Supporting Information

Dimetallaborane Analogues of Pentaborane

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[2]*Department of Chemistry, University of Georgia, Athens, Georgia, 30602*

Complete Gaussian09 Reference (reference 37): Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1. Initial structures of type $Cp_2M_2B_3H_7$ 35 in all.

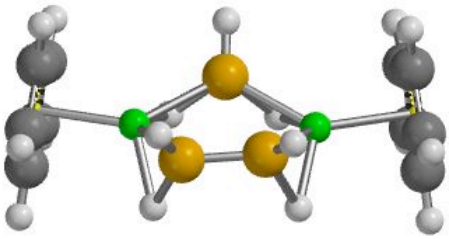
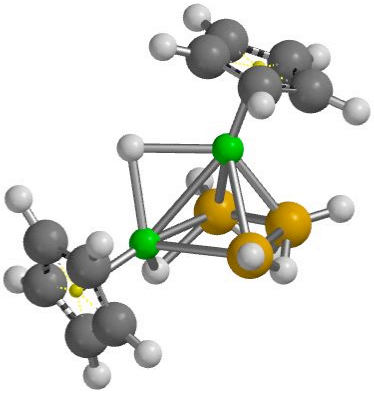
 Pentagonal structure (32 structures)	 Tetragonal pyramid (3 structures)

Table S2A. Distance table for the lowest-lying $Cp_2Pd_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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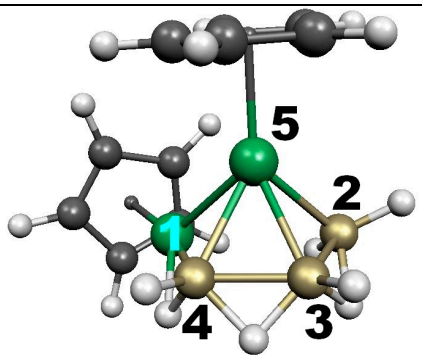
<td> 

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5 Pd 2.603519 2.173146 2.105774 2.130534 0.000000

Pd1-H-B4 Pd1-H 1.71 B4-H 1.31
B2-H-B3 B2-H 1.34 B3-H 1.29
B3-H-B4 B3-H 1.29 B4-H 1.35
B2-H 1.19
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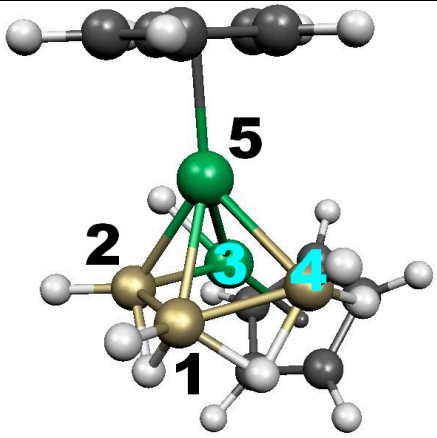
<td> 

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5 Pd 2.127885 2.091344 2.633775 2.167422 0.000000

Pd3-H-Pd5 Pd3-H 1.55 Pd5-H 2.66
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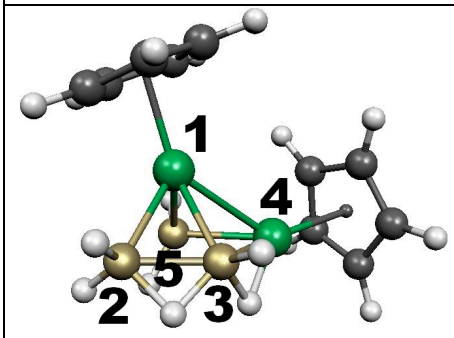
<td> 

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3 B 2.144162 1.790523 0.000000
4 Pd 2.575369 3.551225 2.259891 0.000000
5 B 2.141670 2.959917 2.887507 2.161034 0.000000

Pd4-H-B3 Pd4-H 1.72 B3-H 1.33
B2-H-B3 B2-H 1.33 B3-H 1.30
B2-H 1.19
B5-H 1.19
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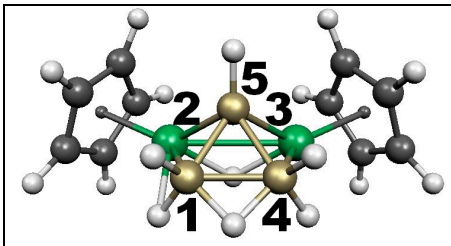
<td> 

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Pd3-H-B4 Pd3-H 2.06 B4-H 1.23
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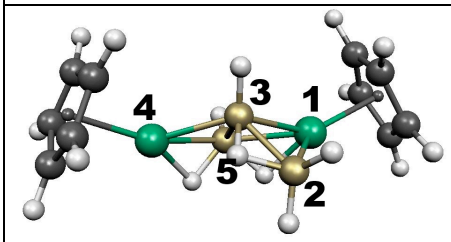
<td> 

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Pd4-H-B5 Pd4-H 1.75 B5-H 1.32
B2-H-B3 B2-H 1.31 B3-H 1.30</td>
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Table S2B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Pd_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	4_Pd_A	-721.67435450	0.00
2	8_Pd_A1.log	-721.66370120	6.69
3	4_Pd_Pentagon-2-Cb	-721.65612630	11.44
4	4_Pd_Pentagon-2-Cg	-721.65515890	12.05
5	4_Pd_Pentagon-2-Ad	-721.65455060	12.43
6	4_Pd_Pentagon-1-Ba	-721.65217520	13.92
7	4_Pd_Pentagon-2-Aa	-721.64831410	16.34
8	4_Pd_C	-721.64585650	17.88
9	4_Pd_Pentagon-1-Bd	-721.64499880	18.42
10	4_Pd_Pentagon-1-Bb	-721.64499880	18.42
11	4_Pd_Pentagon-2-Be	-721.64356710	19.32
12	4_Pd_Pentagon-2-Ca	-721.64351960	19.35
13	4_Pd_Pentagon-2-Ch	-721.64300000	19.68
14	4_Pd_Pentagon-1-Bc	-721.64281530	19.79
15	4_Pd_Pentagon-2-Bd	-721.64099130	20.94
16	4_Pd_Pentagon-2-Ce	-721.63741550	23.18
17	4_Pd_Pentagon-1-Ca	-721.63652830	23.74
18	8_Pd_A2.log	-721.63465600	24.91
19	4_Pd_B	-721.63382280	25.43
20	4_Pd_Pentagon-2-Cc	-721.63380600	25.44
21	4_Pd_Pentagon-2-Ab	-721.63236490	26.35
22	4_Pd_Pentagon-2-Cf	-721.63181570	26.69
23	4_Pd_Pentagon-2-Ba	-721.62624920	30.19
24	4_Pd_Pentagon-1-Be	-721.62199670	32.86
25	4_Pd_Pentagon-2-Ae	-721.61694000	36.03
26	4_Pd_Pentagon-1-Aa	-721.61573630	36.78
27	4_Pd_Pentagon-2-Ac	-721.61350820	38.18
28	4_Pd_Pentagon-2-Cd	-721.61212940	39.05
29	4_Pd_Pentagon-1-Ce	-721.59566550	49.38
30	4_Pd_Pentagon-1-Ac_i1	-721.59049350	52.62
31	4_Pd_Pentagon-1-Ac_i2	-721.59049340	52.62
32	4_Pd_Pentagon-1-Cd	-721.58978480	53.07
33	4_Pd_Pentagon-2-Bc	-721.58799190	54.19
34	4_Pd_Pentagon-1-Cc	-721.58613290	55.36
35	4_Pd_Pentagon-1-Ab	-721.58474150	56.23
36	4_Pd_Pentagon-2-Bb	-721.58461050	56.32
37	4_Pd_Pentagon-1-Cb	-721.58200290	57.95

Table S3A. Distance table for the lowest-lying $Cp_2Pt_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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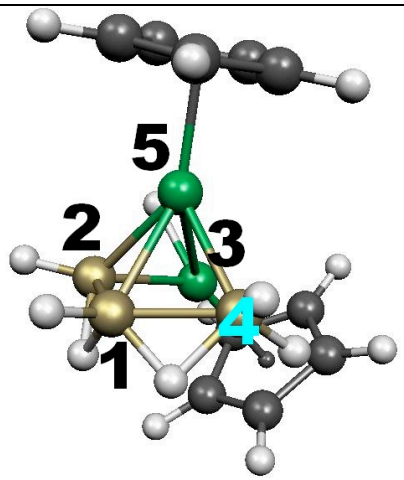
<td> 

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B4-H 1.19
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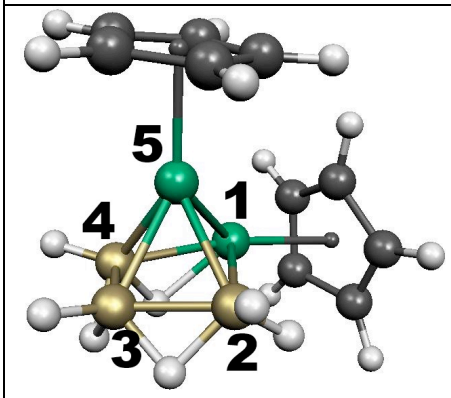
<td> 

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B3-H-B4 B3-H 1.29 B4-H 1.35
B2-H 1.19
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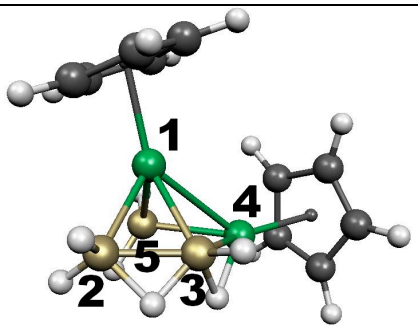
<td> 

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B2-H 1.19
B5-H 1.19
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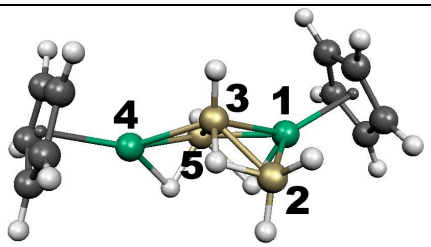
<td> 

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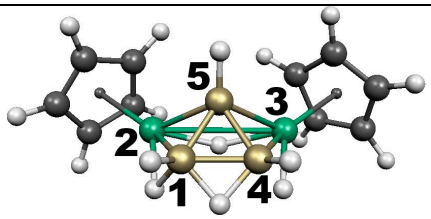
<td> 

