

Supporting Information belonging to the manuscript:

Multimetallocenes. A Theoretical Study

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Cartesian coordinates (in Å) and total energies (in a. u.) of all the metallocenes discussed in the text.

All calculations have been performed at the BP86/TZ2P level of theory.

CpBe₂Cp: E = -4.78364725

Be	0.000000	0.000000	1.038298
Be	0.000000	0.000000	-1.038298
C	-0.373602	-1.149828	-2.589145
C	0.978102	-0.710633	-2.589145
C	0.978102	0.710633	-2.589145
C	-0.373602	1.149828	-2.589145
C	-1.209000	0.000000	-2.589145
C	-0.373602	1.149828	2.589145
C	0.978102	0.710633	2.589145
C	0.978102	-0.710633	2.589145
C	-0.373602	-1.149828	2.589145
C	-1.209000	0.000000	2.589145
H	-0.708146	-2.179449	-2.531073
H	1.853950	-1.346973	-2.531073
H	1.853950	1.346973	-2.531073
H	-0.708146	2.179449	-2.531073
H	-2.291608	0.000000	-2.531073
H	-0.708146	2.179449	2.531073
H	1.853950	1.346973	2.531073
H	1.853950	-1.346973	2.531073
H	-0.708146	-2.179449	2.531073
H	-2.291608	0.000000	2.531073

CpBe₃Cp: E = -4.83280871

Be	0.000000	0.000000	0.000000
Be	0.000000	0.000000	2.112471
Be	0.000000	0.000000	-2.112471
C	-0.373655	1.149992	3.659911
C	0.978242	0.710734	3.659911

C	0.978242	-0.710734	3.659911
C	-0.373655	-1.149992	3.659911
C	-1.209174	0.000000	3.659911
C	-0.373655	1.149992	-3.659911
C	-1.209174	0.000000	-3.659911
C	-0.373655	-1.149992	-3.659911
C	0.978242	-0.710734	-3.659911
C	0.978242	0.710734	-3.659911
H	-0.708211	2.179648	3.602714
H	1.854120	1.347097	3.602714
H	1.854120	-1.347097	3.602714
H	-0.708211	-2.179648	3.602714
H	-2.291818	0.000000	3.602714
H	1.854120	1.347097	-3.602714
H	1.854120	-1.347097	-3.602714
H	-0.708211	-2.179648	-3.602714
H	-2.291818	0.000000	-3.602714
H	-0.708211	2.179648	-3.602714

CpBe₄Cp: E = -4.87956723

Be	0.000000	0.000000	1.085518
Be	0.000000	0.000000	-1.085518
Be	0.000000	0.000000	3.198163
Be	0.000000	0.000000	-3.198163
C	1.209194	0.000000	-4.743202
C	0.373661	1.150012	-4.743202
C	-0.978258	0.710746	-4.743202
C	-0.978258	-0.710746	-4.743202
C	0.373661	-1.150012	-4.743202
C	0.373661	1.150012	4.743202
C	1.209194	0.000000	4.743202
C	0.373661	-1.150012	4.743202
C	-0.978258	-0.710746	4.743202
C	-0.978258	0.710746	4.743202
H	2.291855	0.000000	-4.686295
H	0.708222	2.179683	-4.686295
H	-1.854149	1.347118	-4.686295
H	-1.854149	-1.347118	-4.686295
H	0.708222	-2.179683	-4.686295
H	0.708222	2.179683	4.686295
H	2.291855	0.000000	4.686295
H	0.708222	-2.179683	4.686295
H	-1.854149	-1.347118	4.686295
H	-1.854149	1.347118	4.686295

CpBe₅Cp: E = -4.92620401

Be	0.000000	0.000000	0.000000
Be	0.000000	0.000000	2.175207
Be	0.000000	0.000000	-2.175207
Be	0.000000	0.000000	-4.287596
Be	0.000000	0.000000	4.287596
C	-0.373679	-1.150066	5.831852
C	-1.209251	0.000000	5.831852
C	-0.373679	1.150066	5.831852
C	0.978305	0.710780	5.831852
C	0.978305	-0.710780	5.831852
C	-0.373679	-1.150066	-5.831852
C	0.978305	-0.710780	-5.831852
C	0.978305	0.710780	-5.831852
C	-0.373679	1.150066	-5.831852
C	-1.209251	0.000000	-5.831852

H	-0.708243	2.179748	5.775128
H	-2.291922	0.000000	5.775128
H	-0.708243	-2.179748	5.775128
H	1.854204	-1.347158	5.775128
H	1.854204	1.347158	5.775128
H	1.854204	1.347158	-5.775128
H	1.854204	-1.347158	-5.775128
H	-0.708243	-2.179748	-5.775128
H	-2.291922	0.000000	-5.775128
H	-0.708243	2.179748	-5.775128

