837	H	1.841149240	2.471704707	-0.559169566
C	0.463476851	0.576284869	-2.886308886				
C	0.970372199	1.163463921	-4.051707489				
C	1.838785397	2.249410811	-3.958666413				
C	2.184841678	2.730045876	-2.694453581				
C	1.649734992	2.103245765	-1.572943837				
H	-0.696084687	-0.777486296	-5.025847110				
H	-2.237191843	-2.709656935	-4.857079916				
H	-2.856467081	-3.572711208	-2.572076141				
H	-1.889665935	-2.441161794	-0.571681561				
H	0.696084687	0.777486296	-5.025847110				
H	2.237191843	2.709656935	-4.857079916				
H	2.856467081	3.572711208	-2.572076141				
H	1.889665935	2.441161794	-0.571681561				
=====							
Ru (bpy) 3 - 22(+)							
=====							
Ru	0.000000000	0.000000000	-0.000267133	Ru	0.000000000	0.000000000	0.003706865
N	-1.814849584	1.067950918	0.140563101	N	-1.796186279	1.083380309	0.155816770
N	-1.028711756	-1.067367515	1.498739995	N	-1.037335751	-1.080655285	1.478607873
C	-2.709307852	0.589660643	1.068770401	C	-2.698964065	0.599482097	1.091354766
C	-3.949259570	1.232434890	1.255524630	C	-3.915688652	1.292126830	1.314512854
C	-4.280506839	2.340659864	0.492186566	C	-4.223758026	2.419932882	0.582670160
C	-3.362637467	2.808988595	-0.463838191	C	-3.307627542	2.877990795	-0.393279969
C	-2.152354438	2.144425043	-0.599852336	C	-2.121969203	2.181598624	-0.557948540
C	-2.278085962	-0.587017949	1.813864101	C	-2.301219924	-0.597205483	1.784482627
C	-3.057541512	-1.228901247	2.796473332	C	-3.109042325	-1.290835778	2.720487947
C	-2.562537574	-2.338925270	3.462218156	C	-2.633773372	-2.419866855	3.354449167
C	-1.278135139	-2.810146488	3.139661672	C	-1.328601258	-2.877843507	3.056974149
C	-0.556831848	-2.145949014	2.158126977	C	-0.586790346	-2.180053527	2.118677787
H	-4.647133423	0.860061085	1.995929446	H	-4.603562896	0.933609878	2.072264343
H	-5.235579512	2.836251417	0.632777467	H	-5.155904079	2.948721703	0.757737642
H	-3.580873296	3.667206309	-1.089079479	H	-3.513600025	3.749077705	-1.005001981
H	-1.408624780	2.470143103	-1.318009700	H	-1.379226064	2.498401392	-1.282373175
H	-4.045921970	-0.854197288	3.034306743	H	-4.110706029	-0.932545902	2.930885553
H	-3.160528657	-2.833826952	4.220474765	H	-3.256531173	-2.949818095	4.068890657
H	-0.846618370	3.670714729	3.638031142	H	-0.905604697	-3.750378259	3.541881331
H	0.435121706	-2.473978735	1.869145622	H	0.413211856	-2.497122441	1.842573421
N	1.028711756	1.067367515	1.498739995	N	1.037335751	1.080655285	1.478607873
N	1.814849584	-1.067950918	0.140563101	N	1.796186279	-1.083380309	0.155816770
C	2.78085962	0.587017949	1.813864101	C	2.301219924	0.597205483	1.784482627
C	0.556831848	2.145949014	2.158126977	C	0.586790346	2.180053527	2.118677787
C	2.709307852	-0.589660643	1.068770401	C	2.698964065	-0.599482097	1.091354766
C	2.152354438	-2.144425043	-0.599852336	C	2.121969203	-2.181598624	-0.557948540
C	3.057541512	1.228901247	2.796473332	C	3.109042325	1.290835778	2.720487947
C	1.278135139	2.810146488	3.139661672	C	1.328601258	2.877843507	3.056974149
H	-0.435121706	-2.473978735	1.869145622	H	-0.413211856	-2.497122441	1.842573421
C	3.949259570	-1.232434890	1.255524630	C	3.915688652	-1.292126830	1.314512854
C	3.362637467	-2.808988595	-0.463838191	C	3.307627542	-2.877990795	-0.393279969
				H	1.379226064	-2.498401392	-1.282373175
				C	2.633773372	2.419866855	3.354449167
				H	4.110706029	0.932545902	2.930885553
				H	0.905604697	3.750378259	3.541881331
				C	4.223758026	-2.419932882	0.582670160
				H	4.603562896	-0.933609878	2.072264343
				H	3.513600025	-3.749077705	-1.005001981
				H	3.256531173	2.949818095	4.068890657
				H	5.155904079	-2.948721703	0.757737642
				N	-0.762262284	-1.082189152	-1.628632504
				N	0.762262284	1.082189152	-1.628632504
				C	-0.398431380	-0.598987675	-2.877224253
				C	-0.805790011	-1.294139378	-4.043913984

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C -1.590119212 -2.424561246 -3.947419035
C -1.981890094 -2.882202872 -2.667273008
C -1.539807866 -2.183056274 -1.556703959
C 0.398431380 0.598987675 -2.877224253
C 0.805790011 1.294139378 -4.043913984
C 1.590119212 2.424561246 -3.947419035
C 1.981890094 2.882202872 -2.667273008
C 1.539807866 2.183056274 -1.556703959
H -0.489080541 -0.936198321 -5.017364708
H -1.897817190 -2.955780116 -4.843146875
H -2.611708774 -3.755670810 -2.542003983
H -1.799406717 -2.499801617 -0.552264822
H 0.489080541 0.936198321 -5.017364708
H 1.897817190 2.955780116 -4.843146875
H 2.611708774 3.755670810 -2.542003983
H 1.799406717 2.499801617 -0.552264822

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Ru (bpy)3 - 22 (-1)

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=====
Ru 0.000000000 0.000000000 -0.001258980
N -1.808871383 1.081716087 0.136925990
N -1.024345611 -1.066049854 1.504526381
C -2.723419938 0.568730650 1.065483142
C -3.983794772 1.219825218 1.222279289
C -4.303358320 2.328216645 0.472493709
C -3.363746755 2.825806897 -0.470640723
C -2.150758495 2.160963761 -0.587985841
C -2.300706778 -0.572197575 1.803154549
C -3.073265119 -1.227278773 2.808429118
C -2.569048329 -2.309146343 3.493198112
C -1.259698679 -2.775158364 3.192928947
C -0.550079278 -2.114622090 2.199150415
H -4.695162866 0.831376233 1.944544902
H -5.267301759 2.815310395 0.601840879
H -3.574714307 3.690253989 -1.090859287
H -1.395697073 2.493759749 -1.294065706
H -4.069686784 -0.860394823 3.034846296
H -3.167826812 -2.798295054 4.258328987
H -0.816716514 -3.618545913 3.711626454
H 0.452064165 -2.428899862 1.922767410
N 1.024345611 1.066049854 1.504526381
N 1.808871383 -1.081716087 0.136925990
C 2.300706778 0.572197575 1.803154549
C 0.550079278 2.114622090 2.199150415
C 2.723419938 -0.568730650 1.065483142
C 2.150758495 -2.160963761 -0.587985841
C 3.073265119 1.227278773 2.808429118
C 1.259698679 2.775158364 3.192928947
H -0.452064165 2.428899862 1.922767410
C 3.983794772 -1.219825218 1.222279289
C 3.363746755 -2.825806897 -0.470640723
H 1.395697073 -2.493759749 -1.294065706
C 2.569048329 2.309146343 3.493198112
H 4.069686784 0.860394823 3.034846296
H 0.816716514 3.618545913 3.711626454
C 4.303358320 -2.328216645 0.472493709
H 4.695162866 -0.831376233 1.944544902
H 3.574714307 -3.690253989 -1.090859287
H 3.167826812 -2.798295054 4.258328987
H 5.267301759 -2.815310395 0.601840879
N -0.788950668 -1.075505290 -1.642327942
N 0.788950668 1.075505290 -1.642327942
C -0.420970211 -0.573922174 -2.894971044
C -0.897253590 -1.235883906 -4.067326296
C -1.719290466 -2.334906193 -3.970140120
C -2.097052200 -2.813293125 -2.687634041
C -1.601090519 -2.143258667 -1.575668536
C 0.420970211 0.573922174 -2.894971044
C 0.897253590 1.235883906 -4.067326296
C 1.719290466 2.334906193 -3.970140120
C 2.097052200 2.813293125 -2.687634041
C 1.601090519 2.143258667 -1.575668536
H -0.603342751 -0.864188133 -5.043921957
H -2.075513708 -2.830410320 -4.870737131
H -2.751579585 -3.669248485 -2.562786022
H -1.851534048 -2.463559871 -0.568521557
H 0.603342751 0.864188133 -5.043921957