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Pt2-H-B1 Pt2-H 1.69 B1-H 1.41
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B1-H-B4 B1-H 1.33 B4-H 1.33
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Table S3B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Pt_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	4_Pt_A	-704.61899040	0.00
2	4_Pt_Pentagon-1-Ba	-704.61616310	1.77
3	4_Pt_Pentagon-1-Bc	-704.61510510	2.44
4	4_Pt_Pentagon-1-Bd	-704.61510510	2.44
5	4_Pt_Pentagon-1-Be	-704.61510510	2.44
6	4_Pt_Pentagon-1-Cd	-704.61510510	2.44
7	4_Pt_Pentagon-1-Bb	-704.60474400	8.94
8	4_Pt_Pentagon-2-Aa	-704.60280830	10.15
9	4_Pt_Pentagon-2-Cg	-704.59876450	12.69
10	9_Pt_A1.log	-704.59659350	14.05
11	4_Pt_Pentagon-2-Ab	-704.59501490	15.04
12	4_Pt_Pentagon-2-Bd	-704.59501490	15.04
13	4_Pt_Pentagon-2-Ce	-704.59500000	15.05
14	4_Pt_C	-704.59479700	15.18
15	4_Pt_Pentagon-2-Ad	-704.59290640	16.37
16	4_Pt_Pentagon-2-Cf	-704.58719720	19.95
17	4_Pt_Pentagon-2-Ch	-704.58719710	19.95
18	4_Pt_Pentagon-2-Ac	-704.58719710	19.95
19	4_Pt_B	-704.58705750	20.04
20	4_Pt_Pentagon-2-Ca	-704.58328970	22.40
21	4_Pt_Pentagon-2-Bc	-704.58328970	22.40
22	4_Pt_Pentagon-2-Cc	-704.58328970	22.40
23	4_Pt_Pentagon-2-Cb	-704.58255810	22.86
24	4_Pt_Pentagon-2-Cd	-704.58255810	22.86
25	9_Pt_A2	-704.58175920	23.36
26	4_Pt_Pentagon-2-Ae	-704.58049480	24.16
27	4_Pt_Pentagon-2-Ba	-704.57620480	26.85
28	4_Pt_Pentagon-1-Ab	-704.56787150	32.08
29	4_Pt_Pentagon-1-Aa	-704.56770000	32.19
30	4_Pt_Pentagon-1-Ce	-704.56580750	33.37
31	4_Pt_Pentagon-1-Ca	-704.56580750	33.37
32	4_Pt_Pentagon-1-Cb	-704.56295390	35.16
33	4_Pt_Pentagon-1-Cc	-704.53390160	53.39
34	4_Pt_Pentagon-1-Ac	-704.53022060	55.70
35	4_Pt_Pentagon-2-Be	-704.52742310	57.46
36	4_Pt_Pentagon-2-Bb	-704.52606900	58.31

Table S4A. Distance table for the lowest-lying $Cp_2Rh_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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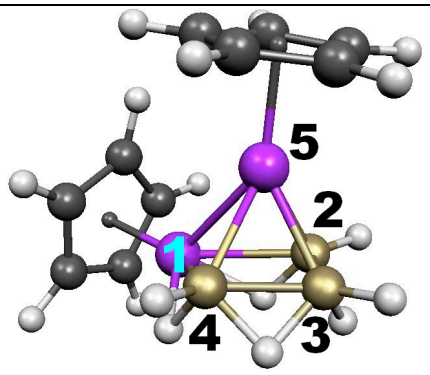
<td> 

1. -686.992314 0.0 Cs
WBI 0.40</td>
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Rh1-H-B2 Rh1-H 1.72 B2-H 1.33
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B4-H-B3 B4-H 1.34 B3-H 1.31
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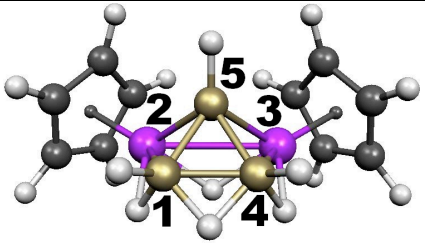
<td> 

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Rh2-H-Rh3 Rh2-H 1.75 Rh3-H 1.75
Rh2-H-B1 Rh2-H 1.72 B1-H 1.33
Rh3-H-B4 Rh3-H 1.72 B4-H 1.33
B1-H-B4 B1-H 1.32 B4-H 1.32
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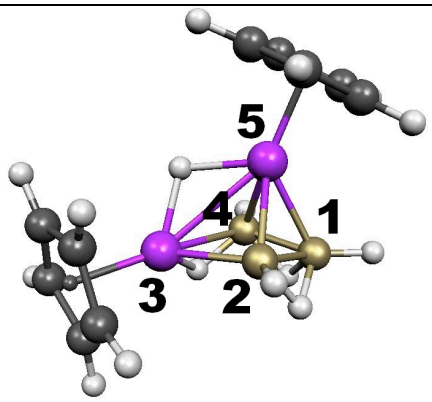
<td> 

3. -686.981545 +6.8 WBI 0.29</td>
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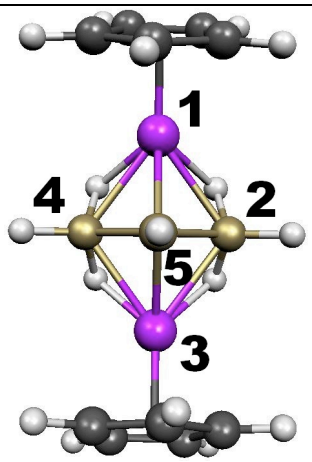
<td> 

4. -686.971052 +13.3 C_{2v}
WBI 0.13</td>
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M-H-B M-H 1.78 B-H 1.31
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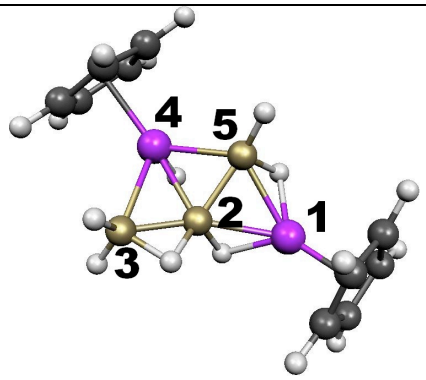
<td> 

5. -686.943349 +30.7
WBI 0.14</td>
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Table S4B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Rh_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	1_Rh_Pentagon-2-Aa	-687.0586914	0.00
2	4_Rh_A_B3LYP	-687.0586295	0.04
3	4_Rh_C	-687.0577297	0.60
4	1_Rh_Pentagon-1-Ce	-687.0577297	0.60
5	10_Rh_A1.log	-687.0503607	5.23
6	1_Rh_Pentagon-2-Ca	-687.0328586	16.21
7	4_Rh_B	-687.0323414	16.53
8	1_Rh_Pentagon-2-Ab	-687.0293014	18.44
9	10_Rh_A2.log	-687.0271476	19.79
10	1_Rh_Pentagon-1-Ca	-687.0141947	27.92
11	1_Rh_Pentagon-1-Bd	-687.0097913	30.69
12	1_Rh_Pentagon-1-Ba	-687.0097723	30.70
13	1_Rh_Pentagon-1-Cc	-687.0096215	30.79
14	1_Rh_Pentagon-2-Ad	-687.0086295	31.41
15	1_Rh_Pentagon-2-Ce	-687.0064029	32.81
16	1_Rh_Pentagon-2-Cg	-687.0058492	33.16
17	1_Rh_Pentagon-1-Cb	-687.0042177	34.18
18	1_Rh_Pentagon-1-Bc	-686.9990396	37.43
19	1_Rh_Pentagon-1-Bb	-686.9978516	38.18
20	1_Rh_Pentagon-2-Cc	-686.9976964	38.27
21	1_Rh_Pentagon-2-Bc	-686.9881967	44.24
22	1_Rh_Pentagon-2-Ac	-686.9881967	44.24
23	1_Rh_Pentagon-1-Aa	-686.9859431	45.65
24	1_Rh_Pentagon-2-Bd	-686.9838902	46.94
25	1_Rh_Pentagon-2-Bb	-686.9834525	47.21
26	1_Rh_Pentagon-2-Ba	-686.982455	47.84
27	1_Rh_Pentagon-2-Ch	-686.9789027	50.07
28	1_Rh_Pentagon-2-Cf	-686.9759588	51.92
29	1_Rh_Pentagon-1-Ac	-686.9758999	51.95
30	1_Rh_Pentagon-2-Be	-686.9737563	53.30
31	1_Rh_Pentagon-2-Cb	-686.9719434	54.44
32	1_Rh_Pentagon-2-Cd	-686.9668802	57.61
33	1_Rh_Pentagon-1-Cd	-686.9662288	58.02
34	1_Rh_Pentagon-2-Ae	-686.9634792	59.75
35	1_Rh_Pentagon-1-Ab	-686.9633903	59.80
36	1_Rh_Pentagon-1-Be	-686.9595764	62.20

Table S5A. Distance table for the lowest-lying $Cp_2Ir_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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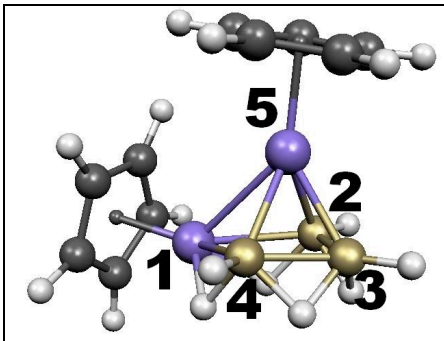
<td> 

1. Ir2B3-1 -674.610910 a.u.
0.0 kcal/mol Cs WBI 0.42</td>
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1 2 3 4 5
1 Ir 0.000000
2 B 2.288238 0.000000
3 B 3.154672 1.817622 0.000000
4 B 2.292945 2.590833 1.816214 0.000000
5 Ir 2.685530 2.103084 2.097907 2.106405

Ir1-H-B2 Ir1-H 1.69 B2-H 1.40
Ir1-H-B4 Ir1-H 1.68 B4-H 1.40
B2-H-B3 B2-H 1.50 B3-H 1.31
B3-H-B4 B3-H 1.31 B4-H 1.35
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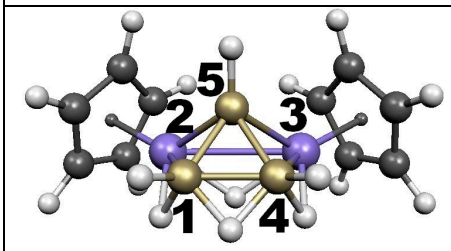
<td> 

2. Ir2B3-2 -674.605693
+3.3 Cs WBI 0.33</td>
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1 2 3 4 5
1 B 0.000000
2 Ir 2.212843 0.000000
3 Ir 3.125033 2.797400 0.000000
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5 B 1.724869 2.157560 2.157560 1.724869

Ir2-H-Ir3 Ir2-H 1.78 Ir3-H 1.78
Ir2-H-B1 Ir2-H 1.70 B1-H 1.39
Ir3-H-B4 Ir3-H 1.70 B4-H 1.39
Ir1-H- Ir4 Ir1-H 1.33 Ir4-H 1.33
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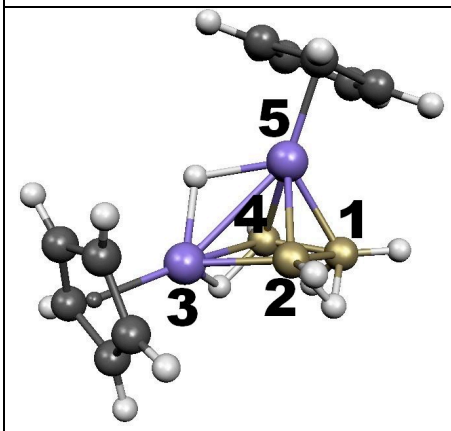
<td> 

3. Ir2B3-3 -674.597810 +8.2
WBI 0.31</td>
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1 B 0.000000
2 B 1.809414 0.000000
3 Ir 3.105776 2.101830 0.000000
4 B 1.808662 2.533696 2.349558 0.000000
5 Ir 2.122327 2.122282 2.763847 2.138065