CpMg₂Cp: E = -4.64612376

Mg	0.000000	0.000000	1.404428
Mg	0.000000	0.000000	-1.404428
C	-0.979814	-0.711876	-3.449159
C	0.374256	-1.151840	-3.449159
C	1.211116	0.000000	-3.449159
C	0.374256	1.151840	-3.449159
C	-0.979814	0.711876	-3.449159
C	0.374256	1.151840	3.449159
C	1.211116	0.000000	3.449159
C	0.374256	-1.151840	3.449159
C	-0.979814	-0.711876	3.449159
C	-0.979814	0.711876	3.449159
H	-1.858080	-1.349974	-3.472716
H	0.709723	-2.184304	-3.472716
H	2.296713	0.000000	-3.472716
H	0.709723	2.184304	-3.472716
H	-1.858080	1.349974	-3.472716
H	0.709723	2.184304	3.472716
H	2.296713	0.000000	3.472716
H	0.709723	-2.184304	3.472716
H	-1.858080	-1.349974	3.472716
H	-1.858080	1.349974	3.472716

CpMg₃Cp: E = -4.65237348

Mg	0.000000	0.000000	0.000000
Mg	0.000000	0.000000	2.893835
Mg	0.000000	0.000000	-2.893835
C	-0.374158	1.151539	4.955206
C	0.979558	0.711690	4.955206
C	0.979558	-0.711690	4.955206
C	-0.374158	-1.151539	4.955206
C	-1.210800	0.000000	4.955206
C	-0.374158	1.151539	-4.955206
C	-1.210800	0.000000	-4.955206
C	-0.374158	-1.151539	-4.955206
C	0.979558	-0.711690	-4.955206
C	0.979558	0.711690	-4.955206
H	-0.709626	2.184004	4.979884
H	1.857825	1.349789	4.979884
H	1.857825	-1.349789	4.979884
H	-0.709626	-2.184004	4.979884
H	-2.296398	0.000000	4.979884
H	1.857825	1.349789	-4.979884
H	1.857825	-1.349789	-4.979884
H	-0.709626	-2.184004	-4.979884
H	-2.296398	0.000000	-4.979884
H	-0.709626	2.184004	-4.979884

CpMg₄Cp: E = -4.65841607

Mg	0.000000	0.000000	1.493145
Mg	0.000000	0.000000	-1.493145
Mg	0.000000	0.000000	4.410940
Mg	0.000000	0.000000	-4.410940
C	1.210635	0.000000	-6.479544
C	0.374107	1.151382	-6.479544
C	-0.979424	0.711593	-6.479544
C	-0.979424	-0.711593	-6.479544
C	0.374107	-1.151382	-6.479544
C	0.374107	1.151382	6.479544
C	1.210635	0.000000	6.479544
C	0.374107	-1.151382	6.479544
C	-0.979424	-0.711593	6.479544
C	-0.979424	0.711593	6.479544
H	2.296271	0.000000	-6.503753
H	0.709587	2.183883	-6.503753
H	-1.857722	1.349714	-6.503753
H	-1.857722	-1.349714	-6.503753
H	0.709587	-2.183883	-6.503753
H	0.709587	2.183883	6.503753
H	2.296271	0.000000	6.503753
H	0.709587	-2.183883	6.503753
H	-1.857722	-1.349714	6.503753
H	-1.857722	1.349714	6.503753

CpMg₅Cp: E = -4.66460949

Mg	0.000000	0.000000	0.000000
Mg	0.000000	0.000000	3.018284
Mg	0.000000	0.000000	-3.018284
Mg	0.000000	0.000000	5.951312
Mg	0.000000	0.000000	-5.951312
C	-0.374082	1.151307	8.024987
C	0.979360	0.711547	8.024987
C	0.979360	-0.711547	8.024987
C	-0.374082	-1.151307	8.024987
C	-1.210556	0.000000	8.024987
C	-0.374082	1.151307	-8.024987
C	-1.210556	0.000000	-8.024987
C	-0.374082	-1.151307	-8.024987
C	0.979360	-0.711547	-8.024987
C	0.979360	0.711547	-8.024987
H	-0.709562	2.183809	8.049509
H	1.857659	1.349668	8.049509
H	1.857659	-1.349668	8.049509
H	-0.709562	-2.183809	8.049509
H	-2.296192	0.000000	8.049509
H	1.857659	-1.349668	-8.049509
H	-0.709562	-2.183809	-8.049509
H	-2.296192	0.000000	-8.049509
H	-0.709562	2.183809	-8.049509
H	1.857659	1.349668	-8.049509