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H 2.075513708 2.830410320 -4.870737131
H 2.751579585 3.669248485 -2.562786022
H 1.851534048 2.463559871 -0.568521557

```

=====

Os (bpy)3 - 23 (+3)

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=====
Os 0.000000000 0.000000000 0.000248565
N -1.850307839 1.017687656 0.093510491
N -1.006216044 -1.017538698 1.554899154
C -2.738630116 0.563892717 1.033223969
C -4.000428845 1.152453510 1.161276112
C -4.359968858 2.211631493 0.327150531
C -3.446847024 2.662459688 -0.629928452
C -2.208272328 2.038231301 -0.720178790
C -2.263499431 -0.562390407 1.855926463
C -3.004242234 -1.150275150 2.885731391
C -2.462027498 -2.210399520 3.612917896
C -1.177704595 -2.663115905 3.298608197
C -0.480696666 -2.039190428 2.270660685
H -4.703319837 0.790677660 1.901943096
H -5.337552244 2.673985733 0.422359723
H -3.685551575 3.482311622 -1.298826519
H -1.471060883 2.353847668 -1.448258495
H -3.996338763 -0.787420109 3.125713991
H -3.032853608 -2.672337737 4.412468812
H -0.718441829 -3.484139655 3.838589851
H 0.517611616 -2.355901924 1.994603805
N 1.006216044 1.017538698 1.554899154
N 1.850307839 -1.017687656 0.093510491
C 2.263499431 0.562390407 1.855926463
C 0.480696666 2.039190428 2.270660685
C 2.738630116 -0.563892717 1.033223969
C 2.208272328 -2.038231301 -0.720178790
C 3.004242234 1.150275150 2.885731391
C 1.177704595 2.663115905 3.298608197
H -0.517611616 2.355901924 1.994603805
C 4.000428845 -1.152453510 1.161276112
C 3.446847024 -2.662459688 -0.629928452
H 1.471060883 -2.353847668 -1.448258495
C 2.462027498 2.210399520 3.612917896
H 3.996338763 0.787420109 3.125713991
H 0.718441829 3.484139655 3.838589851
C 4.359968858 -2.211631493 0.327150531
H 4.703319837 -0.790677660 1.901943096
H 3.685551575 -3.482311622 -1.298826519
H 3.032853608 2.672337737 4.412468812
H 5.337552244 -2.673985733 0.422359723
N -0.844609471 -1.017069090 -1.649340539
N 0.844609471 1.017069090 -1.649340539
C -0.475010528 -0.563143888 -2.888485413
C -0.995020820 -1.151697505 -4.045239188
C -1.896275618 -2.211520448 -3.939641139
C -2.268021283 -2.662935982 -2.670319917
C -1.727633950 -2.038242053 -1.552413603
C 0.475010528 0.563143888 -2.888485413
C 0.995020820 1.151697505 -4.045239188
C 1.896275618 2.211520448 -3.939641139
C 2.268021283 2.662935982 -2.670319917
C 1.727633950 2.038242053 -1.552413603
H -0.705403086 -0.789556913 -5.024262903
H -2.302315127 -2.674018646 -4.833927031
H -2.965782461 -3.483574050 -2.542750567
H -1.989259209 -2.354088160 -0.549923035
H -1.989259209 -2.354088160 -0.549923035

```

=====

Os (bpy)3 - 23 (+2)

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=====
Os 0.000000000 0.000000000 -0.000025431
N -1.827781256 1.038148763 0.124197654
N -1.020709751 -1.037875987 1.518925217

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C	-2.730693352	0.572353387	1.041574124
C	-3.990740906	1.165908405	1.178285018
C	-4.340547495	2.246568592	0.372655790
C	-3.413336595	2.715910673	-0.561418000
C	-2.177182900	2.088260505	-0.654821538
C	-2.266246545	-0.571682986	1.844340799
C	-3.013268384	-1.165125829	2.868080426
C	-2.490406353	-2.246643488	3.572504268
C	-1.218867501	-2.716785445	3.233941838
C	-0.520787039	-2.089006793	2.209601169
H	-4.697252493	0.785232796	1.905891133
H	-5.315922954	2.711437166	0.471361756
H	-3.638445845	3.554675475	-1.210994875
H	-1.428531222	2.420733081	-1.363176787
H	-3.996037997	-0.783811524	3.117597312
H	-3.062769282	-2.711500828	4.368423450
H	-0.768932273	-3.556522743	3.752136553
H	0.466056461	-2.422480650	1.913560819
N	1.020709751	1.037875987	1.518925217
N	1.827781256	-1.038148763	0.124197654
C	2.266246545	0.571682986	1.844340799
C	0.520787039	2.089006793	2.209601169
C	2.730693352	-0.572353387	1.041574124
C	2.177182900	-2.088260505	-0.654821538
C	3.013268384	1.165125829	2.868080426
C	1.218867501	2.716785445	3.233941838
H	-0.466056461	2.422480650	1.913560819
C	3.990740906	-1.165908405	1.178285018
C	3.413336595	-2.715910673	-0.561418000
H	1.428531222	-2.420733081	-1.363176787
C	2.490406353	-2.246643488	3.572504268
H	3.996037997	0.783811524	3.117597312
H	0.768932273	3.556522743	3.752136553
C	4.340547495	-2.246568592	0.372655790
H	4.697252493	-0.785232796	1.905891133
H	3.638445845	-3.554675475	-1.210994875
H	3.062769282	2.711500828	4.368423450
H	5.315922954	-2.711437166	0.471361756
N	-0.805543917	-1.038058980	-1.643677069
N	0.805543917	1.038058980	-1.643677069
C	-0.463979877	-0.571668911	-2.884737098
C	-0.977599113	-1.163839525	-4.044082461
C	-1.850229984	-2.244429682	-3.944187179
C	-2.193185296	-2.715021938	-2.673980916
C	-1.654571633	-2.088527168	-1.556792217
C	0.463979877	0.571668911	-2.884737098
C	0.977599113	1.163839525	-4.044082461
C	1.850229984	2.244429682	-3.944187179
C	2.193185296	2.715021938	-2.673980916
C	1.654571633	2.088527168	-1.556792217
H	-0.702361345	-0.781886939	-5.019706119
H	-2.254097175	-2.708114403	-4.838115959
H	-2.868002333	-3.553989154	-2.543984703
H	-1.892284604	-2.422086775	-0.554348847
H	0.702361345	0.781886939	-5.019706119
H	2.254097175	2.708114403	-4.838115959
H	2.868002333	3.553989154	-2.543984703
H	1.892284604	2.422086775	-0.554348847
=====			
Fe(CN)6 - 24(-3)			
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Fe	-0.000364224	0.001951029	0.000950663
N	3.169638896	-0.023172577	-0.024670763
C	1.995781322	-0.022263545	-0.022959323
N	-3.170751252	0.027499172	0.027236162
C	-1.996788597	0.026284000	0.025164750
N	-0.025216914	3.172061493	-0.026418859
C	-0.025467078	1.998244280	-0.023562760
N	0.025461807	0.030832442	-3.169743250
C	0.024674391	0.027004442	-1.995912942
N	-0.023789721	-0.025148623	3.171797325
C	-0.024210275	-0.022374777	1.997852429
N	0.027171993	-3.168009116	0.029379890