Ir3-H-Ir5 Ir3-H 1.73 Ir5-H 1.80
Ir3-H-B4 Ir3-H 1.73 B4-H 1.32
B1-H-B2 B1-H 1.28 B2-H 1.37
B1-H-B4 B1-H 1.31 B4-H 1.34
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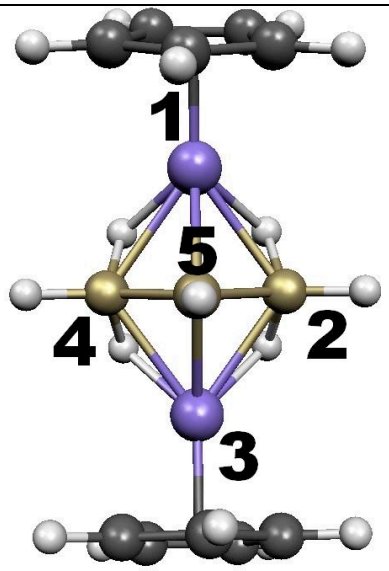
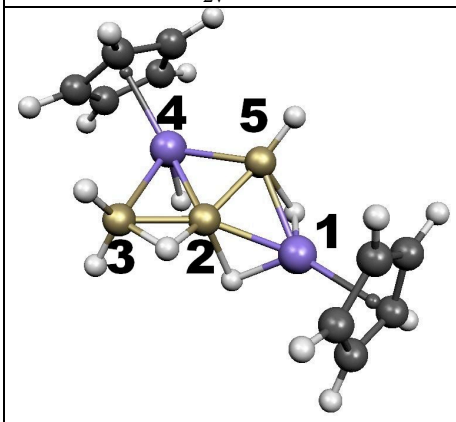
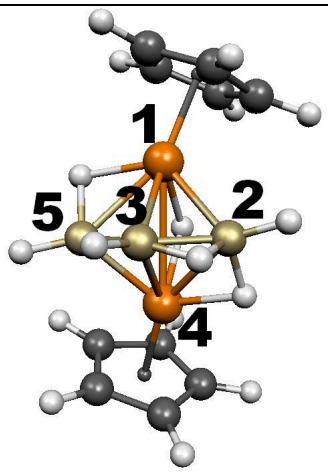
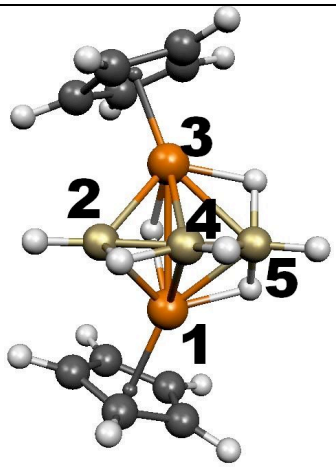
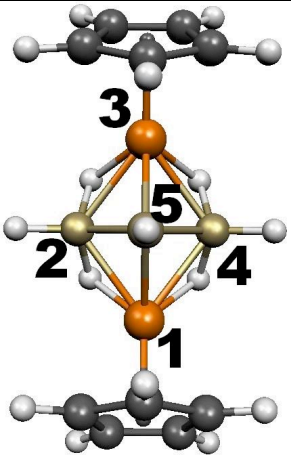
 4. Ir2B3-4 -674.589126 +13.7 C_{2v} WBI 0.10	1 2 3 4 5 1 Ir 0.000000 2 B 2.257224 0.000000 3 Ir 3.660401 2.255221 0.000000 4 B 2.255221 2.638603 2.257224 0.000000 5 B 2.161938 1.738450 2.161938 1.738450 Ir1-H-B2 Ir1-H 1.76 B2-H 1.35 Ir1-H-B4 Ir1-H 1.76 B4-H 1.35 Ir3-H-B2 Ir3-H 1.76 B2-H 1.35 Ir3-H-B4 Ir3-H 1.76 B4-H 1.35
 5. Ir2B3-5 -674.577540 +20.9 WBI 0.11	1 2 3 4 5 1 Ir 0.000000 2 B 2.053244 0.000000 3 B 3.729152 1.741244 0.000000 4 Ir 3.658822 2.025632 2.221878 0.000000 5 B 2.123997 1.781119 3.248526 2.065155 Ir1-H-B2 Ir1-H 1.64 B2-H 1.65 Ir1-H-B5 Ir1-H 1.64 B5-H 1.62 B2-H-B3 B2-H 1.31 B3-H 1.34 Ir4-H 1.59

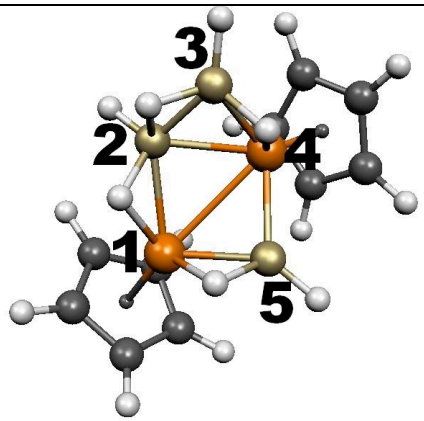
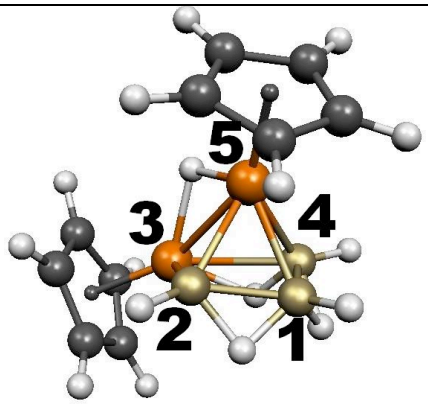
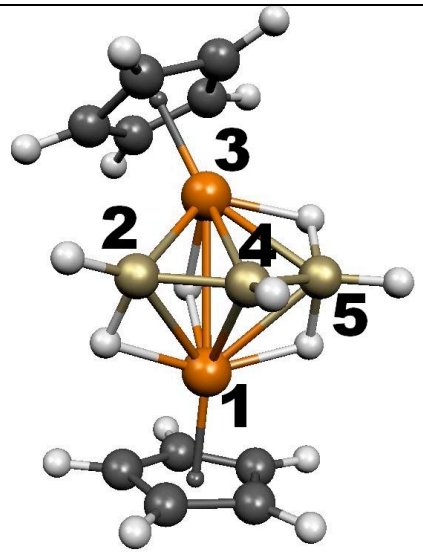
Table S5B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Ir_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	6_Ir_Pentagon-2-Ac	-674.69725693	0.00
2	GES-Ir_M06L_xqc	-674.68285663	9.04
3	5v-Ta2B3-1__Ir_M06L	-674.68285635	9.04
4	GES-mod1	-674.68285619	9.04
5	6_Ir_Pentagon-2-Ac	-674.68157315	9.84
6	6_Ir_Pentagon-1-Ca	-674.68157314	9.84
7	6_Ir_A.	-674.68121122	10.07
8	6_Ir_C.	-674.68093370	10.24

9	GES-mod3	-674.67257323	15.49
10	6_Ir_A1	-674.67112036	16.40
11	6_Ir_Pentagon-1-Ba	-674.65734398	25.05
12	BPT-2	-674.65276462	27.92
13	6_Ir_B.	-674.65192051	28.45
14	6_Ir_Pentagon-1-Bc	-674.65171590	28.58
15	6_Ir_Pentagon-1-Cb	-674.65169052	28.59
16	6_Ir_Pentagon-1-Cd	-674.65081855	29.14
17	GES-mod2	-674.65039508	29.41
18	6_Ir_Pentagon-1-Cc	-674.64642432	31.90
19	6_Ir_Pentagon-1-Bc	-674.64628666	31.98
20	6_Ir_Pentagon-1-Bd	-674.64559598	32.42
21	6_Ir_A2	-674.64557154	32.43
22	BPT-1	-674.63891598	36.61
23	6_Ir_Pentagon-2-Ae	-674.63830313	36.99
24	6_Ir_Pentagon-1-Cb	-674.63534337	38.85
25	6_Ir_Pentagon-1-Aa	-674.63494844	39.10
26	6_Ir_Pentagon-1-Ab	-674.63474747	39.22
27	6_Ir_Pentagon-1-Cd	-674.63408570	39.64
28	6_Ir_Pentagon-1-Bb	-674.63033543	41.99
29	6_Ir_Pentagon-2-Aa	-674.62851562	43.14
30	6_Ir_Pentagon-2-Cg	-674.62211733	47.15
31	6_Ir_Pentagon-2-Ce	-674.62110361	47.79
32	6_Ir_Pentagon-2-Ca	-674.61890358	49.17
33	6_Ir_Pentagon-2-Ba	-674.61849453	49.42
34	6_Ir_Pentagon-2-Cc	-674.61769138	49.93
35	6_Ir_Pentagon-1-Ce	-674.61535985	51.39
36	6_Ir_Pentagon-2-Ab	-674.61535681	51.39
37	6_Ir_Pentagon-2-Bd	-674.61517211	51.51
38	6_Ir_Pentagon-1-Be	-674.61447919	51.94
39	6_Ir_Pentagon-1-Ac	-674.61025260	54.60
40	6_Ir_Pentagon-2-Bc	-674.61016422	54.65
41	6_Ir_Pentagon-2-Ch	-674.61014536	54.66
42	6_Ir_Pentagon-2-Bb	-674.61014535	54.66
43	6_Ir_Pentagon-2-Ad	-674.60749217	56.33
44	6_Ir_Pentagon-2-Cb	-674.60301519	59.14
45	6_Ir_Pentagon-2-Cd	-674.60301519	59.14
46	6_Ir_Pentagon-2-Cf	-674.59964454	61.25
47	6_Ir_Pentagon-2-Be	-674.58651315	69.49

Table S6A. Distance table for the lowest-lying $Cp_2Ru_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 **1. Ru2B3-1 -655.655044 0.0 WBI 0.33**	1 2 3 4 5 1 Ru 0.000000 2 B 2.087627 0.000000 3 B 2.273811 1.740950 0.000000 4 Ru 2.788496 2.161626 2.216283 0.000000 5 B 2.254602 2.881661 1.690872 2.170603 Ru1-H-Ru4 Ru1-H 1.78 Ru4-H 1.79 Ru1-H-B5 Ru1-H 1.69 B5-H 1.34 Ru4-H-B2 Ru4-H 1.73 B2-H 1.32 B2-H-B3 B2-H 1.33 B3-H 1.28
 1b. Ru2B3-2 -655.654042 +0.6 WBI 0.34	1 2 3 4 5 1 Ru 0.000000 2 B 2.162305 0.000000 3 Ru 2.790862 2.123218 0.000000 4 B 2.285484 1.650816 2.220348 0.000000 5 B 2.146021 2.863830 2.230408 1.774336 Ru1-H-Ru3 Ru1-H 1.79 Ru3-H 1.78 Ru1-H-B5 Ru1-H 1.69 B5-H 1.35 Ru3-H-B5 Ru3-H 1.69 B5-H 1.35 B2-H-B4 B2-H 1.32 B4-H 28
 2. Ru2B3-3 -655.644692 +6.5 C_{2v} WBI 0.31	1 2 3 4 5 1 Ru 0.000000 2 B 2.191569 0.000000 3 Ru 3.490200 2.191569 0.000000 4 B 2.191509 2.633300 2.191509 0.000000 5 B 2.068957 1.826597 2.068957 1.826524 Ru1-H-B2 Ru1-H 1.71 B2-H 1.37 Ru1-H-B4 Ru1-H 1.71 B4-H 1.37 Ru3-H-B2 Ru3-H 1.71 B2-H 1.37 Ru3-H-B4 Ru3-H 1.71 B4-H 1.37

 3. Ru2B3-4 -655.640794 +8.9 WBI 0.37	1 2 3 4 5 1 Ru 0.000000 2 B 2.170879 0.000000 3 B 3.475032 1.755597 0.000000 4 Ru 2.750072 2.213195 2.034963 0.000000 5 B 2.028079 3.094321 3.407197 2.092405 Ru1-H-B2 Ru1-H 1.70 B2-H 1.39 Ru1-H-B5 Ru1-H 1.74 B5-H 1.37 Ru4-H-B3 Ru4-H 1.78 B3-H 1.32 B2-H-B3 B2-H 1.42 B3-H 1.28
 4. Ru2B3-5 -655.637966 +10.7 WBI 0.59	1 2 3 4 5 1 B 0.000000 2 B 1.810898 0.000000 3 Ru 3.058189 2.184909 0.000000 4 B 1.783592 2.636913 2.361740 0.000000 5 Ru 2.140896 2.065130 2.612404 2.155360 Ru3-H-Ru5 Ru3-H 1.77 Ru5-H 1.76 Ru3-H-B4 Ru3-H 1.77 B4-H 1.29 B1-H-B2 B1-H 1.29 B2-H 1.38 B1-H-B4 B1-H 1.28 B4-H 1.37
 5. Ru2B3-6 -655.637855 +10.8 WBI 0.35	1 2 3 4 5 1 Ru 0.000000 2 B 2.252444 0.000000 3 Ru 2.779245 2.136590 0.000000 4 B 2.221901 1.647264 2.269262 0.000000 5 B 2.348429 2.903591 2.237051 1.648618 Ru1-H-Ru3 Ru1-H 1.76 Ru3-H 1.80 Ru1-H-B5 Ru1-H 1.73 B5-H 1.35 Ru1-H-B2 Ru1-H 1.75 B2-H 1.32 Ru3-H-B5 Ru3-H 1.76 B5-H 1.31