CpCa₂Cp: E = -4.70616709

Ca	0.000000	0.000000	1.980580
Ca	0.000000	0.000000	-1.980580
C	-0.373538	-1.149631	-4.351733
C	0.977935	-0.710511	-4.351733
C	0.977935	0.710511	-4.351733
C	-0.373538	1.149631	-4.351733

C	-1.208794	0.000000	-4.351733
C	-0.373538	1.149631	4.351733
C	0.977935	0.710511	4.351733
C	0.977935	-0.710511	4.351733
C	-0.373538	-1.149631	4.351733
C	-1.208794	0.000000	4.351733
H	-0.709219	-2.182752	-4.383947
H	1.856760	-1.349015	-4.383947
H	1.856760	1.349015	-4.383947
H	-0.709219	2.182752	-4.383947
H	-2.295081	0.000000	-4.383947
H	-0.709219	2.182752	4.383947
H	1.856760	1.349015	4.383947
H	1.856760	-1.349015	4.383947
H	-0.709219	-2.182752	4.383947
H	-2.295081	0.000000	4.383947

CpCa₃Cp: E = -4.71157556

Ca	0.000000	0.000000	0.000000
Ca	0.000000	0.000000	4.031884
Ca	0.000000	0.000000	-4.031884
C	-0.373507	1.149537	6.407145
C	0.977855	0.710453	6.407145
C	0.977855	-0.710453	6.407145
C	-0.373507	-1.149537	6.407145
C	-1.208695	0.000000	6.407145
C	-0.373507	1.149537	-6.407145
C	-1.208695	0.000000	-6.407145
C	-0.373507	-1.149537	-6.407145
C	0.977855	-0.710453	-6.407145
C	0.977855	0.710453	-6.407145
H	-0.709194	2.182674	6.438633
H	1.856694	1.348967	6.438633
H	1.856694	-1.348967	6.438633
H	-0.709194	-2.182674	6.438633
H	-2.295000	0.000000	6.438633
H	1.856694	1.348967	-6.438633
H	1.856694	-1.348967	-6.438633
H	-0.709194	-2.182674	-6.438633
H	-2.295000	0.000000	-6.438633
H	-0.709194	2.182674	-6.438633

CpCa₄Cp: E = -4.71712932

Ca	0.000000	0.000000	2.074335
Ca	0.000000	0.000000	-2.074335
Ca	0.000000	0.000000	6.152386
Ca	0.000000	0.000000	-6.152386
C	0.977807	0.710418	-8.529311
C	-0.373489	1.149481	-8.529311
C	-1.208636	0.000000	-8.529311
C	-0.373489	-1.149481	-8.529311
C	0.977807	-0.710418	-8.529311
C	-0.373489	1.149481	8.529311
C	0.977807	0.710418	8.529311
C	0.977807	-0.710418	8.529311
C	-0.373489	-1.149481	8.529311
C	-1.208636	0.000000	8.529311
H	1.856628	1.348919	-8.560692
H	-0.709169	2.182597	-8.560692
H	-2.294918	0.000000	-8.560692
H	-0.709169	-2.182597	-8.560692

H	1.856628	-1.348919	-8.560692
H	-0.709169	2.182597	8.560692
H	1.856628	1.348919	8.560692
H	1.856628	-1.348919	8.560692
H	-0.709169	-2.182597	8.560692
H	-2.294918	0.000000	8.560692

CpCa₅Cp: E = -4.72333989

Ca	0.000000	0.000000	0.000000
Ca	0.000000	0.000000	4.195855
Ca	0.000000	0.000000	-4.195855
Ca	0.000000	0.000000	8.285122
Ca	0.000000	0.000000	-8.285122
C	0.373482	1.149459	10.661387
C	1.208613	0.000000	10.661387
C	0.373482	-1.149459	10.661387
C	-0.977788	-0.710405	10.661387
C	-0.977788	0.710405	10.661387
C	0.373482	1.149459	-10.661387
C	-0.977788	0.710405	-10.661387
C	-0.977788	-0.710405	-10.661387
C	0.373482	-1.149459	-10.661387
C	1.208613	0.000000	-10.661387
H	0.709165	2.182585	10.692014
H	2.294906	0.000000	10.692014
H	0.709165	-2.182585	10.692014
H	-1.856618	-1.348912	10.692014
H	-1.856618	1.348912	10.692014
H	0.709165	-2.182585	-10.692014
H	-1.856618	-1.348912	-10.692014
H	-1.856618	1.348912	-10.692014
H	0.709165	2.182585	-10.692014
H	2.294906	0.000000	-10.692014