C	0.025941694	-1.994171807	0.026018145
=====			
Fe(CN)6 - 24(-4)			
=====			
Fe	-0.000021162	0.002108959	0.001185437
N	3.226265839	0.002788787	0.000440118
C	2.043107808	0.002548663	0.000810606
N	-3.226183724	0.001668696	0.001315287
C	-2.043028528	0.001827130	0.001339389
N	-0.000832126	3.228506549	0.001171656
C	-0.000486963	2.045472821	0.001271745
N	-0.000441457	0.001524969	-3.225020334
C	-0.000267356	0.002005228	-2.041981721
N	0.000287661	0.002020630	3.227598624
C	0.000185695	0.002004377	2.044567311
N	0.000536045	-3.223892317	0.001102592
C	0.000343929	-2.040853443	0.001091629
=====			
Fe(CN)5(NO) - 25(-2)			
=====			
Ru	0.000240524	0.000437975	-0.134463023
N	3.257584112	0.001971866	0.097601641
C	2.089662852	0.000783706	0.040038706
N	-3.256689168	0.000255924	0.101731878
C	-2.088870952	-0.000180315	0.042656059
N	0.000505781	3.257666993	0.094115796
C	0.000195475	2.089725454	0.037382779
O	-0.001560843	0.010392895	-3.081428523
N	-0.000913596	0.002589424	-1.917507426
N	0.002540272	0.014671334	3.124887022
C	0.001750293	0.008299810	1.956828001
N	0.001218324	-3.257666311	0.099473917
C	0.000709718	-2.089719112	0.042576937
=====			
Fe(CN)5(NO) - 25(-3)			
=====			
Ru	0.048074531	0.026130489	-0.072231853
N	3.350347758	0.051293331	0.044757118
C	2.173986241	0.042073061	0.021805516
N	-3.235675838	0.038005031	-0.178514599
C	-2.060916982	0.024745392	-0.121580151
N	0.061586469	3.322024992	0.075287516
C	0.055762240	2.146317582	0.040258459
O	-0.510245306	-0.267134395	-3.013985774
N	0.073998053	0.025824898	-2.006368114
N	-0.109216212	-0.061926304	3.207713353
C	-0.043879475	-0.024225735	2.034893929
N	0.052077853	-3.263649292	-0.040392210
C	0.043454314	-2.087720043	-0.032320727
=====			
Ru(CN)6 - 26(-3)			
=====			
Ru	-0.000258263	0.002038490	0.000930242
N	3.281955853	-0.016628509	-0.015481426
C	2.107311522	-0.017545392	-0.016197897
N	-3.281963124	0.014959266	0.018778618
C	-2.107363782	0.019174549	0.020122346
N	-0.016582243	3.286431274	-0.027082250
C	-0.019635507	2.111994727	-0.022170040
N	0.016333883	0.032842948	-3.285664220
C	0.018747475	0.026602538	-2.110025100
N	-0.015448029	-0.022364371	3.287831851
C	-0.017772225	-0.019883719	2.112225248
N	0.016795082	-3.282051940	0.028346930
C	0.019811043	-2.107007754	0.023733985
=====			
Ru(CN)6 - 26(-4)			
=====			
Ru	0.000385919	0.002245632	0.001327913
N	3.311753046	0.003102572	-0.001177117
C	2.128160050	0.002811247	0.000152515
N	-3.310004833	0.001817317	-0.000039677
C	-2.126331616	0.001915652	0.000856491

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N	-0.001963202	3.314897935	0.002633994
C	-0.000548616	2.131133060	0.001742875
N	-0.001366185	-0.001355293	-3.309525884
C	-0.000319443	0.000767227	-2.125841515
N	-0.000912212	0.000715741	3.313069513
C	0.000084916	0.001632140	2.129410680
N	-0.000764317	-3.307950379	0.000586462
C	0.000284130	-2.124270273	0.001351496

Table S2. Computed vibrational frequencies.

=====
 Anthracene - 1(0)
 =====

99.12	129.86	236.91	240.45	275.25	389.70	395.32
396.74	483.37	487.62	509.57	534.72	594.10	615.62
640.17	661.17	750.45	761.94	765.33	777.65	787.93
824.72	854.11	873.57	904.81	918.18	919.04	927.34
977.94	982.73	1000.03	1001.47	1033.54	1037.48	1132.96
1167.90	1177.07	1192.69	1194.87	1215.93	1296.91	1299.48
1300.66	1345.74	1389.72	1421.90	1429.01	1441.76	1492.69
1495.87	1528.22	1590.80	1605.48	1635.12	1681.12	1682.86
3169.98	3171.74	3174.36	3174.80	3178.55	3179.61	3191.90
3192.13	3203.64	3204.17				

=====
 Anthracene - 1(-1)
 =====

97.24	124.39	235.17	256.88	257.22	340.65	390.25
393.97	473.82	477.47	535.08	546.48	580.77	612.98
625.93	660.08	705.85	727.43	740.97	748.47	758.87
769.01	790.10	816.01	816.38	838.29	870.12	873.34
904.95	909.62	915.81	915.83	1049.46	1050.39	1103.10
1140.46	1161.07	1173.20	1185.04	1209.47	1273.33	1283.06
1289.76	1300.80	1372.61	1401.72	1410.45	1427.17	1470.48
1480.18	1512.75	1525.32	1564.55	1567.65	1590.40	1607.56
3124.73	3125.12	3129.02	3130.85	3133.40	3137.37	3146.17
3147.15	3162.56	3164.20				

=====
 Azobenzene - 2(0)
 =====

50.12	71.01	92.39	122.06	223.72	271.20	308.00
311.54	422.56	425.82	496.24	529.86	546.90	564.01
624.51	630.56	683.61	705.92	711.83	784.84	804.43
839.20	864.72	865.58	940.07	954.62	959.90	1002.24
1002.43	1016.07	1016.28	1018.03	1018.35	1044.65	1044.66
1099.59	1103.23	1166.29	1176.53	1184.01	1184.23	1212.66
1261.53	1336.88	1344.09	1364.60	1367.11	1485.02	1493.27
1512.78	1525.73	1554.42	1633.91	1639.85	1651.81	1655.05
3180.31	3180.39	3190.59	3190.60	3201.26	3201.37	3211.55
3211.77	3227.03	3227.08				

=====
 Azobenzene - 2(-1)
 =====

54.43	72.95	92.67	152.97	223.51	264.31	292.32
313.34	432.92	436.93	501.00	531.52	531.61	541.57
623.51	629.71	667.56	702.98	704.64	739.31	744.78
839.80	840.00	841.09	877.63	881.31	916.59	963.50
964.08	978.04	980.77	996.12	997.80	1030.97	1031.17
1084.79	1088.76	1162.50	1163.17	1163.57	1163.59	1203.63
1303.25	1331.87	1332.56	1346.12	1361.70	1376.30	1484.90
1493.31	1510.29	1516.67	1580.31	1585.57	1627.86	1637.53
3126.21	3126.73	3135.72	3135.73	3167.17	3167.36	3177.87
3178.24	3218.83	3218.94				

=====
 Benzophenone - 3(0)
 =====

58.56	76.57	104.98	142.84	219.94	241.89	289.96
383.23	418.31	429.96	448.47	456.13	573.54	628.90
631.37	652.50	701.59	718.64	720.77	731.94	784.28
834.11	869.58	875.06	940.82	962.39	966.64	1001.85
1007.10	1017.15	1017.63	1018.03	1019.40	1053.21	1055.87