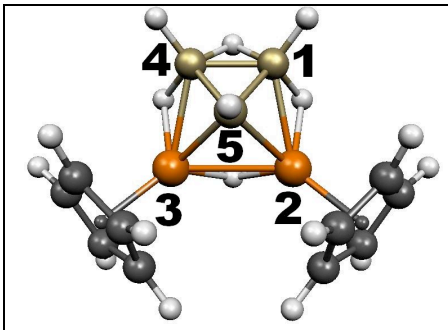
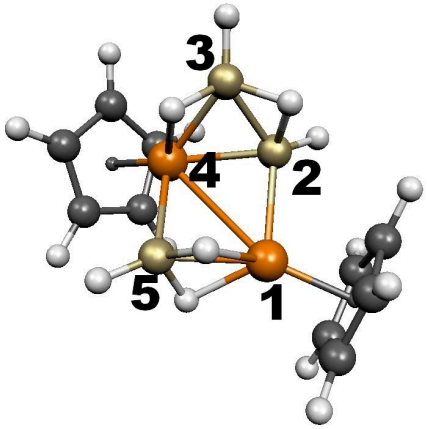
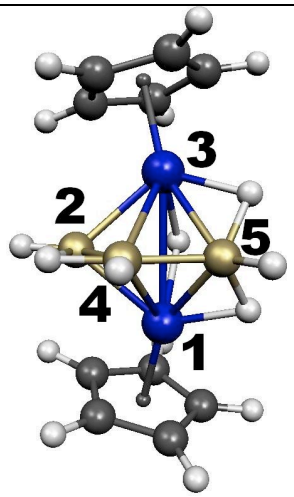
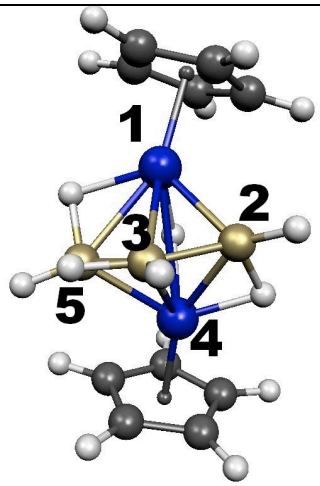
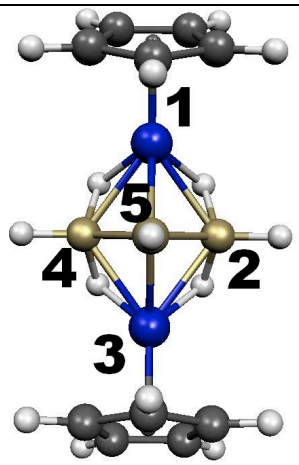
 6. Ru2B3-7 -655.637608 +10.9 Cs WBI 0.72	1 2 3 4 5 1 B 0.000000 2 Ru 2.251423 0.000000 3 Ru 3.091037 2.592200 0.000000 4 B 1.730400 3.091027 2.251437 0.000000 5 B 1.736732 2.129119 2.129180 1.736732 Ru2-H-Ru3 Ru2-H 1.81 Ru3-H 1.81 Ru2-H-B1 Ru2-H 1.72 B1-H 1.34 Ru3-H-B4 Ru3-H 1.72 B4-H 1.34 B1-H-B4 B1-H 1.32 B4-H 1.32
 7. Ru2B3-8 -655.634610 +12.8 WBI 0.32	1 2 3 4 5 1 Ru 0.000000 2 B 2.184046 0.000000 3 B 3.410601 1.747947 0.000000 4 Ru 2.810598 2.093810 2.049231 0.000000 5 B 2.072928 3.148372 3.466984 2.187987 Ru1-H-B5 Ru1-H 1.77 B5-H 1.32 Ru1-H'-B5 Ru1-H' 1.76 B5-H' 1.33 Ru4-H-B3 Ru4-H 1.80 B3-H 1.30 B2-H-B3 B2-H 1.40 B3-H 1.30

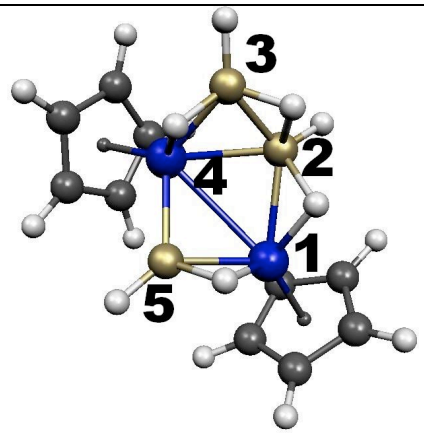
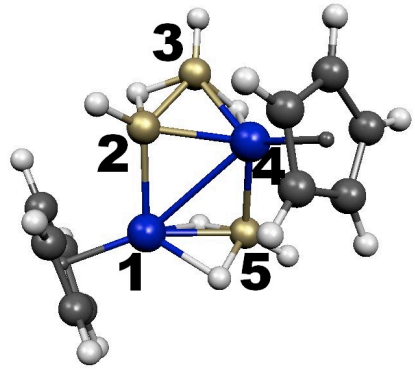
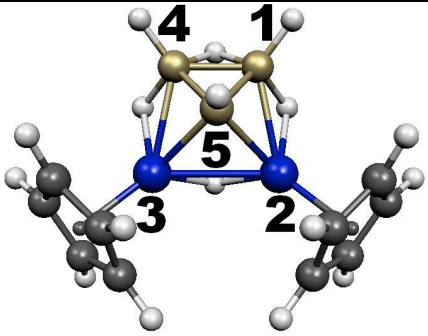
Table S6B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Ru_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	Os2B3-4__Ru	-655.89827647	0.00
2	Os2B3-2__Ru	-655.89827527	0.00
3	7_Ru_Pentagon-1-Ca	-655.73267578	0.00
4	GES-mod3	-655.89731148	0.60
5	BPT-2	-655.89729070	0.62
6	7_Ru_B.	-655.72806412	2.89
7	7_Ru_Pentagon-1-Ba	-655.72600303	4.19
8	7_Ru_Pentagon-1-Ab	-655.72406895	5.40
9	7_Ru_Pentagon-1-Cc	-655.72308811	6.02
10	7_Ru_Pentagon-1-Cb	-655.72039088	7.71
11	7_Ru_C.	-655.71926915	8.41
12	7_Ru_A1-M06L	-655.88311574	9.51

13	7_Ru_Pentagon-2-Ch	-655.71513997	11.00
14	BPT-1	-655.87970680	11.65
15	Os2B3-4__Ru	-655.87933701	11.88
16	Os2B3-5__Ru	-655.87933664	11.88
17	7_Ru_Pentagon-2-Cd	-655.87912017	12.02
18	7_Ru_Pentagon-2-Bb	-655.71227887	12.80
19	7_Ru_Pentagon-2-Ba	-655.71227886	12.80
20	7_Ru_Pentagon-2-Cd	-655.71084283	13.70
21	7_Ru_Pentagon-2-Ca	-655.71051683	13.90
22	7_Ru_Pentagon-2-Cc	-655.71014197	14.14
23	7_Ru_Pentagon-2-Ac	-655.70985165	14.32
24	7_Ru_Pentagon-2-Aa	-655.70940851	14.60
25	7_Ru_A.	-655.70712262	16.03
26	7_Ru_Pentagon-2-Bc	-655.70455566	17.65
27	7_Ru_Pentagon-2-Bd	-655.70452940	17.66
28	7_Ru_Pentagon-2-Ab	-655.70384599	18.09
29	7_Ru_Pentagon-1-Be	-655.70340272	18.37
30	7_Ru_Pentagon-1-Bb	-655.70247710	18.95
31	7_Ru_Pentagon-1-Aa	-655.70215787	19.15
32	GESTAA-Ru-original_M06L	-655.86740099	19.37
33	5v-Ta2B3-1__Ru	-655.86702850	19.61
34	GES-mod1	-655.86702830	19.61
35	7_Ru_A2-M06L	-655.86606270	20.21
36	7_Ru_Pentagon-1-Bc	-655.70034805	20.29
37	7_Ru_Pentagon-2-Be	-655.69843187	21.49
38	7_Ru_Pentagon-1-Bb	-655.86209228	22.70
39	7_Ru_Pentagon-2-Cf	-655.69432071	24.07
40	7_Ru_Pentagon-1-Bd	-655.69215491	25.43
41	7_Ru_Pentagon-1-Ce	-655.68694764	28.69
42	7_Ru_Pentagon-1-Ac	-655.68572934	29.46
43	GES-mod2	-655.84710603	32.11
44	7_Ru_Pentagon-2-Ad	-655.68060145	32.68
45	7_Ru_Pentagon-2-Cg	-655.67408999	36.76
46	7_Ru_Pentagon-2-Cb	-655.67240309	37.82
47	7_Ru_Pentagon-2-Ce	-655.66983024	39.44
48	7_Ru_Pentagon-1-Cd	-655.64627205	54.22
49	7_Ru_Pentagon-2-Ae	-655.63417498	61.81

Table S7A. Distance table for the lowest-lying $Cp_2Os_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 **1. -647.249915 0.0 WBI 0.36**	1 2 3 4 5 1 Os 0.000000 2 B 2.165784 0.000000 3 Os 2.857800 2.165417 0.000000 4 B 2.279764 1.656134 2.279240 0.000000 5 B 2.186676 2.835383 2.187570 1.755421 Os1-H-Os3 Os1-H 1.82 Os3-H 1.82 Os1-H-B5 Os1-H 1.70 B5-H 1.40 Os3-H-B5 Os3-H 1.70 B5-H 1.40 B2-H-B4 B2-H 1.33 B4-H 1.29
 1b. -647.249868 +0.03 WBI 0.34	1 2 3 4 5 1 Os 0.000000 2 B 2.113298 0.000000 3 B 2.279146 1.738894 0.000000 4 Os 2.853019 2.164346 2.262591 0.000000 5 B 2.264159 2.863320 1.689873 2.185771 Os1-H- Os4 Os1-H 1.82 Os4-H 1.82 Os1-H-B5 Os1-H 1.74 B5-H 1.35 Os4-H-B2 Os4-H 1.69 B2-H 1.38 B3-H-B5 B3-H 1.28 B5-H 1.32
 2. -647.244998 +3.1 C_{2v} WBI 0.28	1 2 3 4 5 1 Os 0.000000 2 B 2.192917 0.000000 3 Os 3.530600 2.192917 0.000000 4 B 2.192917 2.590000 2.192917 0.000000 5 B 2.099775 1.808083 2.099775 1.808083 Os1-H-B2 Os1-H 1.70 B2-H 1.43 Os1-H-B4 Os1-H 1.70 B4-H 1.43 Os3-H-B2 Os3-H 1.70 B2-H 1.43 Os3-H-B4 Os3-H 1.70 B4-H 1.43

