Supplementary Information

How Strong are the Metallocene-Metallocene Interactions? Case of Ferrocene, Ruthenocene, and Osmocene

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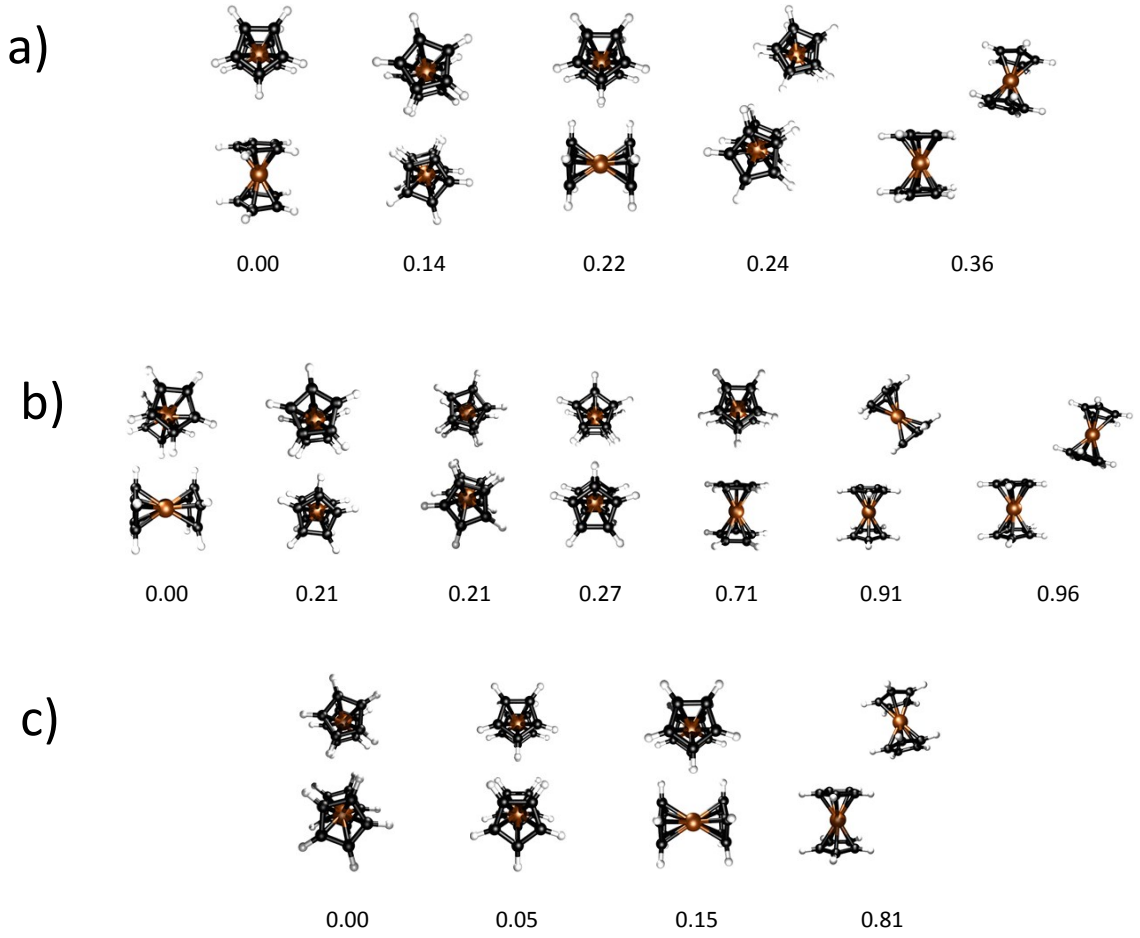


Figure 1-SI. PBE/def2-TZVP local minima on the potential energy surfaces of the MCp_2 dimers (M = Fe, Ru, Os; Cp =cyclopentadienyl). All relative energies in kcal·mol^{-1}, including the ZPE correction. a) ferrocene dimers, b) ruthenocene dimers and c) osmocene dimers.

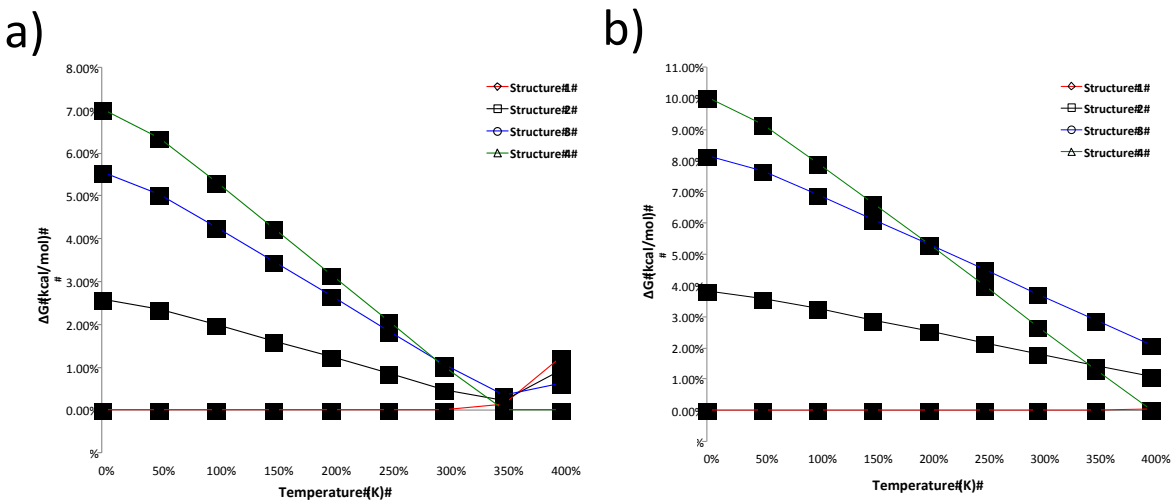


Figure 2-SI. Thermal effects on the relative energies for the a) ruthenocene dimers and b) osmocene dimers. All energy differences are computed at the PBE-D2/def2-TZVP level.

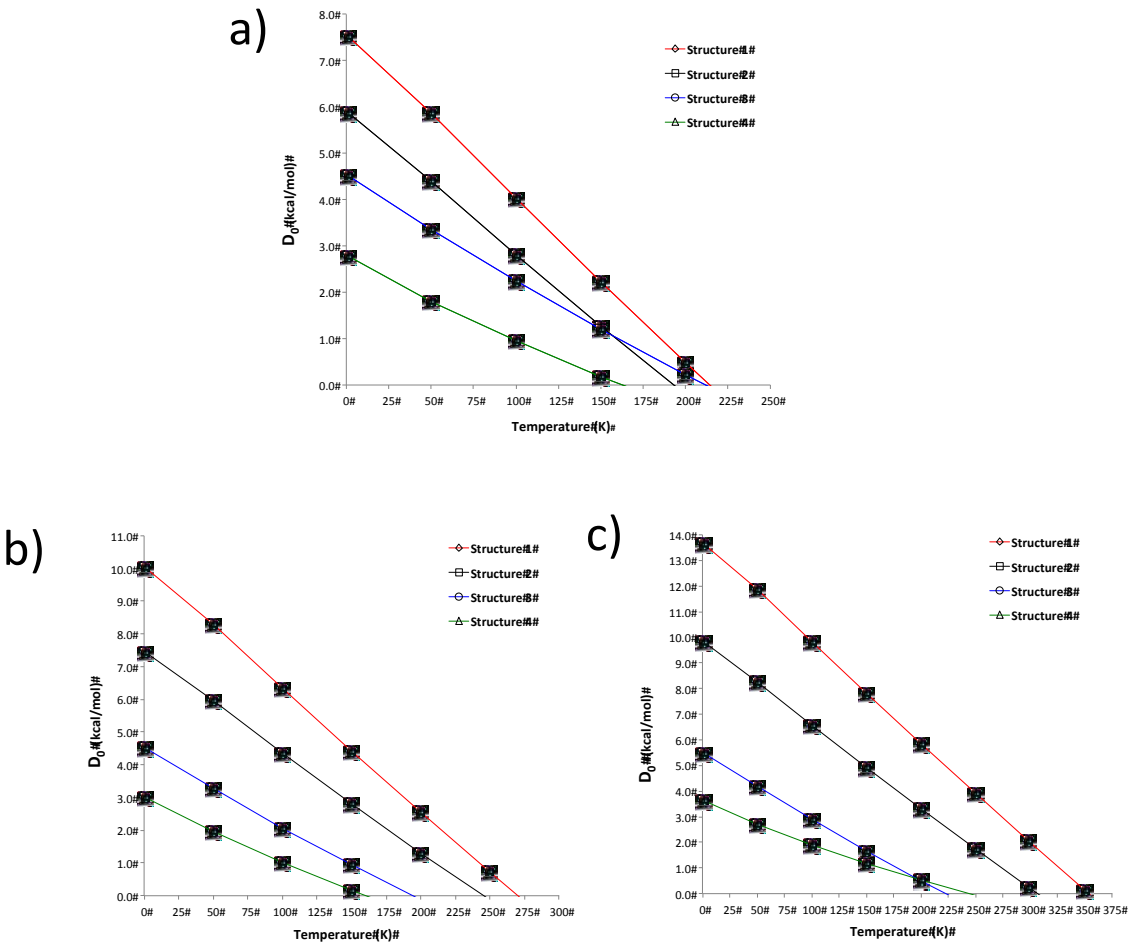
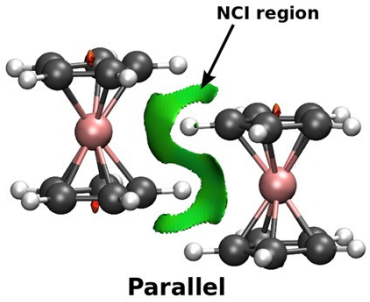
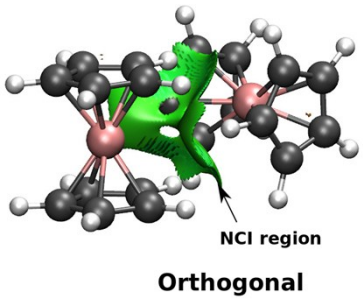


Figure 3-SI. Thermal effects on the dissociation energies for a) ferrocene dimers b) ruthenocene dimers, and c) osmocene dimers.. All energy differences are computed at the PBE-D2/def2-TZVP level.