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1107.52	1111.91	1171.03	1187.04	1187.17	1201.87	1208.56
1297.78	1345.71	1346.64	1361.66	1363.39	1485.61	1486.23
1528.13	1532.09	1629.73	1630.88	1652.00	1653.29	1739.75
3180.93	3181.12	3191.08	3191.64	3200.98	3202.12	3210.65
3214.90	3216.96	3217.52				

=====
Benzophenone - 3(-1)
=====

63.99	77.97	118.78	155.14	223.11	250.50	298.59
384.25	420.21	434.00	442.86	467.81	560.18	624.84
631.19	632.54	641.47	698.74	708.14	721.64	740.91
760.33	832.11	850.61	873.91	879.77	930.41	959.46
979.67	979.82	988.46	988.61	1007.60	1037.13	1040.05
1089.13	1100.24	1153.68	1162.17	1169.16	1175.22	1205.28
1280.10	1316.16	1329.27	1360.57	1364.04	1464.32	1472.19
1505.28	1512.13	1520.18	1566.87	1575.54	1612.50	1652.90
3129.80	3130.60	3136.31	3136.76	3168.99	3169.76	3195.44
3207.41	3208.01	3212.28				

=====
Nitrobenzene - 4(0)
=====

72.13	178.01	262.31	399.06	424.19	454.11	529.01
624.00	695.25	698.40	723.76	815.09	863.98	864.27
970.86	1007.30	1022.38	1023.96	1046.57	1103.52	1126.49
1187.46	1198.83	1339.76	1372.34	1398.84	1498.21	1518.52
1622.80	1643.91	1675.10	3190.99	3203.45	3212.07	3244.50
3244.60						

=====
Nitrobenzene - 4(-1)
=====

127.07	168.10	255.96	403.28	404.90	446.14	525.38
570.10	625.89	651.18	690.37	697.05	795.49	816.09
820.10	941.54	949.40	990.13	1017.72	1076.46	1088.77
1154.80	1181.68	1305.84	1366.89	1401.11	1401.44	1491.60
1505.71	1558.47	1639.06	3127.64	3132.66	3168.26	3229.99
3231.62						

=====
Tetracyano-quinodimethane - 5(0)
=====

53.45	54.75	86.60	119.35	123.31	137.87	139.14
148.65	223.69	287.48	309.07	335.16	377.97	401.02
450.70	473.49	485.09	511.75	531.60	561.65	608.90
610.60	621.68	640.54	674.61	726.10	784.80	822.96
883.01	975.48	990.91	1006.79	1022.58	1024.87	1142.76
1218.37	1231.99	1237.54	1344.09	1383.98	1430.52	1485.81
1497.91	1587.40	1600.78	1678.54	2321.31	2321.75	2336.41
2338.75	3209.96	3210.30	3222.37	3223.65		

=====
Tetracyano-quinodimethane - 5(-1)
=====

43.29	60.04	83.90	103.47	122.07	136.47	143.97
150.44	230.03	289.23	338.30	346.34	386.42	422.15
486.13	488.01	502.92	526.59	544.04	553.96	614.59
626.49	627.14	634.48	640.31	741.01	756.80	834.04
863.19	985.67	996.26	1001.07	1006.18	1033.40	1146.61
1221.38	1238.31	1242.30	1349.29	1352.23	1380.84	1403.66
1517.57	1541.18	1541.96	1660.24	2257.89	2258.32	2290.47
2296.13	3186.10	3187.21	3201.05	3202.85		

=====
Tetracyano-quinodimethane - 5(-2)
=====

27.70	62.83	76.55	79.70	125.90	133.95	146.02
150.11	228.58	288.72	338.08	370.61	393.07	422.24
520.68	526.87	527.52	538.83	542.81	556.92	611.92
624.05	646.91	647.25	654.98	741.11	744.12	841.21
848.89	948.14	970.35	1011.93	1015.77	1056.36	1135.61
1214.06	1257.39	1262.34	1315.57	1324.72	1331.35	1353.48
1466.28	1542.88	1581.03	1664.80	2206.80	2207.90	2248.35
2259.93	3151.74	3152.80	3169.37	3172.32		

=====
Tetrathiafulvalene - 6(+2)
=====

45.46	110.17	113.92	228.80	268.78	277.94	448.04
450.40	453.20	517.52	541.91	553.48	642.60	650.41
758.72	760.79	764.78	771.60	870.11	872.15	872.59
911.00	913.06	940.55	1061.31	1131.51	1131.89	1304.60
1304.67	1309.51	1474.23	1488.94	3218.34	3218.50	3230.93
3231.87						

=====
Tetrathiafulvalene - 6(+1)
=====

65.10	89.90	127.16	149.85	268.59	306.83	331.70
425.91	436.76	473.65	509.58	530.95	631.13	640.65
702.31	703.35	745.43	756.28	824.22	837.28	838.06
888.21	890.13	891.88	1039.64	1130.92	1131.05	1295.26
1299.63	1449.62	1547.67	1567.37	3242.76	3242.92	3258.27
3258.47						

=====
Tetrathiafulvalene - 6(0)
=====

20.03	88.77	97.81	114.90	245.62	254.54	308.77
417.95	421.35	438.67	472.90	511.82	618.38	628.07
650.37	650.60	739.26	741.80	775.15	801.75	810.24
845.05	868.47	868.52	985.93	1125.99	1126.32	1290.03
1292.62	1594.94	1618.94	1641.10	3231.83	3232.04	3250.92
3250.99						

=====
Ferrocene - 7(+1)
=====

33.94	103.68	112.68	283.27	328.43	328.99	350.05
354.21	458.12	530.13	531.03	553.55	553.98	828.68
829.07	836.62	837.92	846.42	846.53	858.54	858.59
864.98	878.77	905.19	908.81	913.43	913.52	1028.83
1028.97	1029.35	1029.41	1079.41	1079.48	1090.72	1115.23
1128.36	1130.94	1293.81	1294.63	1378.44	1382.43	1386.82
1386.85	1457.74	1457.77	1460.68	1461.68	3263.38	3263.49
3264.17	3265.70	3273.74	3273.75	3274.01	3274.10	3283.01
3283.79						

=====
Ferrocene - 7(0)
=====

39.95	57.97	58.25	189.61	279.44	352.16	352.93
384.83	384.92	560.81	561.98	585.95	586.64	806.06
806.30	816.05	825.26	839.29	839.80	841.10	841.17
855.30	855.94	881.41	882.15	885.15	885.19	1024.99
1025.33	1030.71	1030.93	1077.11	1077.20	1077.53	1078.02
1135.92	1136.12	1290.69	1291.45	1385.81	1390.11	1405.21
1405.32	1464.80	1464.84	1465.13	1466.21	3244.79	3244.86
3244.99	3245.08	3258.93	3258.99	3259.63	3259.72	3270.80
3271.08						

=====

Ru(bpy)3 - 22(+3)

=====

47.55	48.00	50.65	52.12	53.60	63.19	94.22
94.43	98.11	114.43	117.27	128.66	152.76	170.57
173.09	173.56	190.49	191.54	227.62	228.87	248.23
266.08	267.25	271.83	283.92	319.54	325.64	337.93
361.13	368.09	431.55	431.61	436.39	437.14	438.27
449.81	457.30	466.43	467.00	475.57	485.72	487.84
559.96	560.07	563.05	649.56	653.32	655.03	655.51
656.82	657.47	666.29	671.38	672.78	739.48	742.90
743.62	755.69	761.48	761.77	764.49	772.74	773.78
790.31	791.46	791.49	821.25	821.69	823.48	912.73
912.94	914.43	917.49	917.75	920.25	991.85	992.23
993.44	994.14	994.44	995.35	1011.80	1023.44	1026.18
1032.51	1036.37	1041.24	1041.32	1041.46	1044.14	1045.17
1045.24	1045.30	1050.82	1055.24	1055.77	1084.12	1085.71
1085.84	1090.46	1093.21	1093.44	1134.35	1135.30	1137.27
1150.48	1152.08	1152.21	1196.67	1196.79	1197.16	1208.44
1208.56	1209.18	1292.34	1294.43	1297.05	1297.13	1297.86
1301.47	1322.97	1323.78	1324.09	1338.32	1342.37	1342.59
1343.03	1343.57	1343.99	1461.98	1462.89	1463.21	1481.59
1483.31	1483.71	1496.72	1500.93	1500.96	1526.41	1526.54
1526.73	1602.10	1602.45	1603.08	1610.59	1610.85	1611.18
1633.41	1633.55	1633.77	1640.11	1640.21	1641.22	3220.24
3220.43	3221.00	3221.03	3221.30	3221.73	3230.19	3230.30
3230.73	3230.86	3230.99	3231.43	3235.53	3235.76	3236.23
3242.51	3242.68	3242.89	3242.93	3243.08	3243.21	3246.57
3246.83	3247.24					