 3. -647.241437 +5.3 WBI 0.39	1 2 3 4 5 1 Os 0.000000 2 B 2.159029 0.000000 3 B 3.476557 1.760191 0.000000 4 Os 2.810891 2.219346 2.059411 0.000000 5 B 2.041697 3.088352 3.431190 2.117499 Os1-H-B2 Os1-H 1.68 B2-H 1.54 Os1-H-B5 Os1-H 1.72 B5-H 1.43 Os4-H-B3 Os4-H 1.78 B3-H 1.34 B2-H-B3 B2-H 1.43 B3-H 1.27
 4. -647.235225 +9.2 WBI 0.36	1 2 3 4 5 1 Os 0.000000 2 B 2.189435 0.000000 3 B 3.430182 1.756662 0.000000 4 Os 2.852896 2.127492 2.062097 0.000000 5 B 2.090595 3.147365 3.463279 2.193063 Os1-H-B5 Os1-H 1.77 B5-H 1.35 Os1-H'-B5 Os1-H' 1.78 B5-H 1.34 Os4-H-B3 Os4-H 1.80 B3-H 1.33 B2-H-B5 B2-H- 1.40 B3-H 1.30
 5. -647.234742 +9.5 Cs WBI 0.80	1 2 3 4 5 1 B 0.000000 2 Os 2.259357 0.000000 3 Os 3.105765 2.624600 0.000000 4 B 1.730200 3.105765 2.259357 0.000000 5 B 1.725252 2.160087 2.160087 1.725252 Os2-H- Os3 Os2-H 1.83 Os3-H 1.82 Os2-H-B1 Os2-H 1.71 B1-H 1.38 Os3-H-B4 Os3-H 1.72 B4-H 1.39 B1-H-B4 B1-H 1.33 B4-H 1.33

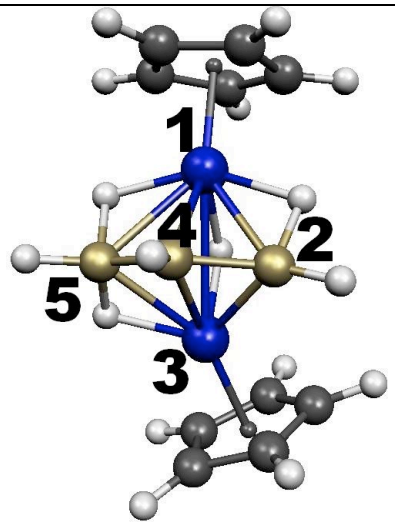
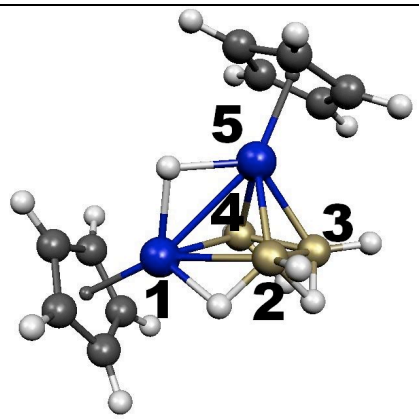
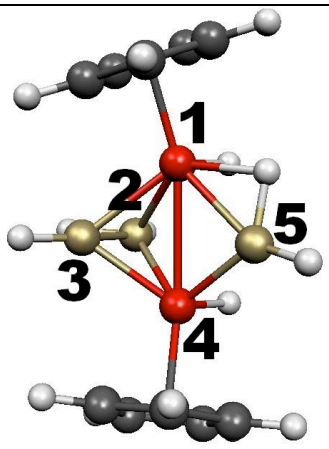
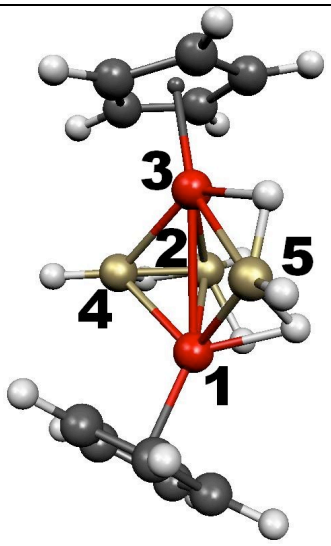
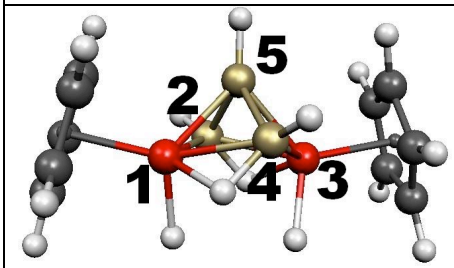
 6. -647.234263 +9.8 WBI 0.37	1 2 3 4 5 1 Os 0.000000 2 B 2.272275 0.000000 3 Os 2.837031 2.136613 0.000000 4 B 2.232478 1.649876 2.293032 0.000000 5 B 2.345122 2.889602 2.252159 1.645834 Os1-H-Os3 Os1-H 1.81 Os3-H 1.82 Os1-H-B2 Os1-H 1.75 B2-H 1.35 Os1-H-B5 Os1-H 1.75 B5-H 1.37 Os3-H-B5 Os3-H 1.77 B5-H 1.33
 7. -647.234258 +9.8 WBI 0.64	1 2 3 4 5 1 Os 0.000000 2 B 2.374757 0.000000 3 B 3.088760 1.798756 0.000000 4 B 2.208964 2.653524 1.828613 0.000000 5 Os 2.657812 2.163985 2.159877 2.096744 Os1-H-Os5 Os1-H 1.79 Os5-H 1.77 Os1-H-B2 Os1-H 1.78 B2-H 1.30 B2-H-B3 B2-H 1.37 B3-H 1.28 B3-H-B4 B3-H 1.29 B4-H 1.39

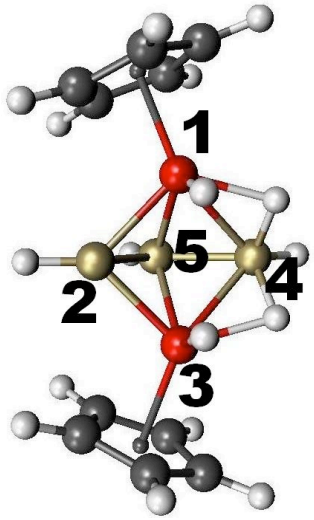
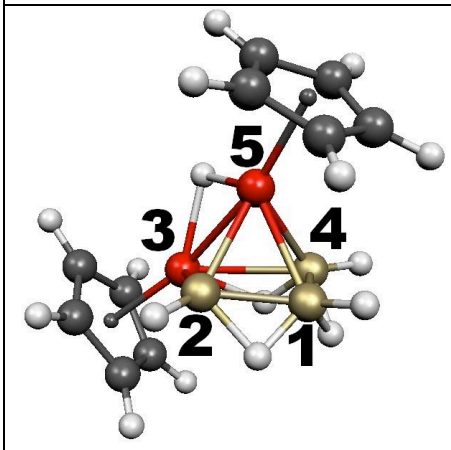
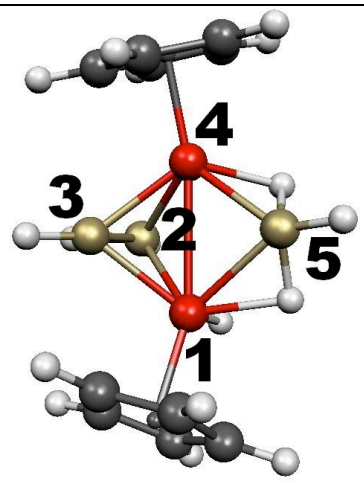
Table S7B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Os_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	BPT-2	-647.32991500	0.00
2	Ru2B3-3__Os	-647.32986900	0.03
3	Ru2B3-1__Os	-647.32986800	0.03
4	GES-mod3	-647.32986600	0.03
5	5_Os_Pentagon-1-Ba	-647.32723868	1.68
6	5_Os_Pentagon-1-Ca	-647.32723868	1.68
7	5_Os_Pentagon-1-Cb	-647.32144528	5.31
8	5_Os_Pentagon-1-Ba	-647.32143700	5.32
9	Ru2B3-4__Os	-647.32133500	5.38
10	5_Os_B	-647.31903892	6.82
11	5_Os_Pentagon-2-Ba	-647.31797993	7.49
12	5_Os_Pentagon-1-Cc	-647.31580555	8.85

13	Ru2B3-7__Os	-647.31426300	9.82
14	5_Os_Pentagon-2-Ab	-647.31425800	9.82
15	Ru2B3-5__Os	-647.31425400	9.83
16	5_Os_Pentagon-2-Ba	-647.31306600	10.57
17	5_Os_Pentagon-1-Bd	-647.31243074	10.97
18	5_Os_Pentagon-1-Ab	-647.30937945	12.89
19	5_Os_Pentagon-1-Cd	-647.30783800	13.85
20	5_Os_C	-647.30723059	14.23
21	5_Os_Pentagon-1-Cd	-647.30576615	15.15
22	5_Os_A1	-647.30456590	15.91
23	5_Os_Pentagon-2-Cb	-647.30456589	15.91
24	5_Os_Pentagon-2-Ch	-647.30320700	16.76
25	5_Os_Pentagon-1-Bc	-647.30298255	16.90
26	5_Os_Pentagon-1-Bc	-647.30236100	17.29
27	5_Os_Pentagon-2-Cf	-647.29949387	19.09
28	5_Os_A	-647.29894554	19.43
29	5_Os_Pentagon-2-Ch	-647.29746597	20.36
30	5_Os_Pentagon-2-Bb	-647.29659434	20.91
31	5_Os_Pentagon-2-Ab	-647.29449342	22.23
32	GESTAA-Os_M06L	-647.29390600	22.60
33	5_Os_Pentagon-2-Cd	-647.29337183	22.93
34	5_Os_Pentagon-1-Bb	-647.29337000	22.93
35	5_Os_Pentagon-2-Bd	-647.29250629	23.47
36	5_Os_Pentagon-2-Bc	-647.29248868	23.49
37	5v5_Os_Pentagon-2-Cc	-647.29171048	23.97
38	5_Os_Pentagon-2-Aa	-647.29087059	24.50
39	5_Os_Pentagon-2-Cd	-647.28991800	25.10
40	5_Os_Pentagon-2-Ca	-647.28966635	25.26
41	5_Os_Pentagon-1-Aa	-647.28814993	26.21
42	5_Os_Pentagon-2-Ad	-647.28470459	28.37
43	5_Os_Pentagon-2-Ce	-647.28386720	28.89
44	5_Os_Pentagon-2-Cg	-647.28228064	29.89
45	5_Os_Pentagon-1-Ce	-647.27977312	31.46
46	5_Os_Pentagon-1-Bb	-647.27950625	31.63
47	5_Os_Pentagon-1-Ac	-647.27708599	33.15
*48	GES-mod2	-647.27536800	34.23
49	5_Os_Pentagon-1-Be	-647.27274101	35.88
50	5_Os_A2	-647.26942009	37.96
51	5_Os_Pentagon-2-Ae	-647.26302736	41.97
52	5_Os_Pentagon-2-Ac	-647.25355094	47.92
53	5_Os_Pentagon-2-Be	-647.23362395	60.42