Table 1-SI. Value of integrals within NCI domain for ferrocene. NCI images are provided as a guide to the eye.



Parallel conformation of ferrocene dimer



Orthogonal conformation of ferrocene dimer

		V_{NCI}	q_{NCI}
Parallel	Fe	87.47	1.78
	Ru	121.80	3.20
	Os	192.17	8.31
Orthogonal	Fe	104.03	1.90
	Ru	142.08	3.29
	Os	258.31	9.07

NCI computational data: Cubic grids with 0.1 a.u. increments
Cutoffs ρ=0.2 a.u., s=2.0

CARTESIAN COORDINATES

Ferrocene with dispersión

ΔE= 0.0 kcal mol^{-1}		Fe_wd_1	
C	-0.7173800	1.6139800	3.4292920
C	-1.1598920	1.6392520	2.0645680
C	0.0000000	1.6569610	1.2211940
C	1.1598920	1.6392520	2.0645680
C	0.7173800	1.6139800	3.4292920
H	-1.3559700	1.5670440	4.3077810
H	-2.1936910	1.6206980	1.7279120
H	2.1936910	1.6206980	1.7279120
H	1.3559700	1.5670440	4.3077810
H	0.0000000	1.6315560	0.1344310
Fe	0.0000000	0.0000000	2.4188670
C	-0.7173800	-1.6139800	3.4292920
C	-1.1598920	-1.6392520	2.0645680
C	0.0000000	-1.6569610	1.2211940
C	1.1598920	-1.6392520	2.0645680
C	0.7173800	-1.6139800	3.4292920
H	-1.3559700	-1.5670440	4.3077810
H	-2.1936910	-1.6206980	1.7279120
H	2.1936910	-1.6206980	1.7279120
H	1.3559700	-1.5670440	4.3077810
H	0.0000000	-1.6315560	0.1344310
C	-1.6139800	-0.7173800	-3.4292920
C	-1.6139800	0.7173800	-3.4292920
C	-1.6392520	1.1598920	-2.0645680
C	-1.6569610	0.0000000	-1.2211940
C	-1.6392520	-1.1598920	-2.0645680
H	-1.5670440	-1.3559700	-4.3077810
H	-1.5670440	1.3559700	-4.3077810
H	-1.6315560	0.0000000	-0.1344310
H	-1.6206980	-2.1936910	-1.7279120
H	-1.6206980	2.1936910	-1.7279120
Fe	0.0000000	0.0000000	-2.4188670
C	1.6139800	0.7173800	-3.4292920
C	1.6392520	1.1598920	-2.0645680
C	1.6569610	0.0000000	-1.2211940

C	1.6392520	-1.1598920	-2.0645680
C	1.6139800	-0.7173800	-3.4292920
H	1.5670440	1.3559700	-4.3077810
H	1.6206980	2.1936910	-1.7279120
H	1.6206980	-2.1936910	-1.7279120
H	1.5670440	-1.3559700	-4.3077810
H	1.6315560	0.0000000	-0.1344310

ΔE= 1.65 kcal mol^{-1} Fe_wd_2

C	2.1801760	1.6974820	-1.2178210
C	1.0430960	1.2696530	-0.4559090
C	1.3729400	1.3951560	0.9355050
C	2.7124520	1.8995650	1.0331110
C	3.2115000	2.0868640	-0.2989890
H	2.2602300	1.6955870	-2.3020600
H	0.1011740	0.8904970	-0.8436940
H	3.2634480	2.0782140	1.9530040
H	4.2081440	2.4300380	-0.5650140
H	0.7276890	1.1255090	1.7682490
C	3.3745950	-1.3314790	-1.2173300
C	2.2394580	-1.7894260	-0.4699880
C	2.5500610	-1.6668150	0.9252070
C	3.8768970	-1.1335570	1.0403680
C	4.3869520	-0.9263300	-0.2846490
H	3.4440090	-1.2707140	-2.3005290
H	1.2964340	-2.1406330	-0.8796520
H	4.3930530	-0.8979120	1.9676160
H	5.3563300	-0.5038820	-0.5370400
H	1.8857610	-1.9141510	1.7495430
Fe	2.6814460	0.1454660	0.0018250
C	-1.3729280	-1.3951390	-0.9355090
C	-1.0430960	-1.2696510	0.4559090
C	-2.1801800	-1.6974940	1.2178070
C	-3.2114950	-2.0868710	0.2989620
C	-2.7124370	-1.8995540	-1.0331320
H	-0.7276710	-1.1254780	-1.7682430
H	-0.1011780	-0.8904960	0.8437040
H	-4.2081390	-2.4300530	0.5649750
H	-3.2634250	-2.0781940	-1.9530310
H	-2.2602430	-1.6956130	2.3020450
C	-2.5500700	1.6668200	-0.9251960
C	-2.2394600	1.7894220	0.4699980
C	-3.3745920	1.3314700	1.2173430

C	-4.3869540	0.9263250	0.2846660
C	-3.8769070	1.1335610	-1.0403540
H	-1.8857740	1.9141620	-1.7495340
H	-1.2964330	2.1406260	0.8796580
H	-5.3563300	0.5038750	0.5370590
H	-4.3930670	0.8979230	-1.9676000
H	-3.4440000	1.2706980	2.3005430
Fe	-2.6814480	-0.1454660	-0.0018240

ΔE= 2.99 kcal mol^{-1} Fe_wd_3

C	-0.7208710	4.7993580	0.7173990
C	0.6225330	4.5603520	1.1608340
C	1.4528040	4.4127100	0.0000000
C	0.6225330	4.5603520	-1.1608340
C	-0.7208710	4.7993580	-0.7173990
H	-1.5913970	4.9249690	1.3562340
H	0.9481520	4.4735490	2.1943240
H	0.9481520	4.4735490	-2.1943240
H	-1.5913970	4.9249690	-1.3562340
H	2.5178170	4.1948710	0.0000000
C	-1.2902590	1.5918970	0.7176520
C	0.0540260	1.3555030	1.1608090
C	0.8827520	1.2056990	0.0000000
C	0.0540260	1.3555030	-1.1608090
C	-1.2902590	1.5918970	-0.7176520
H	-2.1507170	1.7739430	1.3567940
H	0.3878370	1.3174240	2.1945590
H	0.3878370	1.3174240	-2.1945590
H	-2.1507170	1.7739430	-1.3567940
H	1.9572890	1.0400310	0.0000000
Fe	-0.0339280	3.0221590	0.0000000
C	0.8002950	-2.0723970	-1.6227990
C	1.1718800	-3.4584530	-1.6346370
C	-0.0320780	-4.2396860	-1.6361430
C	-1.1465160	-3.3351560	-1.6265990
C	-0.6323460	-1.9955370	-1.6170940
H	1.4784920	-1.2246500	-1.5789840
H	2.1862480	-3.8490110	-1.6120420
H	-2.1961260	-3.6167580	-1.5943860
H	-1.2140900	-1.0794080	-1.5603800
H	-0.0895630	-5.3251700	-1.6162810
Fe	0.0367710	-3.0300700	0.0000000
C	0.8002950	-2.0723970	1.6227990

C	1.1718800	-3.4584530	1.6346370
C	-0.0320780	-4.2396860	1.6361430
C	-1.1465160	-3.3351560	1.6265990
C	-0.6323460	-1.9955370	1.6170940
H	1.4784920	-1.2246500	1.5789840
H	2.1862480	-3.8490110	1.6120420
H	-2.1961260	-3.6167580	1.5943860
H	-1.2140900	-1.0794080	1.5603800
H	-0.0895630	-5.3251700	1.6162810

ΔE= 4.73 kcal mol^{-1} Fe_wd_4

C	4.7503070	-1.2669000	-0.6627100
C	5.0280390	0.0432190	-1.1783270
C	5.2148060	0.9279620	-0.0640930
C	5.0525730	0.1647570	1.1401990
C	4.7655530	-1.1917620	0.7703800
H	4.5335190	-2.1533230	-1.2534750
H	5.0587880	0.3230500	-2.2283630
H	5.1055250	0.5526870	2.1543690
H	4.5624330	-2.0112690	1.4551420
H	5.4124900	1.9953860	-0.1220960
C	1.5631300	-0.5982780	-0.6631250
C	1.8381820	0.7103080	-1.1798740
C	2.0222140	1.5968530	-0.0668200
C	1.8617190	0.8329220	1.1371060
C	1.5775490	-0.5226880	0.7666810
H	1.3890980	-1.4946080	-1.2520000
H	1.9214540	0.9778140	-2.2303470
H	1.9671590	1.2095050	2.1515580
H	1.4175220	-1.3521500	1.4500300
H	2.2734650	2.6530580	-0.1252900
Fe	3.3690760	0.0717280	0.0001530
C	-1.5775470	0.5226830	0.7666800
C	-1.8617220	-0.8329260	1.1371070
C	-2.0222200	-1.5968580	-0.0668180
C	-1.8381840	-0.7103160	-1.1798730
C	-1.5631280	0.5982700	-0.6631270
H	-1.4175160	1.3521450	1.4500270
H	-1.9671630	-1.2095070	2.1515600
H	-1.9214580	-0.9778240	-2.2303460
H	-1.3890920	1.4945990	-1.2520020
H	-2.2734740	-2.6530620	-0.1252860
C	-4.7655490	1.1917610	0.7703880