=====

Ru(bpy)3 - 22(+2)

=====

46.65	46.84	47.79	50.05	50.73	61.79	92.72
92.84	97.08	121.49	121.84	128.66	148.65	169.95
172.06	172.65	191.46	191.70	227.38	228.85	255.25
273.88	274.51	281.60	313.46	321.73	323.74	339.27
363.27	367.33	436.52	436.95	442.23	446.57	446.99
459.61	462.53	477.59	479.48	489.47	490.62	494.06
567.64	567.89	569.60	640.61	646.83	648.79	657.28
659.04	660.81	661.04	665.16	670.38	746.89	749.69
750.44	759.53	762.33	762.52	765.07	776.56	776.92
785.69	786.69	786.80	823.69	824.59	826.09	906.96
907.20	908.75	914.17	914.37	916.72	985.05	985.47
986.87	987.30	987.51	988.81	1012.40	1025.37	1025.52
1025.69	1025.92	1026.10	1029.58	1029.71	1030.05	1030.51
1033.94	1043.79	1050.15	1055.90	1057.25	1084.55	1086.19
1086.39	1090.71	1093.82	1093.95	1132.49	1133.64	1134.81
1147.78	1149.50	1150.10	1190.15	1190.28	1190.48	1202.37
1202.47	1203.00	1291.73	1293.70	1297.56	1297.68	1298.22
1298.70	1318.34	1318.54	1318.63	1330.96	1336.73	1337.17
1339.82	1339.87	1341.25	1461.27	1462.73	1463.22	1480.90
1482.96	1483.06	1499.01	1503.86	1505.12	1522.92	1522.96
1523.61	1606.62	1606.93	1607.42	1616.02	1616.20	1616.96
1642.62	1642.64	1642.92	1647.68	1649.48	1650.02	3215.58
3215.84	3216.04	3216.72	3216.90	3217.07	3225.41	3225.53
3225.78	3226.64	3226.79	3226.91	3231.79	3232.04	3232.37
3237.99	3238.06	3238.27	3238.76	3238.84	3238.94	3242.81
3243.10	3243.53					

=====
 Ru(bpy)3 - 22(+1)
 =====

45.33	45.66	46.00	46.30	47.29	56.63	89.51
89.60	96.04	118.28	118.57	127.96	150.52	172.09
175.63	176.40	188.41	188.79	227.36	228.83	250.86
269.21	269.42	283.34	315.83	321.61	322.61	341.50
365.81	369.09	431.68	432.45	434.82	440.10	440.18
456.41	459.43	469.52	470.88	486.96	489.25	490.84
555.58	555.62	556.83	636.18	640.56	640.99	654.53
656.94	657.83	660.06	664.46	670.07	722.29	724.76
725.59	744.23	744.52	750.87	754.06	766.08	767.03
767.39	772.11	773.02	797.99	798.47	800.55	877.93
878.39	881.82	885.31	885.35	888.07	966.49	968.27
971.01	971.41	974.09	974.41	976.24	977.86	991.05
991.20	991.75	997.94	998.02	998.25	1000.00	1014.45
1016.72	1038.73	1046.91	1051.51	1052.79	1070.83	1072.54
1072.74	1073.92	1077.67	1077.95	1128.36	1129.80	1129.99
1148.72	1149.98	1151.95	1161.69	1162.78	1181.74	1181.80
1182.26	1197.70	1272.04	1274.94	1276.25	1287.50	1289.79
1304.38	1305.01	1307.03	1318.49	1325.45	1326.30	1332.71
1332.89	1333.65	1354.08	1421.74	1422.79	1454.11	1458.38
1459.23	1473.75	1475.82	1476.08	1493.30	1498.96	1500.13
1525.52	1571.51	1572.15	1583.20	1583.27	1586.41	1587.95
1606.97	1607.56	1615.39	1630.37	1632.40	1632.90	3206.75
3206.80	3207.08	3208.47	3208.52	3208.69	3219.03	3219.10
3219.35	3220.36	3220.53	3221.09	3224.46	3224.51	3224.85
3232.19	3232.23	3232.42	3234.52	3234.57	3234.77	3235.73
3235.87	3236.23					

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 Ru(bpy)3 - 22(0)
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43.45	43.81	48.11	49.83	50.17	53.66	86.81
87.00	95.72	117.00	117.16	127.95	151.77	174.61
178.46	179.51	186.65	187.58	226.25	227.82	246.37
264.71	264.77	286.12	314.61	319.76	321.15	345.16
368.16	370.48	419.05	419.75	422.69	438.34	438.48
449.22	458.88	463.72	464.48	485.50	487.84	490.56
543.36	543.43	544.04	630.84	633.60	634.83	652.91
655.53	655.80	660.02	663.96	669.26	698.69	701.87
702.72	729.26	729.41	739.20	747.34	747.91	748.53
750.71	765.35	767.17	770.09	770.85	772.86	841.27
842.06	845.51	845.83	847.75	848.31	956.94	957.11
957.55	960.74	960.98	963.71	964.14	964.30	968.32
969.44	969.52	970.75	982.19	989.14	995.90	1005.38
1006.24	1032.97	1042.19	1044.61	1045.47	1055.12	1056.82
1057.06	1058.25	1063.45	1063.52	1122.52	1124.24	1124.78
1147.94	1149.11	1150.86	1175.25	1175.32	1175.57	1175.72
1176.06	1189.61	1252.18	1256.10	1256.99	1312.26	1312.95
1318.33	1323.17	1325.30	1325.56	1325.82	1327.17	1328.67
1348.13	1351.46	1373.47	1441.49	1441.57	1452.25	1464.39
1464.70	1466.32	1468.89	1469.26	1491.81	1498.53	1499.54
1528.47	1555.40	1555.67	1558.89	1559.71	1560.51	1563.36
1596.76	1597.15	1611.98	1626.06	1628.24	1628.54	3189.04
3189.17	3189.20	3191.20	3191.32	3191.36	3206.22	3206.31
3206.48	3209.03	3209.34	3210.10	3211.20	3211.36	3211.87
3217.71	3217.75	3217.93	3225.18	3225.23	3225.53	3225.65
3225.89	3226.43					

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Ru(bpy)3 - 22(-1)