Table S8A. Distance table for the lowest-lying $Cp_2Re_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 **1. Re2B3-1 -622.432910 a.u. 0.0 WBI 0.89**	1 2 3 4 5 1 Re 0.000000 2 B 2.247672 0.000000 3 B 2.239411 1.622699 0.000000 4 Re 2.593218 2.223737 2.175292 0.000000 5 B 2.223980 3.436494 3.369424 2.046902 Re1-H-B2 Re1-H 1.65 B2-H 2.29 Re1-H-B5 Re1-H 1.81 B5-H 1.28 B2-H-B3 B2-H 1.31 B3-H 1.30
 2. Re2B3-2 -622.428894 +2.5 WBI 0.73	1 2 3 4 5 1 Re 0.000000 2 B 2.299423 0.000000 3 Re 2.670359 2.223827 0.000000 4 B 2.181602 1.690647 2.168226 0.000000 5 B 2.082864 3.369576 2.290554 3.399675 Re1-H-B2 Re1-H 1.74 B2-H 1.47 Re1-H-B5 Re1-H 1.78 B5-H 1.39 Re3-H-B5 Re3-H 1.82 B5-H 1.29 B2-H-B4 B2-H 1.30 B4-H 1.35
 3. Re2B3-3 -622.427727 +3.3 C_2 WBI 0.56	1 2 3 4 5 1 Re 0.000000 2 B 2.159499 0.000000 3 Re 2.966840 2.136334 0.000000 4 B 2.136343 3.012671 2.159523 0.000000 5 B 2.111187 1.878558 2.111201 1.878657 Re1-H-B4 Re1-H 1.79 B4-H 1.35 Re3-H-B2 Re3-H 1.79 B2-H 1.35 Re1-H 1.67 Re3-H 1.67

 4. Re2B3-4 -622.426848 +3.8 Cs WBI 0.58	1 2 3 4 5 1 Re 0.000000 2 B 2.084750 0.000000 3 Re 2.975400 2.084746 0.000000 4 B 2.211585 3.023540 2.211557 0.000000 5 B 2.108943 1.969186 2.108872 1.831042 Re1-H-B4 Re1-H 1.75 B4-H 1.38 Re3-H-B4 Re3-H 1.75 B4-H 1.38 Re1-H 1.68 Re3-H 1.68
 5. Re2B3-5 -622.425195 +4.8 WBI 1.35	1 2 3 4 5 1 B 0.000000 2 B 1.824625 0.000000 3 Re 3.012166 2.177716 0.000000 4 B 1.824468 2.744366 2.383180 0.000000 5 Re 2.216297 2.137221 2.452629 2.159938 Re3-H- Re5 Re3-H 1.82 Re5-H 1.81 Re3-H-B4 Re3-H 1.78 B4-H 1.35 B1-H-B2 B1-H 1.26 B2-H 1.44 B1-H-B4 B1-H 1.30 B4-H 1.36
 6. Re2B3-6 -622.424040 +5.6 (Cs) WBI 0.837	1 2 3 4 5 1 Re 0.000000 2 B 2.280350 0.000000 3 B 2.202071 1.650531 0.000000 4 Re 2.636747 2.235863 2.159706 0.000000 5 B 2.232787 3.372998 3.403117 2.093274 Re1-H-B5 Re1-H 1.79 B5-H 1.31 Re4-H-B5 Re4-H 1.76 B5-H 1.41 B2-H-B3 B2-H 1.30 B3-H 1.33 Re1-H 1.66

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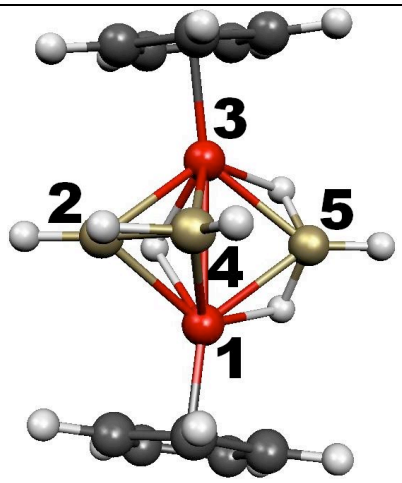
<td> 

7. Re2B3-7 -622.423293
+6.0 Cs WBI 0.70</td>
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2 B 2.201935 0.000000
3 Re 2.628800 2.201984 0.000000
4 B 2.209711 1.665661 2.209479 0.000000
5 B 2.194519 3.489746 2.195042 2.856237

Re1-H- Re3 Re1-H 1.90 Re3-H 1.90
Re1-H-B5 Re1-H 1.79 B5-H 1.34
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B2-H-B4 B2-H 1.33 B4-H 1.31</td>
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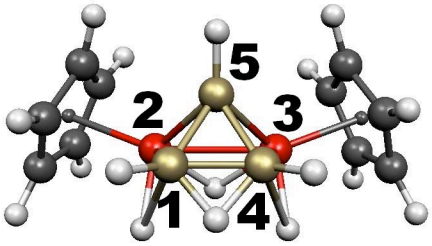
<td> 

8. Re2B3-8 -622.422697
+6.4 Cs WBI 1.40</td>
<td>1 2 3 4 5
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2 Re 2.249149 0.000000
3 Re 3.026596 2.442803 0.000000
4 B 1.674104 3.024468 2.251670 0.000000
5 B 1.715279 2.195887 2.196462 1.713154

Re2-H- Re3 Re2-H 1.82 Re3-H 1.82
Re2-H-B1 Re2-H 1.66 B1-H 2.28
Re3-H-B4 Re3-H 1.66 B4-H 2.25
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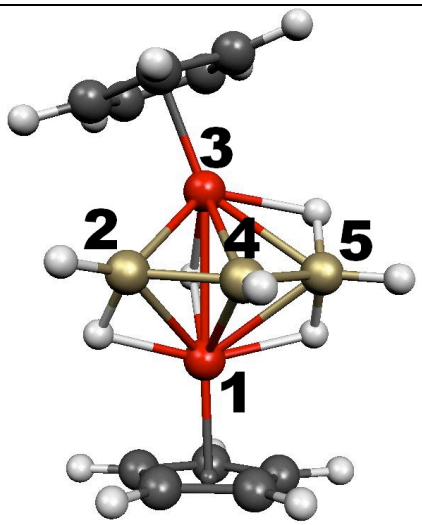
<td> 

9. Re2B3-9 -622.415658
+10.8 (Cs) WBI 0.74</td>
<td>1 2 3 4 5
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2 B 2.210574 0.000000
3 Re 2.684885 2.112370 0.000000
4 B 2.224032 1.748468 2.252812 0.000000
5 B 2.342656 3.027355 2.291281 1.709694

Re1-H-Re3 Re1-H 1.84 Re3-H 1.9
Re1-H-B2 Re1-H 1.76 B2-H 1.39
Re1-H-B5 Re1-H 1.84 B5-H 1.33
Re3-H-B5 Re3-H 1.86 B5-H 1.29</td>
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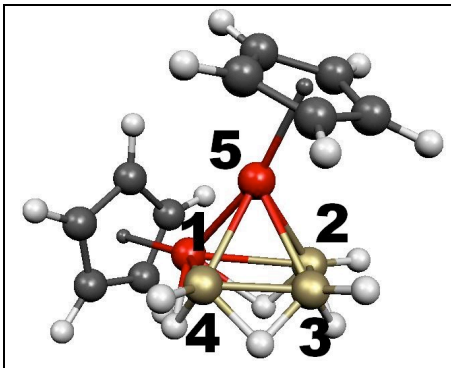


10. Re2B3-10 -622.414866
+11.3 Cs WBI 1.85

	1	2	3	4	5
1 Re	0.000000				
2 B	2.310214	0.000000			
3 B	3.074870	1.840386	0.000000		
4 B	2.312348	2.756705	1.840589	0.000000	
5 Re	2.362610	2.169358	2.188911	2.168877	

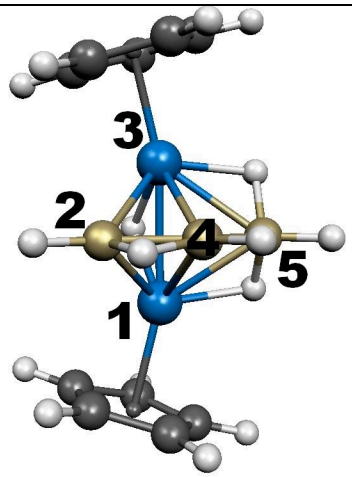
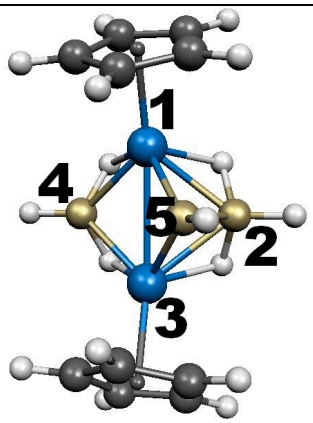
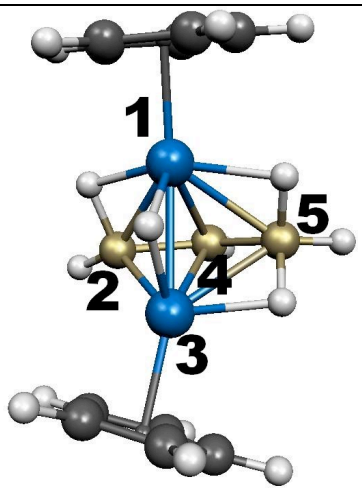
Re1-H-B2 Re1-H 1.79 B2-H 1.36
Re1-H-B4 Re1-H 1.80 B4-H 1.35
B2-H-B3 B2-H 1.39 B3-H 1.29
B3-H-B4 B3-H 1.29 B4-H 1.39

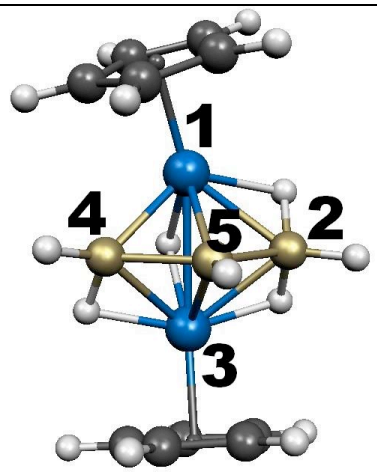
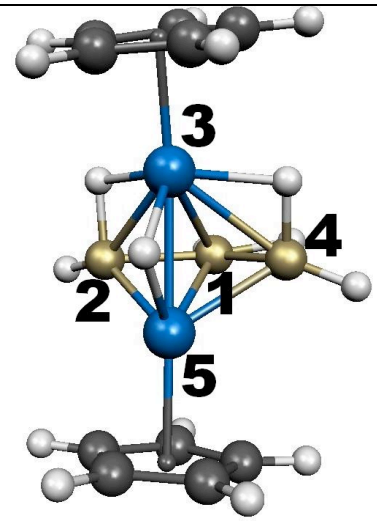
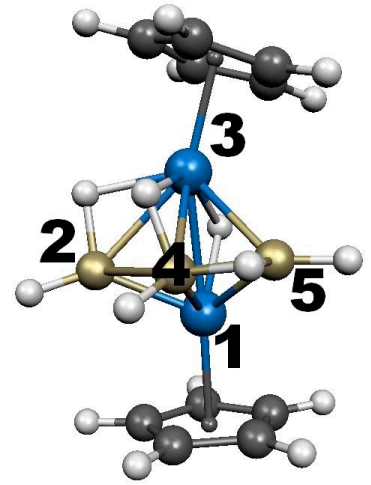
Table S8B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Re_2B_3H_7$ optimized structures.