C	-5.0525750	-0.1647600	1.1401950
C	-5.2148100	-0.9279550	-0.0641030
C	-5.0280370	-0.0432030	-1.1783290
C	-4.7503000	1.2669110	-0.6627010
H	-4.5624270	2.0112620	1.4551580
H	-5.1055300	-0.5526990	2.1543620
H	-5.0587860	-0.3230240	-2.2283680
H	-4.5335070	2.1533380	-1.2534590
H	-5.4124980	-1.9953770	-0.1221160
Fe	-3.3690760	-0.0717290	0.0001520

Ruthenocene with dispersion

ΔE= 0.0 kcal mol^{-1} Ru_wd_1

C	1.1613160	1.7999800	1.9822060
C	0.0000000	1.7983850	1.1360500
C	-1.1613160	1.7999800	1.9822060
C	-0.7183210	1.8011280	3.3495370
C	0.7183210	1.8011280	3.3495370
H	2.1951960	1.8002670	1.6464200
H	0.0000000	1.7558290	0.0486500
H	-1.3569090	1.8000060	4.2287070
H	1.3569090	1.8000060	4.2287070
H	-2.1951960	1.8002670	1.6464200
C	1.1613160	-1.7999800	1.9822060
C	0.0000000	-1.7983850	1.1360500
C	-1.1613160	-1.7999800	1.9822060
C	-0.7183210	-1.8011280	3.3495370
C	0.7183210	-1.8011280	3.3495370
H	2.1951960	-1.8002670	1.6464200
H	0.0000000	-1.7558290	0.0486500
H	-1.3569090	-1.8000060	4.2287070
H	1.3569090	-1.8000060	4.2287070
H	-2.1951960	-1.8002670	1.6464200
Ru	0.0000000	0.0000000	2.3598890
C	1.7999800	-1.1613160	-1.9822060
C	1.8011280	-0.7183210	-3.3495370
C	1.8011280	0.7183210	-3.3495370
C	1.7999800	1.1613160	-1.9822060
C	1.7983850	0.0000000	-1.1360500
H	1.8002670	-2.1951960	-1.6464200
H	1.8000060	-1.3569090	-4.2287070
H	1.8002670	2.1951960	-1.6464200

H	1.7558290	0.0000000	-0.0486500
H	1.8000060	1.3569090	-4.2287070
C	-1.7999800	-1.1613160	-1.9822060
C	-1.8011280	-0.7183210	-3.3495370
C	-1.8011280	0.7183210	-3.3495370
C	-1.7999800	1.1613160	-1.9822060
C	-1.7983850	0.0000000	-1.1360500
H	-1.8002670	-2.1951960	-1.6464200
H	-1.8000060	-1.3569090	-4.2287070
H	-1.8002670	2.1951960	-1.6464200
H	-1.7558290	0.0000000	-0.0486500
H	-1.8000060	1.3569090	-4.2287070
Ru	0.0000000	0.0000000	-2.3598890

ΔE= 2.59 kcal mol^{-1} Ru_wd_2

C	1.2127920	-1.5199860	-0.9355630
C	2.5248790	-2.0973390	-1.0350810
C	3.0145940	-2.3124860	0.2986840
C	2.0047450	-1.8674410	1.2196770
C	0.8903860	-1.3772830	0.4576370
H	0.5694230	-1.2367400	-1.7645750
H	3.0539780	-2.3303640	-1.9551510
H	2.0744750	-1.8961270	2.3038260
H	-0.0416170	-0.9663340	0.8397640
H	3.9803440	-2.7345030	0.5636910
C	2.6783020	1.7820440	-0.9240310
C	3.9807170	1.1870430	-1.0437150
C	4.4852280	0.9548740	0.2814840
C	3.4941450	1.4058820	1.2191560
C	2.3772450	1.9171050	0.4743110
H	2.0346050	2.0847110	-1.7457570
H	4.4941770	0.9539720	-1.9725940
H	3.5757580	1.3668570	2.3020410
H	1.4622950	2.3324460	0.8871260
H	5.4461010	0.5125450	0.5304970
Ru	2.6567220	-0.1885700	-0.0014120
C	-1.2127930	1.5199860	0.9355630
C	-0.8903880	1.3772860	-0.4576380
C	-2.0047480	1.8674440	-1.2196770
C	-3.0145970	2.3124860	-0.2986820
C	-2.5248810	2.0973380	1.0350830
H	-0.5694220	1.2367400	1.7645730
H	0.0416160	0.9663390	-0.8397660
H	-3.9803470	2.7345030	-0.5636880

H	-3.0539780	2.3303610	1.9551540
H	-2.0744780	1.8961330	-2.3038250
C	-2.6782960	-1.7820460	0.9240280
C	-2.3772450	-1.9171050	-0.4743150
C	-3.4941490	-1.4058830	-1.2191550
C	-4.4852290	-0.9548760	-0.2814780
C	-3.9807120	-1.1870460	1.0437180
H	-2.0345960	-2.0847130	1.7457510
H	-1.4622970	-2.3324450	-0.8871360
H	-5.4461020	-0.5125470	-0.5304860
H	-4.4941670	-0.9539760	1.9726000
H	-3.5757660	-1.3668560	-2.3020390
Ru	-2.6567210	0.1885700	0.0014110

ΔE= 5.55 kcal mol^{-1} Ru_wd_3

C	1.0469140	-0.0000220	-0.7345370
C	1.2413010	-1.1622390	0.0858560
C	1.5469570	-0.7190390	1.4184260
C	1.5468300	0.7181210	1.4187470
C	1.2410970	1.1618620	0.0863750
H	0.7941290	0.0001920	-1.7911720
H	1.1599520	-2.1956310	-0.2398940
H	1.7461370	1.3569010	2.2750730
H	1.1595750	2.1953840	-0.2389170
H	1.7463760	-1.3581680	2.2744660
C	4.5493220	0.0004430	-1.5492560
C	4.7417740	-1.1622900	-0.7270360
C	5.0527840	-0.7184200	0.6036930
C	5.0526560	0.7184970	0.6039930
C	4.7415690	1.1628670	-0.7265520
H	4.3025210	0.0006420	-2.6074760
H	4.6658270	-2.1956490	-1.0543690
H	5.2528070	1.3570730	1.4601070
H	4.6654390	2.1963480	-1.0534550
H	5.2530480	-1.3573170	1.4595410
Ru	3.0754520	-0.0000220	0.0495020
C	-3.4800180	1.8063880	-1.1987190
C	-4.2948920	1.8066720	-0.0149970
C	-3.4200940	1.7951780	1.1253890
C	-2.0648460	1.7853740	0.6475140
C	-2.1025990	1.7931340	-0.7888560
H	-3.8422740	1.8142110	-2.2232110
H	-5.3811990	1.8141970	0.0128580
H	-1.1657290	1.7562570	1.2564960

H	-1.2377100	1.7811020	-1.4456500
H	-3.7298830	1.7903610	2.1670020
Ru	-3.0812240	0.0000220	-0.0526180
C	-3.4800010	-1.8062950	-1.1988020
C	-4.2947780	-1.8067040	-0.0150120
C	-3.4198850	-1.7952300	1.1253020
C	-2.0646770	-1.7853150	0.6473160
C	-2.1025500	-1.7929850	-0.7890510
H	-3.8423420	-1.8140740	-2.2232640
H	-5.3810810	-1.8142960	0.0129330
H	-1.1655060	-1.7561830	1.2562180
H	-1.2377150	-1.7808610	-1.4459130
H	-3.7295890	-1.7904970	2.1669410

ΔE= 7.04 kcal mol^{-1} Ru_wd_4

C	-5.1061260	-1.2704410	0.6553230
C	-5.3518080	0.0448640	1.1796660
C	-5.5169250	0.9419580	0.0692790
C	-5.3733580	0.1812420	-1.1414030
C	-5.1194280	-1.1861470	-0.7793830
H	-4.9405320	-2.1708620	1.2406500
H	-5.4043100	0.3136570	2.2312370
H	-5.4455270	0.5712080	-2.1531160
H	-4.9656250	-2.0116030	-1.4691350
H	-5.7165800	2.0081650	0.1338600
C	-1.5708110	-0.6156970	0.6672410
C	-1.8141340	0.7016140	1.1838140
C	-1.9743250	1.5932550	0.0685170
C	-1.8313010	0.8240210	-1.1366520
C	-1.5813610	-0.5401930	-0.7649670
H	-1.3941940	-1.5106360	1.2566450
H	-1.8639870	0.9766040	2.2339670
H	-1.8971890	1.2078820	-2.1511770
H	-1.4151030	-1.3683640	-1.4476700
H	-2.1703000	2.6606370	0.1262970
Ru	-3.5249160	0.0698960	-0.0001920
C	1.5813790	0.5402190	-0.7650250
C	1.8313230	-0.8239870	-1.1367390
C	1.9743180	-1.5932510	0.0684130
C	1.8141050	-0.7016390	1.1837290
C	1.5707980	0.6156860	0.6671840
H	1.4151410	1.3684080	-1.4477110
H	1.8972330	-1.2078220	-2.1512730
H	1.8639340	-0.9766560	2.2338770