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48.65	51.56	52.89	57.43	61.20	63.24	82.80
87.19	93.96	115.78	117.31	120.19	151.88	169.92
174.06	175.98	184.07	185.03	225.33	225.84	249.12
259.97	260.51	276.89	306.90	313.64	316.33	344.75
364.10	371.52	403.06	405.43	406.28	431.74	433.59
446.59	448.72	458.46	461.87	481.54	482.75	484.77
525.95	526.84	528.08	624.23	626.91	627.56	650.81
653.11	653.58	657.17	660.93	667.21	672.39	673.31
674.86	712.13	713.28	715.61	719.33	720.76	722.03
728.26	728.83	730.39	740.75	755.55	758.65	795.08
795.80	796.40	797.11	798.44	798.48	927.37	928.46
931.44	941.37	942.98	944.15	952.65	952.92	953.23
953.58	956.25	957.71	963.37	980.89	984.01	989.97
1004.50	1021.55	1031.28	1032.33	1032.82	1040.75	1041.33
1042.88	1048.38	1053.96	1054.26	1113.76	1114.31	1116.13
1135.46	1139.12	1140.85	1164.04	1167.99	1168.37	1169.27
1172.86	1177.11	1232.74	1235.07	1238.15	1311.76	1312.36
1314.03	1323.74	1327.21	1330.44	1332.88	1335.06	1337.22
1367.13	1381.48	1385.39	1434.56	1451.46	1456.19	1457.12
1458.32	1458.70	1467.46	1490.02	1498.83	1500.10	1510.20
1517.59	1523.08	1524.64	1526.22	1538.14	1539.51	1543.06
1585.60	1608.94	1621.11	1623.08	1623.19	1625.65	3160.75
3160.96	3161.09	3162.40	3162.58	3163.06	3186.56	3186.99
3189.08	3192.77	3193.22	3193.50	3193.91	3194.10	3194.33
3198.37	3199.02	3201.53	3210.68	3210.90	3211.14	3211.30
3211.81	3212.75					

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Fe(CN)6 - 24(-3)

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100.41	100.55	110.29	123.58	124.03	124.49	134.15
152.11	189.20	283.07	318.14	319.52	319.91	339.91
347.74	355.95	358.86	389.53	412.67	426.98	449.61
458.50	464.90	466.54	478.38	496.19	657.34	2201.36
2201.55	2202.90	2206.10	2206.35	2211.64		

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Fe(CN)6 - 24(-4)

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77.36	77.42	77.58	102.98	103.21	103.26	123.97
124.19	124.21	231.62	231.80	232.03	240.80	256.63
256.78	361.42	362.32	362.39	469.41	469.69	469.71
490.65	491.09	491.14	520.25	520.46	520.48	2120.87
2121.55	2121.61	2125.56	2126.11	2143.34		

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Fe(CN)5(NO) - 25(-2)

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53.74	53.81	85.29	101.34	101.35	102.58	115.31
116.03	116.09	309.28	309.34	318.19	344.27	344.62
358.83	365.38	381.97	411.13	420.94	421.01	425.30
452.23	461.56	461.63	603.58	657.67	657.74	1911.49
2238.40	2238.43	2246.12	2250.66	2259.31		

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Fe(CN)5(NO) - 25(-3)

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22.13	83.21	89.19	96.79	103.30	105.23	113.47
115.64	123.19	204.89	279.03	292.61	295.35	326.33
333.84	344.59	350.87	359.58	392.73	437.38	443.76
447.16	455.78	490.40	498.74	508.61	552.87	1685.24
2174.78	2177.76	2186.01	2188.69	2202.85		

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Ru(CN)6 - 26(-3)

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75.84	76.63	77.46	92.83	98.82	101.38	107.02
118.16	120.32	295.60	297.83	299.83	320.28	324.88
328.49	349.77	350.95	363.13	372.88	393.37	394.03
404.54	420.17	420.45	467.30	507.83	511.65	2175.30
2181.56	2183.44	2186.41	2192.37	2203.96		

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Ru(CN)6 - 26(-4)

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88.86	88.93	88.97	106.43	106.50	106.50	122.74
122.80	122.84	247.57	247.67	248.34	325.65	325.90
332.18	357.86	357.92	357.98	469.40	469.40	469.48
485.91	485.98	486.01	544.63	544.66	544.67	2108.51
2108.89	2109.20	2121.07	2121.47	2153.02		

Table S3. Computed energy components at B3LYP/6-31G** level of theory

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
1	Anthracene	0	DMF	-14681.254	-4.68	-14681.457				
1	Anthracene	-1	DMF	-14681.376	-46.04	-14683.372	-1.915	0.165	-2.591	-1.92
2	Azobenzene	0	DMF	-15585.482	-4.88	-15585.694				
2	Azobenzene	-1	DMF	-15586.253	-50.36	-15588.436	-2.742	0.096	-1.833	-1.36
3	Benzophenone	0	AN	-15690.831	-7.99	-15691.177				
3	Benzophenone	-1	AN	-15691.044	-52.27	-15693.311	-2.134	0.112	-2.426	-1.88
4	Nitrobenzene	0	AN	-11884.395	-7.62	-11884.725				
4	Nitrobenzene	-1	AN	-11884.932	-62.74	-11887.653	-2.928	0.110	-1.633	-1.15
5	Tetracyano- quinodimethane	0	AN	-18464.518	-17.28	-18465.267				
5	Tetracyano- quinodimethane	-1	AN	-18467.870	-48.10	-18469.955	-4.688	0.024	0.041	0.127
5	Tetracyano- quinodimethane	-2	AN	-18466.852	-158.81	-18473.739	-3.784	0.032	-0.855	-0.291
6	Tetrathiafulvalene	+2	AN	-49608.359	-180.07	-49616.167				
6	Tetrathiafulvalene	+1	AN	-49619.287	-48.68	-49621.398	-5.231	0.068	0.628	0.66
6	Tetrathiafulvalene	0	AN	-49625.429	-6.66	-49625.717	-4.319	0.106	-0.246	0.3
7	Fc-(COCH3)2	+1	DMF	-22192.700	-53.09	-22195.003				
7		0	DMF	-22199.451	-10.90	-22199.924	-4.921	from 8	0.340	0.74
8	Ferrocene	+1	AN	-13884.803	-49.72	-13886.959				
8		0	AN	-13891.896	-3.71	-13892.057	-5.098	0.090	0.517	0.307
9	Cp*2Fe	+1	DMF	-24584.881	-39.10	-24586.577				
9		0	DMF	-24590.954	-2.44	-24591.060	-4.483	from 8	-0.098	-0.1
10	Cp2Co	+1	DMF	-14474.735	-46.53	-14476.752				
10		0	DMF	-14480.264	-1.14	-14480.314	-3.562	from 8	-1.019	-0.91
11	[Me3(Ph)]2Cr	+1	DMF	-21402.643	-41.73	-21404.453				
11		0	DMF	-21407.508	-0.60	-21407.534	-3.081	from 8	-1.500	-0.98
12	CpFePh - [+1]	+1	DMF	-14939.634	-48.02	-14941.716				
12		0	DMF	-14944.458	-4.17	-14944.639	-2.923	from 8	-1.658	-1.36
13	Cp*2Co - [0]	+1	DMF	-25174.900	-36.40	-25176.478				
13		0	DMF	-25179.436	-2.90	-25179.562	-3.084	from 8	-1.497	-1.43
14	CpFeAr*	+1	DMF	-21359.255	-42.56	-21361.101				
14		0	DMF	-21363.558	-4.13	-21363.737	-2.636	from 8	-1.945	-1.57
15	Cp*FeAr*	+1	DMF	-20289.683	-44.84	-20291.627				
15		0	DMF	-20294.012	-3.91	-20294.181	-2.554	from 8	-2.027	-1.85
16	Rh(Cp)2	+1	AN	-13507.490	-48.30	-13509.584				
16		0	AN	-13512.325	-3.76	-13512.488	-2.904	from 8	-1.677	-1.41
16		-1	AN	-13511.667	-51.07	-13513.877	-1.389	from 8	-3.192	-2.18
17	Cr(Cp*)2	+1	AN	-23574.418	-38.71	-23576.097				
17		0	AN	-23579.702	-3.01	-23579.833	-3.736	from 8	-0.845	-1.04
17		-1	AN	-23580.027	-37.99	-23581.675	-1.842	from 8	-2.739	-2.3
18	Mn(Cp*)2	+1	AN	-24053.187	-38.86	-24054.873				
18		0	AN	-24058.719	0.35	-24058.705	-3.832	from 8	-0.749	-0.56
18		-1	AN	-24059.283	-39.90	-24061.014	-2.309	from 8	-2.272	-2.5
19	Ru(Cp*)2	+1	CH2Cl2	-23781.312	-35.79	-23782.864				
19		0	CH2Cl2	-23787.567	-2.18	-23787.662	-4.798	from 8	0.217	0.55
20	Os(Cp*)2	+1	CH2Cl2	-23703.918	-35.80	-23705.470				
20		0	CH2Cl2	-23710.160	1.06	-23710.123	-4.653	from 8	0.072	0.46