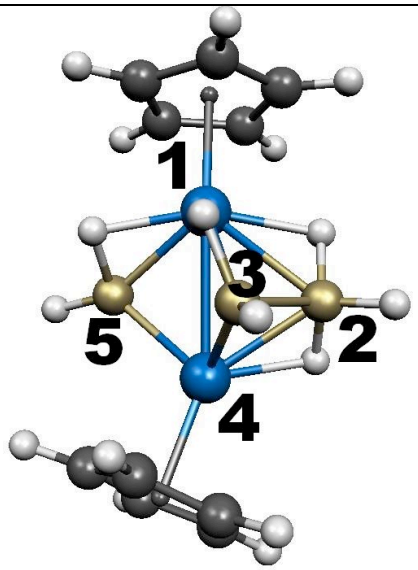
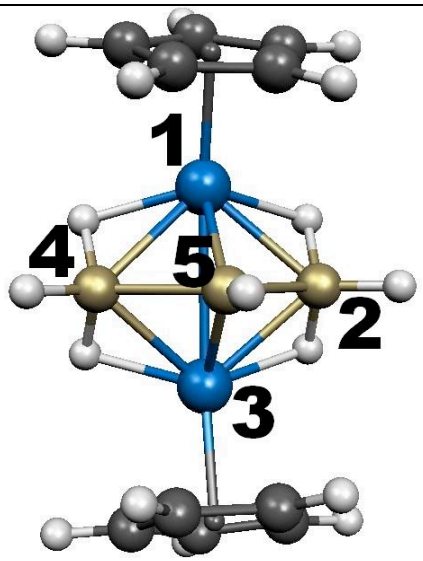
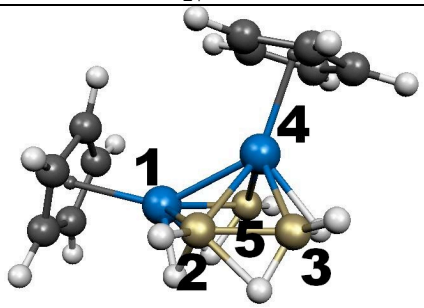
Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	3_Re_Pentagon-1-Ce	-622.54402683	0.00
2	GES-mod3	-622.54047474	2.23
3	BPT-2	-622.53382886	6.40
4	BPT-1	-622.52546120	11.65
5	GES-mod2	-622.52419503	12.44
6	3_Re_Pentagon-1-Ce	-622.52240807	13.57
7	3_Re_Pentagon-1-Bd	-622.52219080	13.70
8	3_Re_Pentagon-2-Cc	-622.52036111	14.85
9	3_Re_Pentagon-1-Ca	-622.51244935	19.82
10	3_Re_C.	-622.51203652	20.07
11	3_Re_Pentagon-1-Cb	-622.51180169	20.22
12	3_Re_Pentagon-1-Cc	-622.51180168	20.22
13	3_Re_B.	-622.50852164	22.28
14	3_Re_Pentagon-1-Ba	-622.50826490	22.44
15	3_Re_Pentagon-1-Bd	-622.50693771	23.27
16	3_Re_A1	-622.50631498	23.66

17	3_Re_A.	-622.50257927	26.01
18	3_Re_Pentagon-1-Be	-622.49824520	28.73
19	3_Re_Pentagon-1-Ca	-622.49649935	29.82
20	3_Re_Pentagon-2-Bd	-622.48777868	35.30
21	3_Re_Pentagon-2-Cc	-622.48576485	36.56
22	GES-mod1	-622.48536783	36.81
23	GESTAA-Re	-622.48536609	36.81
24	3_Re_Pentagon-2-Ch	-622.48529560	36.85
25	5v-Ta2B3-1__Re	-622.48489843	37.10
26	3_Re_Pentagon-2-Cg	-622.48345400	38.01
27	3_Re_Pentagon-2-Bc	-622.48316362	38.19
28	3_Re_Pentagon-2-Cb	-622.48286604	38.38
29	3_Re_Pentagon-1-Ab	-622.48103891	39.53
30	3_Re_Pentagon-1-Bc	-622.48089706	39.61
31	3_Re_Pentagon-2-Be	-622.47951338	40.48
32	3_Re_Pentagon-2-Bb	-622.47635707	42.46
33	3_Re_Pentagon-1-Bb	-622.47279380	44.70
34	3_Re_Pentagon-1-Aa	-622.47214676	45.11
35	3_Re_Pentagon-2-Ca	-622.46980275	46.58
36	3_Re_Pentagon-2-Ab	-622.46914180	46.99
37	3_Re_Pentagon-2-Ba	-622.46823838	47.56
38	3_Re_Pentagon-2-Ad	-622.46805632	47.67
39	3_Re_Pentagon-2-Cf	-622.46663692	48.56
40	3_Re_Pentagon-2-Ac	-622.46469906	49.78
41	3_Re_Pentagon-2-Aa	-622.45024054	58.85
42	3_Re_Pentagon-1-Ac	-622.43829251	66.35
43	3_Re_Pentagon-2-Ce	-622.42882032	72.29
44	3_Re_Pentagon-1-Cd	-622.41182859	82.96
45	3_Re_Pentagon-2-Cd	-622.39111910	95.95
46	3_Re_Pentagon-2-Ae	-622.38692223	98.58

Table S9A. Distance table for the lowest-lying $Cp_2Mo_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 **1. Mo2B3-1 -602.205202 a.u. 0.0 kcal/mol Cs WBI 1.51**	1 2 3 4 1 Mo 0.000000 2 B 2.208838 0.000000 3 Mo 2.521025 2.195478 0.000000 4 B 2.334313 1.647130 2.283135 0.000000 5 B 2.232485 2.986099 2.270133 1.807554 Mo1-H-Mo3 Mo1-H 1.85 Mo3-H 1.86 Mo3-H- B5 Mo3-H 1.78 B5-H 1.33 Mo1-H-B5 Mo1-H 1.78 B5-H 1.32 B2-H-B4 B2-H 1.31 B4-H 1.3
 2. Mo2B3-2 -602.201032 +2.6 Cs WBI 1.07	1 2 3 4 1 Mo 0.000000 2 B 2.224601 0.000000 3 Mo 2.739400 2.224601 0.000000 4 B 2.232622 3.312813 2.232622 0.000000 5 B 2.091595 1.817785 2.091595 3.253731 Mo1-H-B2 Mo1-H 1.8 B2-H 1.37 Mo1-H-B4 Mo1-H 1.85 B4-H 1.31 Mo3-H-B2 Mo3-H 1.81 B2-H 1.37 Mo3-H-B4 Mo3-H 1.85 B4-H 1.31
 3. Mo2B3-3 -602.200268 +3.1 WBI 1.53	1 2 3 4 5 1 Mo 0.000000 2 B 2.254699 0.000000 3 Mo 2.499594 2.181048 0.000000 4 B 2.231627 1.682766 2.328636 0.000000 5 B 2.335395 3.012209 2.352697 1.675619 Mo1-H-Mo3 Mo1-H 1.82 Mo3-H 1.87 Mo1-H-B2 Mo1-H 1.81 B2-H 1.31 Mo1-H-B5 Mo1-H-B5 1.92 B5-H 1.27 Mo3-H-B5 Mo3-H 1.85 B5-H 1.31

 4. Mo2B3-4 -602.196157 +5.7 WBI 1.00	1 2 3 4 5 1 Mo 0.000000 2 B 2.221345 0.000000 3 Mo 2.759137 2.272786 0.000000 4 B 2.127448 3.180906 2.182075 0.000000 5 B 2.119247 1.855653 2.173906 1.904741 Mo1-H-Mo3 Mo1-H 1.97 Mo3-H 1.95 Mo1-H-B2 Mo1-H 1.87 B2-H 1.29 Mo3-H-B2 Mo3-H 1.8 B2-H 1.35 Mo3-H-B4 Mo3-H 1.82 B4-H 1.31
 5. Mo2B3-5 -602.191516 +8.6 WBI 1.46	1 2 3 4 5 1 B 0.000000 2 B 1.878642 0.000000 3 Mo 2.345514 2.282161 0.000000 4 B 1.696849 3.095683 2.364944 0.000000 5 Mo 2.217469 2.065060 2.500134 2.221692 Mo3-H- Mo5 Mo3-H 1.82 Mo5-H 1.87 Mo3-H-B2 Mo3-H 1.84 B2-H 1.31 Mo3-H-B4 Mo3-H 1.79 B4-H 1.32 B1-H-B2 B1-H 1.34 B2-H 1.3
 6. Mo2B3-6 -602.190959 +8.9 WBI 1.36	1 2 3 4 5 1 Mo 0.000000 2 B 2.048360 0.000000 3 Mo 2.513308 2.322126 0.000000 4 B 2.277069 2.156764 2.350410 0.000000 5 B 2.164182 3.193773 2.318361 1.686842 Mo1-H- Mo3 Mo1-H 1.86 Mo3-H 1.84 Mo3-H-B2 Mo3-H 1.81 B2-H 1.34 Mo3-H-B4 Mo3-H 1.85 B4-H 1.33 B4-H-B5 B4-H 1.33 B5-H 1.31

 7. Mo2B3-7 -602.186609 +11.7 WBI 1.11	1 2 3 4 5 1 Mo 0.000000 2 B 2.352769 0.000000 3 B 2.294930 1.871944 0.000000 4 Mo 2.657690 2.222004 2.081299 0.000000 5 B 2.133980 3.515805 3.095076 2.143441 Mo1-H-B2 Mo1-H 1.89 B2-H 1.26 Mo1-H-B3 Mo1-H 1.78 B3-H 1.37 Mo1-H-B5 Mo1-H 1.83 B5-H 1.32 Mo4-H-B2 Mo4-H 1.88 B2-H 1.29
 8. Mo2B3-8 -602.185979 +12.1 C_{2v} WBI 1.15	1 2 3 4 5 1 Mo 0.000000 2 B 2.213918 0.000000 3 Mo 2.911200 2.213918 0.000000 4 B 2.213880 3.245900 2.213880 0.000000 5 B 2.109621 1.984201 2.109621 1.984168 Mo1-H-B2 Mo1-H 1.82 B2-H 1.31 Mo1-H-B4 Mo1-H 1.82 B4-H 1.31 Mo3-H-B2 Mo3-H 1.82 B2-H 1.31 Mo3-H-B4 Mo3-H 1.82 B4-H 1.31
 9. Mo2B3-9 -602.171797 +21.0 WBI 1.94	1 2 3 4 5 1 Mo 0.000000 2 B 2.237273 0.000000 3 B 3.440791 1.763772 0.000000 4 Mo 2.375418 2.279928 2.175859 0.000000 5 B 2.120740 3.375697 3.539944 2.202109 Mo1-H-B2 Mo1-B2 1.82 B2-H 1.36 Mo1-H-B5 Mo1-H 1.82 B5-H 1.32 Mo4-H-B3 Mo4-H 1.91 B3-H 1.29 B2-H-B3 B2-H 1.6 B3-H 1.24

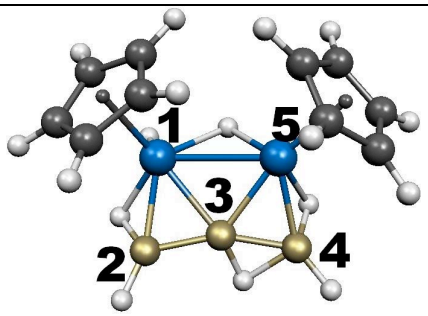
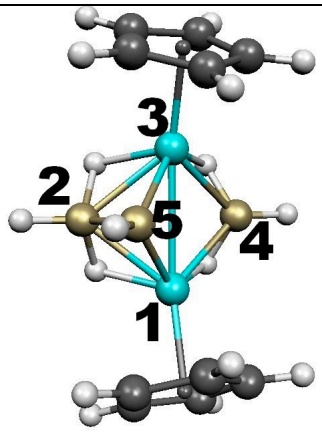
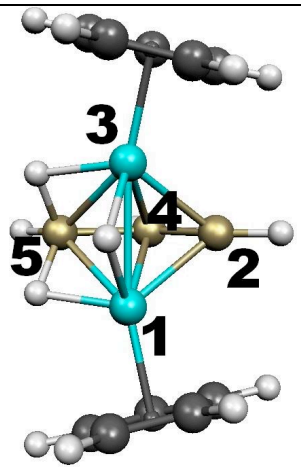
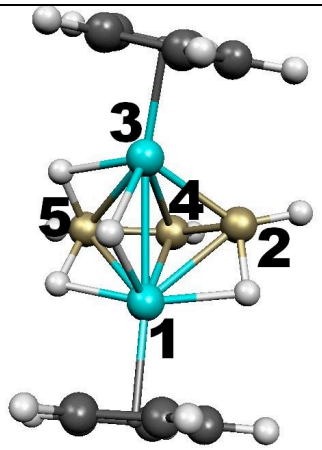
 10. Mo2B3-10 -602.171199 +21.3 (Cs) WBI 1.01	1 2 3 4 5 1 Mo 0.000000 2 B 2.061866 0.000000 3 B 2.198391 1.696859 0.000000 4 B 3.640721 3.327603 1.689144 0.000000 5 Mo 2.661011 3.568181 2.130637 2.058366 Mo1-H- Mo5 Mo1-H 1.93 Mo5-H 1.84 Mo1-H-B2 Mo1-H 1.83 B2-H 1.28 Mo5-H-B4 Mo5-H 1.85 B4-H 1.35 B3-H-B4 B3-H 1.26 B4-H 1.46