H	1.3941700	1.5106100	1.2566080
H	2.1702880	-2.6606370	0.1261700
C	5.1194510	1.1861590	-0.7793480
C	5.3733860	-0.1812220	-1.1413920
C	5.5169220	-0.9419650	0.0692770
C	5.3517800	-0.0448940	1.1796790
C	5.1061140	1.2704230	0.6553590
H	4.9656670	2.0116300	-1.4690860
H	5.4455780	-0.5711670	-2.1531110
H	5.4042560	-0.3137110	2.2312470
H	4.9405080	2.1708310	1.2407010
H	5.7165720	-2.0081740	0.1338400
Ru	3.5249170	-0.0698960	-0.0002230

Osmocene with dispersion

ΔE= 0.0 kcal mol^{-1} Os_wd_1

C	0.0000000	1.8240110	1.0956010
C	-1.1634970	1.8229680	1.9437190
C	-0.7198300	1.8207300	3.3141100
C	0.7198300	1.8207300	3.3141100
C	1.1634970	1.8229680	1.9437190
H	0.0000000	1.7939880	0.0077100
H	-2.1973500	1.8346290	1.6078600
H	1.3583390	1.8265370	4.1933770
H	2.1973500	1.8346290	1.6078600
H	-1.3583390	1.8265370	4.1933770
C	0.0000000	-1.8240110	1.0956010
C	-1.1634970	-1.8229680	1.9437190
C	-0.7198300	-1.8207300	3.3141100
C	0.7198300	-1.8207300	3.3141100
C	1.1634970	-1.8229680	1.9437190
H	0.0000000	-1.7939880	0.0077100
H	-2.1973500	-1.8346290	1.6078600
H	1.3583390	-1.8265370	4.1933770
H	2.1973500	-1.8346290	1.6078600
H	-1.3583390	-1.8265370	4.1933770
Os	0.0000000	0.0000000	2.3182760
C	-1.8229680	1.1634970	-1.9437190
C	-1.8207300	0.7198300	-3.3141100
C	-1.8207300	-0.7198300	-3.3141100
C	-1.8229680	-1.1634970	-1.9437190
C	-1.8240110	0.0000000	-1.0956010

H	-1.8346290	2.1973500	-1.6078600
H	-1.8265370	1.3583390	-4.1933770
H	-1.8346290	-2.1973500	-1.6078600
H	-1.7939880	0.0000000	-0.0077100
H	-1.8265370	-1.3583390	-4.1933770
C	1.8229680	1.1634970	-1.9437190
C	1.8207300	0.7198300	-3.3141100
C	1.8207300	-0.7198300	-3.3141100
C	1.8229680	-1.1634970	-1.9437190
C	1.8240110	0.0000000	-1.0956010
H	1.8346290	2.1973500	-1.6078600
H	1.8265370	1.3583390	-4.1933770
H	1.8346290	-2.1973500	-1.6078600
H	1.7939880	0.0000000	-0.0077100
H	1.8265370	-1.3583390	-4.1933770
Os	0.0000000	0.0000000	-2.3182760

ΔE= 3.83 kcal mol^{-1} Os_wd_2

C	-2.6473340	-1.8387610	0.9240000
C	-3.9538940	-1.2463630	1.0477870
C	-4.4636480	-1.0144860	-0.2787590
C	-3.4715950	-1.4626220	-1.2214680
C	-2.3487710	-1.9721660	-0.4781700
H	-2.0047470	-2.1493980	1.7436610
H	-4.4695360	-1.0241230	1.9781490
H	-3.5604960	-1.4327240	-2.3040990
H	-1.4383020	-2.3949010	-0.8930430
H	-5.4302940	-0.5831040	-0.5248450
C	-1.1539130	1.5001150	0.9140560
C	-2.4688100	2.0699080	1.0564760
C	-2.9963830	2.2995100	-0.2638570
C	-2.0072570	1.8703370	-1.2190970
C	-0.8678780	1.3763490	-0.4916290
H	-0.4801830	1.2174770	1.7187520
H	-2.9706030	2.2976330	1.9930790
H	-2.1022080	1.9210450	-2.3005610
H	0.0600630	0.9837390	-0.9011020
H	-3.9675780	2.7276410	-0.4975880
Os	-2.6256360	0.1528930	0.0006660
C	2.0072580	-1.8703300	1.2191040
C	0.8678780	-1.3763430	0.4916370
C	1.1539090	-1.5001160	-0.9140480
C	2.4688040	-2.0699130	-1.0564690
C	2.9963800	-2.2995100	0.2638630

H	2.1022130	-1.9210320	2.3005680
H	-0.0600610	-0.9837310	0.9011120
H	2.9705920	-2.2976450	-1.9930730
H	3.9675760	-2.7276420	0.4975940
H	0.4801740	-1.2174840	-1.7187420
C	3.4715960	1.4626210	1.2214650
C	2.3487720	1.9721640	0.4781670
C	2.6473330	1.8387610	-0.9240020
C	3.9538940	1.2463620	-1.0477910
C	4.4636490	1.0144850	0.2787550
H	3.5604980	1.4327230	2.3040960
H	1.4383040	2.3949030	0.8930420
H	4.4695350	1.0241240	-1.9781530
H	5.4302950	0.5831050	0.5248400
H	2.0047460	2.1493980	-1.7436630
Os	2.6256370	-0.1528930	-0.0006680

ΔE= 8.16 kcal mol^{-1} Os_wd_3

C	-1.5393870	0.5505480	1.5449730
C	-1.5843430	-0.8845900	1.4319120
C	-1.2288740	-1.2349410	0.0804630
C	-0.9575990	-0.0181640	-0.6375610
C	-1.1568200	1.0851650	0.2634620
H	-1.7493760	1.1275060	2.4417060
H	-1.8331980	-1.5810300	2.2282650
H	-0.6391870	0.0538500	-1.6734560
H	-1.0193650	2.1364030	0.0257970
H	-1.1531670	-2.2429410	-0.3180800
C	-5.0433300	0.7338040	0.5641650
C	-5.0873330	-0.7007300	0.4466580
C	-4.7250460	-1.0480870	-0.9030630
C	-4.4572580	0.1720060	-1.6199270
C	-4.6539590	1.2733220	-0.7129480
H	-5.2751980	1.3090330	1.4564390
H	-5.3583240	-1.3980450	1.2347630
H	-4.1699420	0.2489050	-2.6650860
H	-4.5408470	2.3269360	-0.9536150
H	-4.6749580	-2.0534550	-1.3123700
Os	-3.0424780	-0.0078340	0.0475940
C	3.4304900	-1.8063170	-1.2262260
C	4.2532740	-1.8250240	-0.0444180
C	3.3824900	-1.8265960	1.1030390
C	2.0218410	-1.8063800	0.6318240
C	2.0525320	-1.7947850	-0.8078620

H	3.7871550	-1.8116740	-2.2527100
H	5.3395880	-1.8452410	-0.0223860
H	1.1257270	-1.7943650	1.2457640
H	1.1847500	-1.7842360	-1.4605430
H	3.6976640	-1.8466010	2.1428970
C	3.4246220	1.8492730	-1.1841930
C	4.2807210	1.8220770	-0.0264350
C	3.4431800	1.8022090	1.1451550
C	2.0696230	1.8147350	0.7126790
C	2.0587830	1.8444670	-0.7271860
H	3.7521610	1.8798320	-2.2198860
H	5.3674000	1.8262680	-0.0351290
H	1.1928490	1.7970670	1.3535840
H	1.1732720	1.8653620	-1.3556520
H	3.7877780	1.7877930	2.1757230
Os	3.0438410	0.0076590	-0.0507920

ΔE= 10.05 kcal mol^{-1} Os_wd_4

C	5.1303900	1.2669960	0.6786490
C	5.3702560	-0.0631220	1.1763940
C	5.5265890	-0.9403470	0.0449650
C	5.3833990	-0.1526020	-1.1521600
C	5.1385430	1.2117050	-0.7607400
H	4.9825750	2.1581300	1.2827250
H	5.4346220	-0.3517870	2.2220560
H	5.4598520	-0.5205790	-2.1717910
H	4.9979320	2.0537840	-1.4330510
H	5.7298360	-2.0070180	0.0871600
C	1.5480860	0.6261060	0.6882380
C	1.7860580	-0.7051070	1.1793360
C	1.9374000	-1.5775910	0.0437120
C	1.7951200	-0.7823100	-1.1482850
C	1.5537690	0.5785110	-0.7481710
H	1.3691300	1.5086630	1.2953200
H	1.8268190	-1.0029660	2.2236460
H	1.8451750	-1.1484900	-2.1702380
H	1.3805980	1.4190680	-1.4137480
H	2.1168360	-2.6488870	0.0799630
Os	3.5177470	-0.0560850	-0.0001610
C	-1.5077800	-0.7908820	0.2471940
C	-1.6146370	-0.2057630	-1.0613070
C	-1.8771280	1.2004120	-0.9010870
C	-1.9313930	1.4837630	0.5098310
C	-1.7035970	0.2513410	1.2184290