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
21	Fe(bpy)3	3+	Water	-43778.964	-277.56	-43791.000				
21	Fe(bpy)3	2+	Water	-43790.939	-124.22	-43796.326	-5.325	from 22	0.744	1.12
22	Ru(bpy)3	+3	AN	-42974.947	-273.53	-42986.809				
22	Ru(bpy)3	+2	AN	-42987.019	-125.17	-42992.447	-5.638	0.090	1.057	1.32
22	Ru(bpy)3	+1	AN	-42993.433	-38.52	-42995.103	-2.656	0.091	-1.923	-1.3
22	Ru(bpy)3	0	AN	-42996.937	-10.32	-42997.385	-2.281	0.133	-2.257	-1.49
22	Ru(bpy)3	-1	AN	-42997.878	-44.21	-42999.795	-2.411	0.136	-2.125	-1.73
23	Os(bpy)3	3+	Water	-42898.256	-275.17	-42910.189				
23	Os(bpy)3	2+	Water	-42909.928	-123.60	-42915.288	-5.099	from 22	0.518	0.84
24	Fe(CN)6	3-	Water	-18514.385	-376.54	-18530.714				
24	Fe(CN)6	4-	Water	-18505.486	-667.69	-18534.440	-3.727	0.166	-0.778	0.358
25	Fe(CN)5(NO)	2-	Water	-18724.815	-177.45	-18732.510				
25	Fe(CN)5(NO)	3-	Water	-18720.113	-378.95	-18736.546	-4.036	0.136	-0.499	-0.075
26	Ru(CN)6	3-	Water	-17711.361	-370.10	-17727.410				
26	Ru(CN)6	4-	Water	-17703.345	-660.82	-17732.002	-4.591	-0.061	-0.141	0.86

Table S4. Computed energy components at B3LYP/cc-pVTZ(-f) level of theory

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
1	Anthracene	0	DMF	-14685.492	-5.81	-14685.744				
1	Anthracene	-1	DMF	-14685.953	-48.97	-14688.077	-2.333	0.165	-2.173	-1.92
2	Azobenzene	0	DMF	-15590.186	-5.70	-15590.434				
2	Azobenzene	-1	DMF	-15591.281	-52.85	-15593.572	-3.138	0.096	-1.437	-1.36
3	Benzophenone	0	AN	-15695.607	-8.11	-15695.959				
3	Benzophenone	-1	AN	-15696.176	-54.38	-15698.534	-2.575	0.112	-1.985	-1.88
4	Nitrobenzene	0	AN	-11888.346	-8.09	-11888.697				
4	Nitrobenzene	-1	AN	-11889.262	-63.83	-11892.030	-3.333	0.110	-1.228	-1.15
5	Tetracyano- quinodimethane	0	AN	-18470.372	-17.88	-18471.148				
5	Tetracyano- quinodimethane	-1	AN	-18473.986	-47.26	-18476.035	-4.887	0.024	0.240	0.127
5	Tetracyano- quinodimethane	-2	AN	-18473.331	-157.27	-18480.150	-4.115	0.032	-0.524	-0.291
6	Tetrathiafulvalene	+2	AN	-49614.093	-181.89	-49621.981				
6	Tetrathiafulvalene	+1	AN	-49625.043	-49.23	-49627.178	-5.197	0.068	0.594	0.66
6	Tetrathiafulvalene	0	AN	-49631.294	-7.07	-49631.600	-4.422	0.106	-0.143	0.3
7	Fc-(COCH ₃) ₂	+1	DMF	-22199.238	-55.10	-22201.627				
7		0	DMF	-22206.028	-12.56	-22206.573	-4.945	from 8	0.364	0.74
8	Ferrocene	+1	AN	-13888.672	-49.73	-13890.829				
8		0	AN	-13895.753	-5.30	-13895.983	-5.154	0.090	0.573	0.307
9	Cp* ₂ Fe	+1	DMF	-24591.510	-39.53	-24593.224				
9		0	DMF	-24597.615	-2.33	-24597.716	-4.492	from 8	-0.089	-0.1
10	Cp ₂ Co	+1	DMF	-14478.535	-49.85	-14480.697				
10		0	DMF	-14484.065	-3.52	-14484.218	-3.521	from 8	-1.060	-0.91
11	[Me ₃ (Ph)] ₂ Cr	+1	DMF	-21408.613	-42.27	-21410.446				
11		0	DMF	-21413.489	-4.17	-21413.670	-3.224	from 8	-1.357	-0.98
12	CpFePh - [+1]	+1	DMF	-14943.721	-49.70	-14945.876				
12		0	DMF	-14948.568	-5.51	-14948.807	-2.931	from 8	-1.651	-1.36
13	Cp* ₂ Co - [0]	+1	DMF	-25181.485	-39.55	-25183.200				
13		0	DMF	-25186.048	-2.93	-25186.175	-2.975	from 8	-1.606	-1.43
14	CpFeAr*	+1	DMF	-21364.985	-43.50	-21366.871				
14		0	DMF	-21369.323	-4.02	-21369.497	-2.626	from 8	-1.955	-1.57
15	Cp*FeAr*	+1	DMF	-20295.121	-45.73	-20297.104				
15		0	DMF	-20299.523	-4.59	-20299.722	-2.618	from 8	-1.963	-1.85
16	Rh(Cp) ₂	+1	AN	-11160.151	-48.77	-11162.266				
16		0	AN	-11165.363	-3.15	-11165.500	-3.234	from 8	-1.348	-1.41
16		-1	AN	-11165.290	-49.40	-11167.432	-1.933	from 8	-2.649	-2.18
17	Cr(Cp*) ₂	+1	AN	-23580.880	-38.94	-23582.569				
17		0	AN	-23586.138	-2.91	-23586.264	-3.696	from 8	-0.886	-1.04
17		-1	AN	-23586.679	-37.01	-23588.284	-2.020	from 8	-2.561	-2.3
18	Mn(Cp*) ₂	+1	AN	-24059.705	-39.13	-24061.402				
18		0	AN	-24065.385	-3.40	-24065.532	-4.131	from 8	-0.451	-0.56
18		-1	AN	-24066.063	-38.39	-24067.728	-2.195	from 8	-2.386	-2.5
19	Ru(Cp*) ₂	+1	CH ₂ Cl ₂	-21698.322	-35.41	-21699.858				
19		0	CH ₂ Cl ₂	-21704.904	-2.23	-21705.001	-5.143	from 8	0.562	0.55
20	Os(Cp*) ₂	+1	CH ₂ Cl ₂	-21661.451	-35.42	-21662.987				
20		0	CH ₂ Cl ₂	-21667.960	-2.10	-21668.051	-5.064	from 8	0.483	0.46

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
21	Fe(bpy)3	3+	Water	-43790.995	-278.24	-43803.061				
21	Fe(bpy)3	2+	Water	-43802.878	-125.17	-43808.306	-5.245	from 22	0.664	1.12
22	Ru(bpy)3	+3	AN	-42986.386	-275.29	-42998.324				
22	Ru(bpy)3	+2	AN	-42998.519	-126.53	-43004.006	-5.682	0.090	1.101	1.32
22	Ru(bpy)3	+1	AN	-43005.162	-38.99	-43006.853	-2.847	0.091	-1.733	-1.3
22	Ru(bpy)3	0	AN	-43008.778	-11.59	-43009.281	-2.428	0.133	-2.110	-1.49
22	Ru(bpy)3	-1	AN	-43010.079	-43.57	-43011.968	-2.688	0.136	-1.848	-1.73
23	Os(bpy)3	3+	Water	-42909.682	-275.26	-42921.619				
23	Os(bpy)3	2+	Water	-42921.433	-124.68	-42926.840	-5.221	from 22	0.640	0.84
24	Fe(CN)6	3-	Water	-18521.470	-373.90	-18537.684				
24	Fe(CN)6	4-	Water	-18512.946	-664.50	-18541.762	-4.078	0.166	-0.427	0.358
25	Fe(CN)5(NO)	2-	Water	-18731.587	-176.92	-18739.259				
25	Fe(CN)5(NO)	3-	Water	-18727.144	-376.18	-18743.457	-4.198	0.136	-0.337	-0.075
26	Ru(CN)6	3-	Water	-17718.022	-368.08	-17733.984				
26	Ru(CN)6	4-	Water	-17710.377	-655.44	-17738.800	-4.816	-0.061	0.085	0.86