CpZn₂Cp: E = -4.57544053

Zn	0.000000	0.000000	1.138421
Zn	0.000000	0.000000	-1.138421
C	-0.982206	-0.713615	-3.109426
C	0.375169	-1.154653	-3.109426
C	1.214074	0.000000	-3.109426
C	0.375169	1.154653	-3.109426
C	-0.982206	0.713615	-3.109426
C	0.375169	1.154653	3.109426
C	1.214074	0.000000	3.109426
C	0.375169	-1.154653	3.109426
C	-0.982206	-0.713615	3.109426
C	-0.982206	0.713615	3.109426
H	-1.860425	-1.351678	-3.121394
H	0.710619	-2.187061	-3.121394
H	2.299612	0.000000	-3.121394
H	0.710619	2.187061	-3.121394
H	-1.860425	1.351678	-3.121394
H	0.710619	2.187061	3.121394
H	2.299612	0.000000	3.121394
H	0.710619	-2.187061	3.121394
H	-1.860425	-1.351678	3.121394
H	-1.860425	1.351678	3.121394

CpZn₃Cp: E = -4.58319077

Zn	0.000000	0.000000	0.000000
Zn	0.000000	0.000000	2.339580
Zn	0.000000	0.000000	-2.339580
C	-0.374899	1.153819	4.339436
C	0.981497	0.713099	4.339436
C	0.981497	-0.713099	4.339436
C	-0.374899	-1.153819	4.339436
C	-1.213197	0.000000	4.339436
C	-0.374899	1.153819	-4.339436
C	-1.213197	0.000000	-4.339436
C	-0.374899	-1.153819	-4.339436
C	0.981497	-0.713099	-4.339436
C	0.981497	0.713099	-4.339436
H	-0.710348	2.186227	4.353147
H	1.859715	1.351162	4.353147
H	1.859715	-1.351162	4.353147
H	-0.710348	-2.186227	4.353147
H	-2.298735	0.000000	4.353147
H	1.859715	1.351162	-4.353147
H	1.859715	-1.351162	-4.353147
H	-0.710348	-2.186227	-4.353147
H	-2.298735	0.000000	-4.353147
H	-0.710348	2.186227	-4.353147

CpZn₄Cp: E = -4.58621039

Zn	0.000000	0.000000	1.214421
Zn	0.000000	0.000000	-1.214421
Zn	0.000000	0.000000	3.576521
Zn	0.000000	0.000000	-3.576521
C	1.212782	0.000000	-5.593373
C	0.374770	1.153424	-5.593373
C	-0.981161	0.712855	-5.593373
C	-0.981161	-0.712855	-5.593373
C	0.374770	-1.153424	-5.593373
C	0.374770	1.153424	5.593373
C	1.212782	0.000000	5.593373
C	0.374770	-1.153424	5.593373
C	-0.981161	-0.712855	5.593373
C	-0.981161	0.712855	5.593373
H	2.298325	0.000000	-5.608154
H	0.710221	2.185837	-5.608154
H	-1.859384	1.350921	-5.608154
H	-1.859384	-1.350921	-5.608154
H	0.710221	-2.185837	-5.608154
H	0.710221	2.185837	5.608154
H	2.298325	0.000000	5.608154
H	0.710221	-2.185837	5.608154
H	-1.859384	-1.350921	5.608154
H	-1.859384	1.350921	5.608154

CpZn₅Cp: E = -4.58621133

Zn	0.000000	0.000000	0.000000
Zn	0.000000	0.000000	2.454133
Zn	0.000000	0.000000	-2.454133
Zn	0.000000	0.000000	4.827500
Zn	0.000000	0.000000	-4.827500
C	-0.374702	1.153213	6.854899
C	0.980982	0.712725	6.854899
C	0.980982	-0.712725	6.854899

C	-0.374702	-1.153213	6.854899
C	-1.212560	0.000000	6.854899
C	-0.374702	1.153213	-6.854899
C	-1.212560	0.000000	-6.854899
C	-0.374702	-1.153213	-6.854899
C	0.980982	-0.712725	-6.854899
C	0.980982	0.712725	-6.854899
H	-0.710164	2.185659	6.870040
H	1.859233	1.350812	6.870040
H	1.859233	-1.350812	6.870040
H	-0.710164	-2.185659	6.870040
H	-2.298138	0.000000	6.870040
H	1.859233	-1.350812	-6.870040
H	-0.710164	-2.185659	-6.870040
H	-2.298138	0.000000	-6.870040
H	-0.710164	2.185659	-6.870040
H	1.859233	1.350812	-6.870040