H	-1.2866080	-1.8317200	0.4637010
H	-1.4955380	-0.7300060	-2.0052750
H	-2.1025290	2.4579870	0.9600750
H	-1.6664290	0.1324400	2.2978490
H	-1.9996700	1.9234550	-1.7031470
C	-5.0849940	-1.4590100	0.2461870
C	-5.1929530	-0.8765250	-1.0667820
C	-5.4584680	0.5302400	-0.9090200
C	-5.5146990	0.8172830	0.5011340
C	-5.2840390	-0.4120740	1.2151690
H	-4.8994170	-2.5067560	0.4667880
H	-5.1029630	-1.4077140	-2.0104980
H	-5.7097100	1.7884750	0.9479400
H	-5.2746450	-0.5314350	2.2952300
H	-5.6039280	1.2467450	-1.7129700
Os	-3.5177660	0.0559860	0.0000050

Ferrocene without dispersion

ΔE= 0.0 kcal mol^{-1} Fe_wod_1

C	-0.9882890	5.1033430	0.7169280
C	0.3753700	5.1048060	1.1599940
C	1.2181540	5.1056730	0.0000000
C	0.3753700	5.1048060	-1.1599940
C	-0.9882890	5.1033430	-0.7169280
H	-1.8676030	5.0845990	1.3558350
H	0.7113320	5.0875510	2.1937190
H	0.7113320	5.0875510	-2.1937190
H	-1.8676030	5.0845990	-1.3558350
H	2.3051120	5.0893540	0.0000000
C	-0.9854180	1.8184730	0.7170800
C	0.3790090	1.8198840	1.1604630
C	1.2220380	1.8205710	0.0000000
C	0.3790090	1.8198840	-1.1604630
C	-0.9854180	1.8184730	-0.7170800
H	-1.8647410	1.8354540	1.3561070
H	0.7149370	1.8398790	2.1942950
H	0.7149370	1.8398790	-2.1942950
H	-1.8647410	1.8354540	-1.3561070
H	2.3089650	1.8391010	0.0000000
Fe	0.0002280	3.4611000	0.0000000
C	1.1613550	-3.0883230	-1.6393630
C	0.7116280	-4.4501860	-1.6488520

C	-0.7224300	-4.4425720	-1.6488640
C	-1.1576770	-3.0760050	-1.6394090
C	0.0063150	-2.2382500	-1.6328560
H	2.1968400	-2.7578390	-1.6168430
H	1.3459460	-5.3330620	-1.6381890
H	-2.1896020	-2.7345660	-1.6168320
H	0.0120820	-1.1515250	-1.5918270
H	-1.3660940	-5.3186540	-1.6381520
Fe	-0.0002200	-3.4689320	0.0000000
C	1.1613550	-3.0883230	1.6393630
C	0.7116280	-4.4501860	1.6488520
C	-0.7224300	-4.4425720	1.6488640
C	-1.1576770	-3.0760050	1.6394090
C	0.0063150	-2.2382500	1.6328560
H	2.1968400	-2.7578390	1.6168430
H	1.3459460	-5.3330620	1.6381890
H	-2.1896020	-2.7345660	1.6168320
H	0.0120820	-1.1515250	1.5918270
H	-1.3660940	-5.3186540	1.6381520

ΔE= 0.14 kcal mol^{-1} Fe_wod_2

C	2.6068170	1.7031070	-1.2172580
C	1.4569660	1.3179410	-0.4522250
C	1.7927530	1.4307570	0.9378010
C	3.1493610	1.8857610	1.0312410
C	3.6523010	2.0542700	-0.3008910
H	2.6799460	1.7090690	-2.3019220
H	0.5027470	0.9832990	-0.8517560
H	3.7049140	2.0546400	1.9502740
H	4.6564770	2.3728860	-0.5690440
H	1.1397930	1.1958510	1.7750060
C	3.6666970	-1.4065840	-1.2173930
C	2.5214560	-1.8051580	-0.4525690
C	2.8554030	-1.6898730	0.9370470
C	4.2069760	-1.2207270	1.0312160
C	4.7086480	-1.0458390	-0.3006550
H	3.7283420	-1.3667050	-2.3020300
H	1.5627980	-2.1255000	-0.8531150
H	4.7496580	-1.0153420	1.9505210
H	5.6983290	-0.6842590	-0.5682720
H	2.1948500	-1.9072400	1.7727960
Fe	3.0557150	0.1207420	0.0006170
C	-1.7927500	-1.4307640	-0.9377870
C	-1.4569730	-1.3179440	0.4522410

C	-2.6068310	-1.7031050	1.2172670
C	-3.6523090	-2.0542670	0.3008930
C	-3.1493590	-1.8857640	-1.0312350
H	-1.1397830	-1.1958630	-1.7749880
H	-0.5027560	-0.9833040	0.8517780
H	-4.6564880	-2.3728790	0.5690400
H	-3.7049050	-2.0546450	-1.9502730
H	-2.6799680	-1.7090630	2.3019300
C	-2.8553890	1.6898690	-0.9370500
C	-2.5214550	1.8051580	0.4525690
C	-3.6667040	1.4065900	1.2173830
C	-4.7086470	1.0458440	0.3006360
C	-4.2069620	1.2207280	-1.0312310
H	-2.1948270	1.9072320	-1.7727940
H	-1.5628000	2.1254980	0.8531230
H	-5.6983320	0.6842690	0.5682450
H	-4.7496360	1.0153410	-1.9505400
H	-3.7283600	1.3667140	2.3020190
Fe	-3.0557150	-0.1207420	-0.0006170

ΔE= 0.22 kcal mol^{-1} Fe_wod_3

C	-0.7169620	1.6374750	3.8946110
C	-1.1600030	1.6466930	2.5309750
C	0.0000000	1.6533990	1.6880080
C	1.1600030	1.6466930	2.5309750
C	0.7169620	1.6374750	3.8946110
H	-1.3558830	1.6143630	4.7738260
H	-2.1940740	1.6335370	2.1954300
H	2.1940740	1.6335370	2.1954300
H	1.3558830	1.6143630	4.7738260
H	0.0000000	1.6456260	0.6006170
Fe	0.0000000	0.0000000	2.8997320
C	-0.7169620	-1.6374750	3.8946110
C	-1.1600030	-1.6466930	2.5309750
C	0.0000000	-1.6533990	1.6880080
C	1.1600030	-1.6466930	2.5309750
C	0.7169620	-1.6374750	3.8946110
H	-1.3558830	-1.6143630	4.7738260
H	-2.1940740	-1.6335370	2.1954300
H	2.1940740	-1.6335370	2.1954300
H	1.3558830	-1.6143630	4.7738260
H	0.0000000	-1.6456260	0.6006170
C	-1.6374750	-0.7169620	-3.8946110
C	-1.6374750	0.7169620	-3.8946110

C	-1.6466930	1.1600030	-2.5309750
C	-1.6533990	0.0000000	-1.6880080
C	-1.6466930	-1.1600030	-2.5309750
H	-1.6143630	-1.3558830	-4.7738260
H	-1.6143630	1.3558830	-4.7738260
H	-1.6456260	0.0000000	-0.6006170
H	-1.6335370	-2.1940740	-2.1954300
H	-1.6335370	2.1940740	-2.1954300
Fe	0.0000000	0.0000000	-2.8997320
C	1.6374750	0.7169620	-3.8946110
C	1.6466930	1.1600030	-2.5309750
C	1.6533990	0.0000000	-1.6880080
C	1.6466930	-1.1600030	-2.5309750
C	1.6374750	-0.7169620	-3.8946110
H	1.6143630	1.3558830	-4.7738260
H	1.6335370	2.1940740	-2.1954300
H	1.6335370	-2.1940740	-2.1954300
H	1.6143630	-1.3558830	-4.7738260
H	1.6456260	0.0000000	-0.6006170

ΔE= 0.24 kcal mol^{-1} Fe_wod_4

C	1.6446050	-1.3836840	-0.7173230
C	1.6446020	-1.3836820	0.7173210
C	2.9438800	-1.7978800	1.1601370
C	3.7465620	-2.0541390	0.0000050
C	2.9438840	-1.7978850	-1.1601310
H	0.8111750	-1.1026950	-1.3566290
H	0.8111690	-1.1026900	1.3566230
H	4.7875140	-2.3675570	0.0000080
H	3.2691050	-1.8840400	-2.1938500
H	3.2690960	-1.8840320	2.1938570
Fe	3.0856110	-0.1180580	0.0000000
C	2.6663280	1.7555870	-0.7168940
C	2.6663420	1.7555840	0.7169100
C	3.9596370	1.3238510	1.1600360
C	4.7593180	1.0574740	-0.0000140
C	3.9596140	1.3238570	-1.1600480
H	1.8278190	2.0237020	-1.3549020
H	1.8278460	2.0236960	1.3549360
H	5.7851260	0.6975430	-0.0000250
H	4.2729850	1.2015780	-2.1937940
H	4.2730280	1.2015680	2.1937760
C	-4.5631150	-1.1039660	0.7169630
C	-3.2771480	-1.5580680	1.1597120