Table S5. Computed energy components at B3LYP/cc-pVTZ(-f)++ level of theory

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
1	Anthracene	0	DMF	-14686.201	-6.67	-14686.490				
1	Anthracene	-1	DMF	-14686.772	-48.10	-14688.858	-2.368	0.165	-2.138	-1.92
2	Azobenzene	0	DMF	-15590.950	-6.22	-15591.220				
2	Azobenzene	-1	DMF	-15592.174	-52.71	-15594.460	-3.240	0.096	-1.335	-1.36
3	Benzophenone	0	AN	-15696.351	-8.70	-15696.728				
3	Benzophenone	-1	AN	-15697.075	-55.13	-15699.466	-2.738	0.112	-1.822	-1.88
4	Nitrobenzene	0	AN	-11888.959	-7.88	-11889.300				
4	Nitrobenzene	-1	AN	-11890.128	-63.44	-11892.878	-3.578	0.110	-0.983	-1.15
5	Tetracyano- quinodimethane	0	AN	-18471.254	-18.43	-18472.054				
5	Tetracyano- quinodimethane	-1	AN	-18474.983	-47.31	-18477.034	-4.980	0.024	0.333	0.127
5	Tetracyano- quinodimethane	-2	AN	-18474.556	-155.44	-18481.296	-4.262	0.032	-0.377	-0.291
6	Tetrathiafulvalene	+2	AN	-49614.133	-180.18	-49621.947				
6	Tetrathiafulvalene	+1	AN	-49625.075	-48.36	-49627.172	-5.226	0.068	0.623	0.66
6	Tetrathiafulvalene	0	AN	-49631.968	-5.41	-49632.203	-5.030	0.106	0.465	0.3
7	Fc-(COCH ₃) ₂	+1	DMF	-22199.354	-55.82	-22201.775				
7		0	DMF	-22206.152	-12.89	-22206.711	-4.936	from 8	0.355	0.74
8	Ferrocene	+1	AN	-13888.830	-49.95	-13890.996				
8		0	AN	-13895.814	-4.34	-13896.002	-5.006	0.090	0.425	0.307
9	Cp* ₂ Fe	+1	DMF	-24591.591	-39.26	-24593.294				
9		0	DMF	-24597.692	-3.00	-24597.822	-4.529	from 8	-0.053	-0.1
10	Cp ₂ Co	+1	DMF	-14478.575	-50.16	-14480.750				
10		0	DMF	-14484.149	-4.16	-14484.329	-3.579	from 8	-1.002	-0.91
11	[Me ₃ (Ph)] ₂ Cr	+1	DMF	-21408.492	-42.13	-21410.319				
11		0	DMF	-21413.365	-4.24	-21413.549	-3.230	from 8	-1.351	-0.98
12	CpFePh - [+1]	+1	DMF	-14943.690	-49.92	-14945.855				
12		0	DMF	-14948.601	-5.24	-14948.828	-2.973	from 8	-1.608	-1.36
13	Cp* ₂ Co - [0]	+1	DMF	-25181.565	-39.56	-25183.281				
13		0	DMF	-25186.158	-2.82	-25186.280	-3.000	from 8	-1.581	-1.43
14	CpFeAr*	+1	DMF	-21364.965	-42.68	-21366.816				
14		0	DMF	-21369.380	-4.45	-21369.573	-2.757	from 8	-1.824	-1.57
15	Cp*FeAr*	+1	DMF	-20295.120	-44.52	-20297.051				
15		0	DMF	-20299.546	-4.02	-20299.720	-2.670	from 8	-1.911	-1.85
16	Rh(Cp) ₂	+1	AN	-11160.178	-48.82	-11162.295				
16		0	AN	-11165.438	-4.14	-11165.618	-3.322	from 8	-1.259	-1.41
16		-1	AN	-11165.605	-49.31	-11167.743	-2.126	from 8	-2.455	-2.18
17	Cr(Cp*) ₂	+1	AN	-23580.894	-39.04	-23582.587				
17		0	AN	-23586.137	-2.80	-23586.258	-3.671	from 8	-0.910	-1.04
17		-1	AN	-23586.772	-37.01*	-23588.377	-2.119	from 8	-2.463	-2.3
18	Mn(Cp*) ₂	+1	AN	-24059.77	-39.13*	-24061.47				
18		0	AN	-24065.41	-2.95	-24065.54	-4.072	from 8	-0.509	-0.56
18		-1	AN	-24066.20	-38.39*	-24067.87	-2.329	from 8	-2.252	-2.5
19	Ru(Cp*) ₂	+1	CH ₂ Cl ₂	-21698.36	-34.76	-21699.87				
19		0	CH ₂ Cl ₂	-21704.95	-2.09	-21705.04	-5.175	from 8	0.594	0.55
20	Os(Cp*) ₂	+1	CH ₂ Cl ₂	-21661.45	-36.35	-21663.03				
20		0	CH ₂ Cl ₂	-21667.96	-2.10	-21668.05	-5.024	from 8	0.443	0.46

* : Owing to technical difficulties with diffuse function, we were unable to reach convergence in SCRF calculations for 4 molecules marked with *. We used the solvation energy from B3LYP/cc-pVTZ(-f) calculations in these cases.

	Molecule	Chrg.	Solvent	H(SCF) eV	G(Solv) kcal/mol	H(SCF) + G(Solv) eV	Δ eV	ZPE-Entropy Correction eV	E0(Calc) V	E0(Exp) vs SCE V
21	Fe(bpy)3	3+	Water	-43791.016	-278.35	-43803.087				
21	Fe(bpy)3	2+	Water	-43802.878	-125.17	-43808.306	-5.219	from 22	0.638	1.12
22	Ru(bpy)3	+3	AN	-42986.303	-275.44	-42998.247				
22	Ru(bpy)3	+2	AN	-42998.424	-126.58	-43003.913	-5.666	0.090	1.084	1.32
22	Ru(bpy)3	+1	AN	-43005.095	-38.82	-43006.778	-2.865	0.091	-1.715	-1.3
22	Ru(bpy)3	0	AN	-43008.799	-10.87	-43009.270	-2.492	0.133	-2.046	-1.49
22	Ru(bpy)3	-1	AN	-43009.58	-43.57*	-43011.469	-2.199	0.136	-2.337	-1.73
23	Os(bpy)3	3+	Water	-42909.666	-275.4	-42921.609				
23	Os(bpy)3	2+	Water	-42921.414	-124.81	-42926.826	-5.218	from 22	0.636	0.84
24	Fe(CN)6	3-	Water	-18522.363	-368.19	-18538.33				
24	Fe(CN)6	4-	Water	-18514.429	-650.44	-18542.64	-4.306	0.166	-0.199	0.358
25	Fe(CN)5(NO)	2-	Water	-18732.102	-175.45	-18739.71				
25	Fe(CN)5(NO)	3-	Water	-18728.020	-370.18	-18744.07	-4.362	0.136	-0.172	-0.075
26	Ru(CN)6	3-	Water	-17718.823	-361.46	-17734.50				
26	Ru(CN)6	4-	Water	-17711.794	-642.40	-17739.65	-5.154	-0.061	0.422	0.86