C	-2.4822810	-1.8393870	-0.0000090
C	-3.2771610	-1.5580620	-1.1597200
C	-4.5631230	-1.1039620	-0.7169550
H	-5.3867070	-0.7954110	1.3559650
H	-2.9557100	-1.6555030	2.1936870
H	-2.9557340	-1.6554930	-2.1936990
H	-5.3867220	-0.7954040	-1.3559460
H	-1.4533480	-2.1909940	-0.0000150
Fe	-3.0877340	0.1185210	-0.0000010
C	-3.4863480	1.9927370	0.7169140
C	-2.1963930	1.5500510	1.1597580
C	-1.3981550	1.2766910	0.0000140
C	-2.1963700	1.5500470	-1.1597460
C	-3.4863340	1.9927340	-0.7169290
H	-4.3236610	2.2620350	1.3558220
H	-1.8852440	1.4253880	2.1940580
H	-1.8852000	1.4253810	-2.1940400
H	-4.3236340	2.2620300	-1.3558560
H	-0.3737690	0.9114780	0.0000250

ΔE= 0.36 kcal mol^{-1} Fe_wod_5

C	-2.8586400	-1.6862100	0.9070710
C	-3.0167570	-1.9472390	-0.4941430
C	-2.3860080	-0.8813250	-1.2172670
C	-1.8381350	0.0390300	-0.2635810
C	-2.1300670	-0.4589960	1.0493990
H	-3.2419010	-2.2998990	1.7184780
H	-3.5408390	-2.7935210	-0.9311900
H	-1.3078120	0.9598370	-0.4928880
H	-1.8657340	0.0226460	1.9876240
H	-2.3494690	-0.7775890	-2.2988840
Fe	-3.8582910	-0.1491650	-0.0001680
C	-4.9521190	1.2206370	1.0551620
C	-5.6822410	-0.0056740	0.9159970
C	-5.8428110	-0.2692370	-0.4843540
C	-5.2118490	0.7941520	-1.2104860
C	-4.6613760	1.7150010	-0.2590530
H	-4.6531700	1.6835350	1.9922670
H	-6.0346100	-0.6353500	1.7291280
H	-5.1448760	0.8771550	-2.2923570
H	-4.1031670	2.6180430	-0.4928770
H	-6.3384690	-1.1336010	-0.9191300
C	5.1311820	-0.9006070	1.2104340
C	4.2278950	-1.7895400	0.5394570

C	4.4055590	-1.6184490	-0.8730550
C	5.4185880	-0.6238340	-1.0751530
C	5.8670920	-0.1800890	0.2125970
H	5.2267260	-0.7793640	2.2865470
H	3.5176300	-2.4597350	1.0170880
H	5.7704060	-0.2562600	-2.0358580
H	6.6186530	0.5828320	0.3995530
H	3.8536740	-2.1365700	-1.6532760
C	2.8255400	1.4394710	1.2052510
C	1.9243270	0.5491030	0.5331490
C	2.1027280	0.7221470	-0.8792250
C	3.1141470	1.7189050	-1.0801050
C	3.5609160	2.1624590	0.2084890
H	2.9458610	1.5345720	2.2815590
H	1.2379940	-0.1491380	1.0056990
H	3.4909180	2.0629980	-2.0400940
H	4.3353400	2.9019000	0.3966360
H	1.5776390	0.1752120	-1.6583850
Fe	3.8589600	0.1493210	0.0000470

Ruthenocene without dispersion

ΔE= 0.0 kcal mol^{-1} Ru_wod_1

C	1.1615550	1.8104840	2.4089930
C	0.0000000	1.8138100	1.5640730
C	-1.1615550	1.8104840	2.4089930
C	-0.7180390	1.8049040	3.7749760
C	0.7180390	1.8049040	3.7749760
H	2.1956510	1.8243350	2.0744920
H	0.0000000	1.8210190	0.4766170
H	-1.3568060	1.8115300	4.6541890
H	1.3568060	1.8115300	4.6541890
H	-2.1956510	1.8243350	2.0744920
C	1.1615550	-1.8104840	2.4089930
C	0.0000000	-1.8138100	1.5640730
C	-1.1615550	-1.8104840	2.4089930
C	-0.7180390	-1.8049040	3.7749760
C	0.7180390	-1.8049040	3.7749760
H	2.1956510	-1.8243350	2.0744920
H	0.0000000	-1.8210190	0.4766170
H	-1.3568060	-1.8115300	4.6541890
H	1.3568060	-1.8115300	4.6541890
H	-2.1956510	-1.8243350	2.0744920
Ru	0.0000000	0.0000000	2.7813570

C	1.8104840	-1.1615550	-2.4089930
C	1.8049040	-0.7180390	-3.7749760
C	1.8049040	0.7180390	-3.7749760
C	1.8104840	1.1615550	-2.4089930
C	1.8138100	0.0000000	-1.5640730
H	1.8243350	-2.1956510	-2.0744920
H	1.8115300	-1.3568060	-4.6541890
H	1.8243350	2.1956510	-2.0744920
H	1.8210190	0.0000000	-0.4766170
H	1.8115300	1.3568060	-4.6541890
C	-1.8104840	-1.1615550	-2.4089930
C	-1.8049040	-0.7180390	-3.7749760
C	-1.8049040	0.7180390	-3.7749760
C	-1.8104840	1.1615550	-2.4089930
C	-1.8138100	0.0000000	-1.5640730
H	-1.8243350	-2.1956510	-2.0744920
H	-1.8115300	-1.3568060	-4.6541890
H	-1.8243350	2.1956510	-2.0744920
H	-1.8210190	0.0000000	-0.4766170
H	-1.8115300	1.3568060	-4.6541890
Ru	0.0000000	0.0000000	-2.7813570

ΔE= 0.21 kcal mol^{-1} Ru_wod_2

C	-3.9224510	-1.4262330	-1.1945690
C	-2.6967520	-1.9140100	-0.6275340
C	-2.8204630	-1.8683240	0.8026320
C	-4.1225530	-1.3524230	1.1194630
C	-4.8039330	-1.0795660	-0.1149920
H	-4.1482420	-1.3453530	-2.2545450
H	-1.8328530	-2.2719890	-1.1815200
H	-4.5262110	-1.2061460	2.1178370
H	-5.8133080	-0.6892030	-0.2146700
H	-2.0673240	-2.1867290	1.5186950
Ru	-3.0101050	0.1551280	0.0007310
C	-2.6148120	1.9405840	-1.1902360
C	-1.3823300	1.4730060	-0.6207380
C	-1.5091090	1.5200900	0.8097000
C	-2.8195440	2.0166380	1.1234710
C	-3.5027810	2.2768720	-0.1126590
H	-2.8332930	2.0351710	-2.2506400
H	-0.5007070	1.1523830	-1.1700200
H	-3.2196020	2.1788580	2.1208250
H	-4.5111210	2.6693120	-0.2146320
H	-0.7407640	1.2422300	1.5267040

C	1.8544660	-1.6434220	-1.1007960
C	3.1663340	-2.1646650	-0.8361040
C	3.3374730	-2.2309080	0.5882840
C	2.1314080	-1.7503750	1.2025310
C	1.2135100	-1.3874080	0.1591150
H	1.4184780	-1.4827400	-2.0834990
H	3.8966030	-2.4669920	-1.5820650
H	1.9425760	-1.6846870	2.2708930
H	0.2055000	-1.0010560	0.2943890
H	4.2201210	-2.5921170	1.1094660
C	3.2120800	1.7156050	-1.1065260
C	4.5179030	1.1805020	-0.8401330
C	4.6873270	1.1129930	0.5844340
C	3.4861590	1.6063430	1.1979070
C	2.5743200	1.9793050	0.1530000
H	2.7872280	1.9027630	-2.0892300
H	5.2532850	0.8889930	-1.5853600
H	3.3047440	1.6950820	2.2657990
H	1.5825270	2.4027320	0.2899160
H	5.5734050	0.7614000	1.1063160
Ru	3.0121830	-0.1557980	-0.0000990

ΔE= 0.21 kcal mol^{-1} Ru_wod_3

C	2.9577350	1.8078330	0.9526850
C	4.2869550	1.2685120	1.0202820
C	4.7564870	1.0767310	-0.3233440
C	3.7172160	1.4973400	-1.2209280
C	2.6055480	1.9495430	-0.4324660
H	2.3344810	2.0786820	1.8009710
H	4.8445780	1.0551030	1.9283640
H	3.7683810	1.4873380	-2.3064710
H	1.6681930	2.3458790	-0.8142030
H	5.7313130	0.6913250	-0.6102780
C	1.6257480	-1.5677350	0.9619450
C	2.9624570	-2.0905000	1.0122800
C	3.4193630	-2.2686630	-0.3375620
C	2.3650990	-1.8555740	-1.2211830
C	1.2557730	-1.4224950	-0.4186750
H	0.9979290	-1.3356170	1.8184970
H	3.5248060	-2.3223540	1.9129060
H	2.3974530	-1.8785200	-2.3072980
H	0.2969570	-1.0613120	-0.7831970
H	4.3886000	-2.6582660	-0.6375070
Ru	2.9877820	-0.1575310	0.0008240

C	-4.2868770	-1.2685540	-1.0203240
C	-2.9576620	-1.8078710	-0.9526060
C	-2.6055790	-1.9495260	0.4325770
C	-3.7173060	-1.4972910	1.2209380
C	-4.7565100	-1.0767190	0.3232590
H	-4.8444320	-1.0551810	-1.9284560
H	-2.3343450	-2.0787540	-1.8008340
H	-3.7685520	-1.4872450	2.3064770
H	-5.7313570	-0.6913010	0.6101050
H	-1.6682530	-2.3458460	0.8144000
C	-2.9623650	2.0904560	-1.0123640
C	-1.6256610	1.5676950	-0.9618820
C	-1.2558140	1.4225160	0.4187780
C	-2.3652140	1.8556280	1.2211660
C	-3.4193970	2.2686770	0.3374280
H	-3.5246310	2.3222700	-1.9130520
H	-0.9977610	1.3355400	-1.8183650
H	-2.3976680	1.8786200	2.3072760
H	-4.3886620	2.6582910	0.6372670
H	-0.2970310	1.0613490	0.7834060
Ru	-2.9877820	0.1575310	-0.0008250

ΔE= 0.27 kcal mol^{-1} Ru_wod_4

C	-2.1988670	-3.2758140	0.7180750
C	-1.7029840	-2.0028010	1.1611430
C	-1.3968650	-1.2145260	0.0000000
C	-1.7029840	-2.0028010	-1.1611430
C	-2.1988670	-3.2758140	-0.7180750
H	-2.5274660	-4.0912950	1.3569370
H	-1.5911500	-1.6870490	2.1951890
H	-1.5911500	-1.6870490	-2.1951890
H	-2.5274660	-4.0912950	-1.3569370
H	-1.0153370	-0.1955120	0.0000000
Ru	-0.1557890	-3.0142010	0.0000000
C	1.1547320	-4.6031860	-0.7180770
C	1.1547320	-4.6031860	0.7180770
C	1.6644270	-3.3359140	1.1615810
C	1.9798800	-2.5524420	0.0000000
C	1.6644270	-3.3359140	-1.1615810
H	0.8364340	-5.4227840	-1.3568980
H	0.8364340	-5.4227840	1.3568980
H	2.3990550	-1.5495000	0.0000000
H	1.8013020	-3.0296610	-2.1953500
H	1.8013020	-3.0296610	2.1953500

C	1.4830460	1.4337640	0.7184270
C	1.4830460	1.4337640	-0.7184270
C	1.9769780	2.7070890	-1.1620330
C	2.2823860	3.4939150	0.0000000
C	1.9769780	2.7070890	1.1620330
H	1.1757130	0.6073170	1.3542090
H	1.1757130	0.6073170	-1.3542090
H	2.6841030	4.5037550	0.0000000
H	2.1082910	3.0167230	2.1954610
H	2.1082910	3.0167230	-2.1954610
Ru	0.1551400	3.0121580	0.0000000
C	-1.3810330	4.0377600	1.1619290
C	-1.8945440	2.7723590	0.7181240
C	-1.8945440	2.7723590	-0.7181240
C	-1.3810330	4.0377600	-1.1619290
C	-1.0641330	4.8201550	0.0000000
H	-1.2647120	4.3530350	2.1954400
H	-2.2401150	1.9630130	1.3559790
H	-1.2647120	4.3530350	-2.1954400
H	-0.6645510	5.8308500	0.0000000
H	-2.2401150	1.9630130	-1.3559790

ΔE= 0.71 kcal mol^{-1} Ru_wod_5

C	-5.3933240	-0.2020520	-1.1618870
C	-5.4745720	-1.0422790	-0.0000180
C	-5.3933350	-0.2020740	1.1618680
C	-5.2617430	1.1574170	0.7180930
C	-5.2617360	1.1574310	-0.7180860
H	-5.4359770	-0.5353030	-2.1954220
H	-5.5895800	-2.1229460	-0.0000290
H	-5.1878310	2.0335690	1.3568100
H	-5.1878190	2.0335940	-1.3567860
H	-5.4359980	-0.5353430	2.1953960
C	-1.7957250	-0.5518110	-1.1622860
C	-1.8784100	-1.3924790	-0.0000030
C	-1.7957350	-0.5518290	1.1622950
C	-1.6625040	0.8075780	0.7182570
C	-1.6624980	0.8075890	-0.7182260
H	-1.8178280	-0.8869690	-2.1958590
H	-1.9751450	-2.4750520	-0.0000120
H	-1.5674830	1.6813940	1.3575780
H	-1.5674710	1.6814160	-1.3575330
H	-1.8178480	-0.8870040	2.1958620
Ru	-3.5575320	-0.0006600	0.0000010

C	3.3428650	1.8325120	1.1617470
C	4.7042610	1.7180410	0.7181180
C	4.7042570	1.7180420	-0.7181250
C	3.3428580	1.8325140	-1.1617440
C	2.5009730	1.9026470	0.0000040
H	3.0089880	1.8692360	2.1953680
H	5.5812970	1.6556030	1.3568980
H	3.0089750	1.8692390	-2.1953640
H	1.4175220	1.9913040	0.0000070
H	5.5812890	1.6556050	-1.3569100
Ru	3.5639100	0.0005680	-0.0000010
C	3.0133080	-1.7612590	1.1611950
C	4.3731930	-1.8950820	0.7181350
C	4.3731880	-1.8950810	-0.7181440
C	3.0133010	-1.7612580	-1.1611950
C	2.1720330	-1.6779870	0.0000030
H	2.6781330	-1.7365480	2.1947720
H	5.2469690	-1.9924850	1.3570430
H	2.6781200	-1.7365460	-2.1947700
H	1.0901620	-1.5697070	0.0000060
H	5.2469600	-1.9924840	-1.3570570

ΔE= 0.91 kcal mol^{-1} Ru_wod_6

C	5.3278170	1.4953100	0.2434290
C	5.5201550	0.5281770	1.2876230
C	5.8771470	-0.7210170	0.6754770
C	5.9053760	-0.5260310	-0.7471130
C	5.5658090	0.8437120	-1.0141150
H	5.0603850	2.5395980	0.3813540
H	5.4243930	0.7124100	2.3543930
H	6.1526040	-1.2794300	-1.4903180
H	5.5103860	1.3086620	-1.9948580
H	6.0991440	-1.6478590	1.1977600
C	1.8344690	0.5955970	0.0499090
C	2.0250250	-0.3713620	1.0949030
C	2.3798720	-1.6221140	0.4840600
C	2.4081450	-1.4286780	-0.9388190
C	2.0708590	-0.0583010	-1.2071020
H	-1.3811930	0.5934640	1.4589070
H	1.9118790	-0.1906680	2.1607100
H	2.6333020	-2.1886080	-1.6824300
H	1.9981010	0.4014090	-2.1893160
H	2.5800580	-2.5540750	1.0060610
Ru	3.8914670	-0.1276030	-0.0074550

C	-3.2002500	1.8807900	1.1060470
C	-2.0712220	1.0621490	0.7622120
C	-2.0014010	0.9799740	-0.6697250
C	-3.0875260	1.7479990	-1.2114270
C	-3.8286000	2.3050330	-0.1140770
H	-3.5169420	2.1431840	2.1120820
H	1.5450210	1.6342990	0.1848380
H	-3.3046020	1.8919050	-2.2666080
H	-4.7033300	2.9452150	-0.1931270
H	-1.2485310	0.4398190	-1.2376980
Ru	-3.8928710	0.1278450	0.0073940
C	-5.3084390	-1.0570280	1.1703000
C	-4.1764430	-1.8726520	0.8291700
C	-4.1045600	-1.9556250	-0.6028530
C	-5.1921540	-1.1912600	-1.1467590
C	-5.9361660	-0.6357910	-0.0509390
H	-5.6391210	-0.8116930	2.1760860
H	-3.4992420	-2.3519020	1.5311640
H	-5.4194740	-1.0653890	-2.2020530
H	-6.8251300	-0.0158030	-0.1314940
H	-3.3634260	-2.5084480	-1.1739890

ΔE= 0.96 kcal mol^{-1} Ru_wod_7

C	6.0200340	-0.1639730	0.8301130
C	6.0935600	-0.3365300	-0.5938020
C	5.5260440	0.8290900	-1.2119280
C	5.1017080	1.7219880	-0.1701000
C	5.4069470	1.1081680	1.0919070
H	6.3768810	-0.8671140	1.5780310
H	6.5158810	-1.1931110	-1.1124710
H	4.6408020	2.6959400	-0.3117510
H	5.2180510	1.5365440	2.0726920
H	5.4432450	1.0093010	-2.2804670
C	2.7641700	-1.7367060	0.8511510
C	2.8357630	-1.9070290	-0.5732040
C	2.2688720	-0.7395350	-1.1887430
C	1.8471710	0.1530610	-0.1453830
C	2.1530710	-0.4637700	1.1154680
H	3.1022180	-2.4505490	1.5976670
H	3.2371910	-2.7725370	-1.0936620
H	1.3659300	1.1175090	-0.2842130
H	1.9495200	-0.0442670	2.0973000
H	2.1675060	-0.5663170	-2.2569220
Ru	4.0019810	-0.1545970	0.0003530

C	-4.6735820	-1.7193630	-0.8922760
C	-4.4928770	-1.9056210	0.5202900
C	-5.3927800	-1.0188310	1.2034800
C	-6.1295060	-0.2844230	0.2131530
C	-5.6850100	-0.7174190	-1.0821370
H	-4.1454500	-2.2514440	-1.6790810
H	-3.8036600	-2.6027880	0.9893520
H	-6.8973450	0.4592340	0.4094440
H	-6.0573990	-0.3587380	-2.0380730
H	-5.5052910	-0.9283470	2.2806410
C	-2.1280130	0.8435150	-0.8776570
C	-1.9483120	0.6564890	0.5350390
C	-2.8456240	1.5465700	1.2175210
C	-3.5799810	2.2832260	0.2268190
C	-3.1363450	1.8485990	-1.0683920
H	-1.5866560	0.3216070	-1.6623910
H	-1.2457350	-0.0296540	1.0007100
H	-4.3303240	3.0446310	0.4228300
H	-3.4928760	2.2230920	-2.0243430
H	-2.9437560	1.6528170	2.2947020
Ru	-4.0029040	0.1550320	-0.0005330

Osmocene without dispersion

ΔE= 0.0 kcal mol^{-1}		Os_wod_1	
C	1.2479510	1.4163150	-0.4189080
C	2.3612890	1.8441340	-1.2241740
C	3.4206300	2.2532580	-0.3396910
C	2.9629210	2.0777090	1.0135400
C	1.6206040	1.5607450	0.9642980
H	0.2848960	1.0649920	-0.7814990
H	2.3907990	1.8720270	-2.3099900
H	3.5246530	2.3131590	1.9132960
H	0.9898680	1.3379400	1.8208370
H	4.3891180	2.6433090	-0.6405030
Os	2.9830430	0.1256900	0.0007920
C	2.5932940	-1.9977700	-0.4316340
C	3.7084990	-1.5513590	-1.2240610
C	4.7539960	-1.1354490	-0.3265710
C	4.2848470	-1.3243400	1.0208880
C	2.9495940	-1.8572110	0.9558400
H	1.6554570	-2.3941600	-0.8114270
H	3.7600880	-1.5479870	-2.3093560

H	4.8475540	-1.1197600	1.9275310
H	2.3289070	-2.1296890	1.8051450
H	5.7323960	-0.7613870	-0.6152950
C	-2.9495900	1.8572140	-0.9558330
C	-2.5932970	1.9977690	0.4316430
C	-3.7085060	1.5513550	1.2240630
C	-4.7539980	1.1354480	0.3265670
C	-4.2848430	1.3243430	-1.0208900
H	-2.3288990	2.1296950	-1.8051340
H	-1.6554630	2.3941570	0.8114420
H	-5.7324000	0.7613840	0.6152850
H	-4.8475450	1.1197660	-1.9275360
H	-3.7601000	1.5479790	2.3093580
Os	-2.9830430	-0.1256910	-0.0007920
C	-1.2479530	-1.4163160	0.4189130
C	-2.3612950	-1.8441390	1.2241710
C	-3.4206300	-2.2532600	0.3396800
C	-2.9629140	-2.0777040	-1.0135480
C	-1.6205970	-1.5607390	-0.9642960
H	-0.2849000	-1.0649930	0.7815110
H	-2.3908110	-1.8720360	2.3099860
H	-3.5246400	-2.3131510	-1.9133080
H	-0.9898570	-1.3379300	-1.8208300
H	-4.3891200	-2.6433140	0.6404850

ΔE= 0.05 kcal mol^{-1} Os_wod_2

C	1.7149930	-3.3231040	1.1641260
C	1.2111350	-4.5958450	0.7196170
C	1.2111350	-4.5958450	-0.7196170
C	1.7149930	-3.3231040	-1.1641260
C	2.0267130	-2.5361730	0.0000000
H	1.8560800	-3.0186170	2.1975730
H	0.9032190	-5.4192070	1.3582200
H	1.8560800	-3.0186170	-2.1975730
H	2.4458180	-1.5335310	0.0000000
H	0.9032190	-5.4192070	-1.3582200
C	-1.6949050	-1.9936010	1.1635530
C	-2.1852600	-3.2719630	0.7196250
C	-2.1852600	-3.2719630	-0.7196250
C	-1.6949050	-1.9936010	-1.1635530
C	-1.3922630	-1.2018990	0.0000000
H	-1.5904570	-1.6751530	2.1972600
H	-2.5153740	-4.0866340	1.3582860
H	-1.5904570	-1.6751530	-2.1972600

H	-1.0214020	-0.1789340	0.0000000
H	-2.5153740	-4.0866340	-1.3582860
Os	-0.1248750	-3.0045810	0.0000000
C	1.9649610	2.6955320	1.1645780
C	1.4726710	1.4184480	0.7199770
C	1.4726710	1.4184480	-0.7199770
C	1.9649610	2.6955320	-1.1645780
C	2.2695450	3.4846290	0.0000000
H	2.1014510	3.0031380	2.1976600
H	1.1724460	0.5888830	1.3546760
H	2.1014510	3.0031380	-2.1976600
H	2.6746610	4.4928230	0.0000000
H	1.1724460	0.5888830	-1.3546760
C	-1.4315290	4.0332900	1.1644610
C	-1.9431310	2.7639720	0.7196850
C	-1.9431310	2.7639720	-0.7196850
C	-1.4315290	4.0332900	-1.1644610
C	-1.1159160	4.8180980	0.0000000
H	-1.3218910	4.3511100	2.1976360
H	-2.2921810	1.9562890	1.3573230
H	-1.3218910	4.3511100	-2.1976360
H	-0.7243850	5.8316470	0.0000000
H	-2.2921810	1.9562890	-1.3573230
Os	0.1243890	3.0029980	0.0000000

ΔE= 0.15 kcal mol^{-1} Os_wod_3

C	1.5167160	1.2946580	-1.2944900
C	2.3638210	2.1163310	-0.4701740
C	3.7328100	1.7998880	-0.7821660
C	3.7327850	0.7823530	-1.7998250
C	2.3637900	0.4704130	-2.1162700
H	0.4292400	1.2991620	-1.2989300
H	2.0296350	2.8612150	0.2470510
H	4.6116330	0.3415050	-2.2621810
H	2.0295810	-0.2467450	-2.8612120
H	4.6116830	2.2621910	-0.3413140
C	1.5167570	-1.2945910	1.2945730
C	2.3639460	-0.4704150	2.1163120
C	3.7329040	-0.7824020	1.7997410
C	3.7327930	-1.7999260	0.7820700
C	2.3637720	-2.1163050	0.4701930
H	0.4292790	-1.2991070	1.2991780
H	2.0298360	0.2467650	2.8612770
H	4.6116080	-2.2622410	0.3411180

H	2.0295010	-2.8610990	-0.2470870
H	4.6118140	-0.3416170	2.2620400
Os	2.7394500	0.0000120	0.0000090
C	-2.3639280	2.1163160	0.4703280
C	-3.7329050	1.7997880	0.7822850
C	-3.7328540	0.7821660	1.7998560
C	-2.3638470	0.4702760	2.1163040
C	-1.5167990	1.2946140	1.2945910
H	-2.0297690	2.8612810	-0.2468300
H	-4.6117820	2.2620920	0.3414400
H	-2.0296160	-0.2469400	2.8611760
H	-0.4293240	1.2991350	1.2990720
H	-4.6117010	0.3412600	2.2621600
C	-2.3639230	-0.4702580	-2.1163350
C	-3.7328540	-0.7823630	-1.7997850
C	-3.7326640	-1.7999720	-0.7821980
C	-2.3636200	-2.1162660	-0.4703390
C	-1.5166660	-1.2944210	-1.2946500
H	-2.0298600	0.2470350	-2.8612090
H	-4.6117970	-0.3416040	-2.2620430
H	-2.0293020	-2.8610940	0.2468870
H	-0.4291880	-1.2988520	-1.2992850
H	-4.6114410	-2.2623850	-0.3412680
Os	-2.7394530	-0.0000020	-0.0000110

ΔE= 0.81 kcal mol^{-1} Os_wod_4

C	5.8315000	0.1517980	-1.2793280
C	5.1026510	1.3907780	-1.2057210
C	5.0861790	1.8162400	0.1691350
C	5.8049880	0.8402320	0.9453220
C	6.2656580	-0.1884330	0.0501300
H	6.0349540	-0.4167490	-2.1825920
H	4.6592260	1.9217980	-2.0435320
H	5.9849940	0.8825230	2.0159950
H	6.8547040	-1.0586170	0.3264240
H	4.6272580	2.7240070	0.5510360
C	2.7303870	-1.7049100	-0.7397880
C	2.0027840	-0.4646210	-0.6702950
C	1.9847680	-0.0351690	0.7037430
C	2.7012610	-1.0104380	1.4832120
C	3.1621700	-2.0421070	0.5913270
H	2.9060430	-2.2931690	-1.6362480
H	1.5332810	0.0495980	-1.5044940
H	2.8518150	-0.9823310	2.5589000

H	3.7210380	-2.9294590	0.8755750
H	1.4961110	0.8569070	1.0858020
Os	4.0676200	-0.1258500	0.0045920
C	-1.8852490	0.3510040	0.1514970
C	-2.3617880	1.1313350	-0.9603770
C	-3.2697450	2.1256080	-0.4510560
C	-3.3546280	1.9600540	0.9763180
C	-2.4991230	0.8636840	1.3482790
H	-1.1698750	-0.4652390	0.1001420
H	-2.0734290	1.0035310	-2.0002220
H	-3.9454290	2.5683810	1.6556410
H	-2.3318900	0.4979520	2.3576840
H	-3.7850430	2.8808330	-1.0381630
C	-4.6698880	-1.9702100	-0.2875740
C	-5.1500140	-1.1885820	-1.3967610
C	-6.0583320	-0.1974560	-0.8825890
C	-6.1396660	-0.3665330	0.5444820
C	-5.2816550	-1.4621680	0.9121590
H	-3.9810070	-2.8082810	-0.3475780
H	-4.8879790	-1.3340070	-2.4411420
H	-6.7557170	0.2174940	1.2226590
H	-5.1361130	-1.8501540	1.9165420
H	-6.6021390	0.5367330	-1.4706100
Os	-4.0678080	0.1258180	-0.0047830