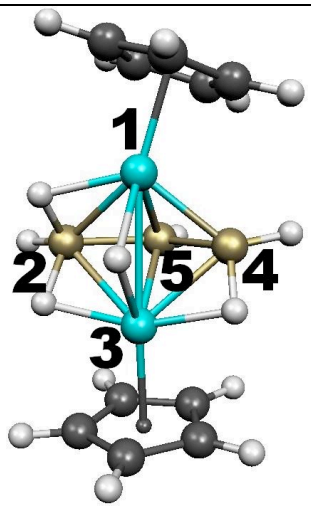
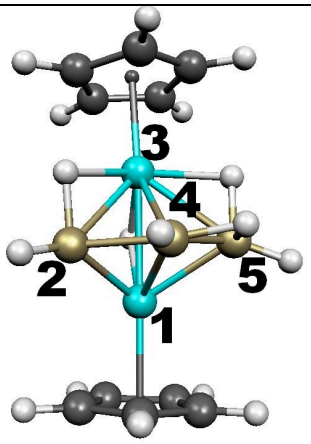
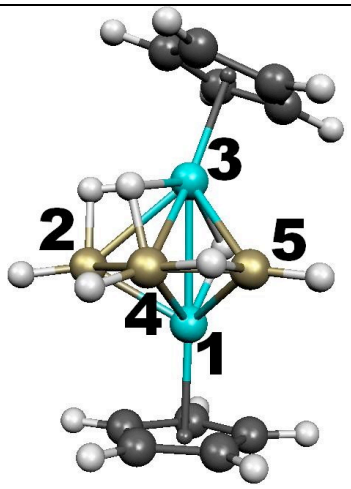
Table S9B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Mo_2B_3H_7$ optimized structures.

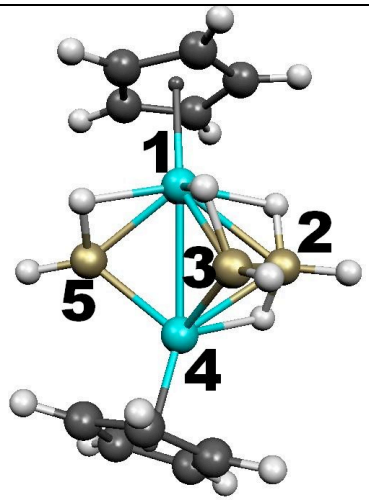
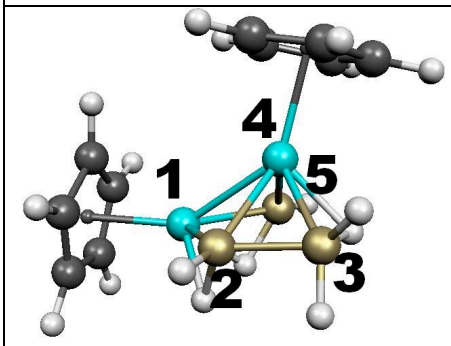
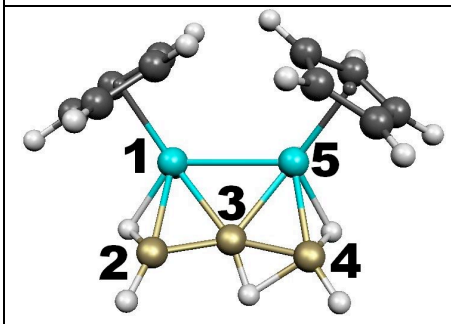
Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	BPT-2	-602.32513420	0.00
2	BPT-1	-602.31925725	3.69
3	1-W__Mo	-602.31485497	6.45
4	GES-mod2	-602.31066223	9.08
5	5v-Ta2B3-1__Mo_	-602.31066201	9.08
6	GES-mod1	-602.31066114	9.08
7	Ges-Mo_M06L	-602.31066102	9.08
8	1_Mo_Pentagon-1-Bd	-602.31065658	9.08
9	GES-mod3	-602.30665105	11.60
10	4-W__Mo	-602.30664537	11.60
11	1_Mo_B_B3LYP	-602.30451754	12.94
12	1_Mo_B.	-602.30451703	12.94
13	1_Mo_Pentagon-1-Cb	-602.29263858	20.39
14	6-W__Mo	-602.28807301	23.26
15	1_Mo_Pentagon-1-Ca	-602.28805977	23.26
16	1_Mo_Pentagon-1-Bd	-602.27924279	28.80
17	1_Mo_Pentagon-1-Aa	-602.27862423	29.19
18	1_Mo_Pentagon-1-Bc	-602.27794965	29.61
19	1_Mo_Pentagon-1-Cb	-602.27761615	29.82
20	1_Mo_Pentagon-1-Ba	-602.27569375	31.02
21	1_Mo_Pentagon-1-Bb	-602.27410103	32.02
22	1_Mo_Pentagon-1-Bc	-602.27153065	33.64

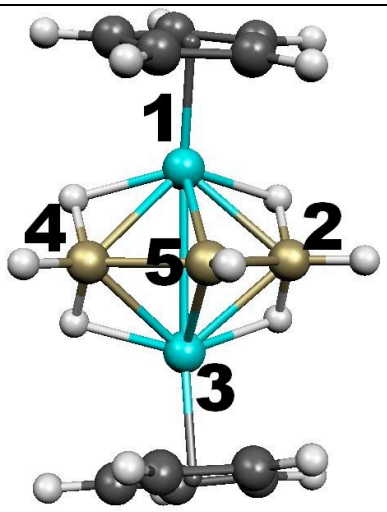
23	1_Mo_Pentagon-2-Cf	-602.26997260	34.61
24	1_Mo_A.	-602.26923814	35.07
25	1_Mo_Pentagon-1-Ce	-602.26697039	36.50
26	1_Mo_Pentagon-2-Ad	-602.26420817	38.23
27	1_Mo_Pentagon-2-Ad	-602.26420817	38.23
28	1_Mo_Pentagon-2-Aa	-602.26420809	38.23
29	1_Mo_Pentagon-2-Ac	-602.26420809	38.23
30	1_Mo_Pentagon-2-Ab	-602.26420808	38.23
31	1_Mo_A1-M06L	-602.26307494	38.94
32	1_Mo_Pentagon-1-Be	-602.25954017	41.16
33	1_Mo_C.	-602.25631939	43.18
34	1_Mo_Pentagon-1-Ab	-602.25609191	43.32
35	1_Mo_Pentagon-2-Cd	-602.25539643	43.76
36	1_Mo_Pentagon-1-Cd	-602.25520777	43.88
37	1_Mo_Pentagon-2-Bd	-602.25090502	46.58
38	1_Mo_Pentagon-2-Ch	-602.25090501	46.58
39	1_Mo_Pentagon-1-Cc	-602.25073637	46.68
40	1_Mo_A2-M06L	-602.24998129	47.16
41	1_Mo_Pentagon-2-Cg	-602.24540030	50.03
42	1_Mo_Pentagon-2-Bb	-602.23870037	54.24
43	1_Mo_Pentagon-2-Cb	-602.22932435	60.12
44	1_Mo_Pentagon-2-Ba	-602.22932434	60.12
45	1_Mo_Pentagon-2-Ce	-602.22739978	61.33
46	1_Mo_Pentagon-2-Cc	-602.22673063	61.75
47	1_Mo_Pentagon-2-Bc	-602.22482331	62.95
48	1_Mo_Pentagon-2-Be	-602.22482331	62.95
49	1_Mo_Pentagon-1-Ac	-602.22028828	65.79
50	1_Mo_Pentagon-2-Ca	-602.20269327	76.83
51	1_Mo_Pentagon-2-Ae	-602.18130636	90.25

Table S10A. Distance table for the lowest-lying $Cp_2W_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 **1. W2B3-1 -600.005158 a.u. 0.0 kcal/mol Cs WBI 1.05**	1 2 3 4 5 1 W 0.000000 2 B 2.228523 0.000000 3 W 2.762000 2.228581 0.000000 4 B 2.231339 3.290531 2.231261 0.000000 5 B 2.111307 1.815766 2.111377 3.266915 W1-H-B2 W1-H 1.79 B2-H 1.42 W1-H-B4 W1-H 1.85 B4-H 1.32 W3-H-B2 W3-H 1.79 B2-H 1.42 W3-H-B4 W3-H 1.85 B4-H 1.32
 2. W2B3-2 -600.003473 +1.1 Cs WBI 1.50	1 2 3 4 5 1 W 0.000000 2 B 2.213541 0.000000 3 W 2.556102 2.209411 0.000000 4 B 2.338541 1.658182 2.323339 0.000000 5 B 2.246761 2.972402 2.257420 1.799184 W1-H-W3 W1-H 1.87 W3-H 1.87 W1-H-B5 W1-H 1.79 B5-H 1.35 W3-H-B5 W3-H 1.79 B5-H 1.36 B2-H-B4 B2-H 1.31 B4-H 1.3
 3. W2B3-3 -600.000438 +3.0 WBI 1.53	1 2 3 4 5 1 W 0.000000 2 B 2.264922 0.000000 3 W 2.537747 2.174427 0.000000 4 B 2.261324 1.692057 2.340646 0.000000 5 B 2.346383 3.001547 2.350455 1.674504 W1-H-W3 W1-H 1.83 W3-H 1.88 W1-H-B2 W1-H 1.80 B2-H 1.34 W1-H-B5 W1-H 1.91 B5-H 1.29 W3-H-B5 W3-H 1.86 B5-H 1.32

 4. W2B3-4 -599.996771 +5.3 WBI 1.01	1 2 3 4 5 1 W 0.000000 2 B 2.221126 0.000000 3 W 2.779651 2.262277 0.000000 4 B 2.135981 3.182836 2.201291 0.000000 5 B 2.138154 1.862803 2.189902 1.925052 W1-H-W3 W1-H 1.97 W3-H 1.95 W1-H-B2 W1-H 1.86 B2-H 1.31 W3-H-B2 W3-H 1.80 B2-H 1.39 W3-H-B4 W3-H 1.84 B4-H 1.32
 5. W2B3-5 -599.990363 +9.3 WBI 1.45	1 2 3 4 5 1 W 0.000000 2 B 2.071279 0.000000 3 W 2.535955 2.297885 0.000000 4 B 2.230762 1.898698 2.371379 0.000000 5 B 2.229273 3.105979 2.372739 1.706202 W1-H-W3 W1-H 1.88 W3-H 1.83 W3-H-B2 W3-H 1.79 B2-H 1.35 W3-H-B5 W3-H 1.84 W5-H 1.33 B4-H-B5 B4-H 1.36 B5-H 1.29
 6. W2B3-6 -599.990321 +9.3 WBI 1.36	1 2 3 4 5 1 W 0.000000 2 B 2.057212 0.000000 3 W 2.545169 2.342947 0.000000 4 B 2.290229 2.178888 2.373280 0.000000 5 B 2.180023 3.207985 2.323198 1.690980 W1-H-W3 W1-H 1.86 W3-H 1.86 W3-H-B2 W3-H 1.81 B2-H 1.38 W3-H-B4 W3-H 1.85 B4-H 1.36 B4-H-B5 B4-H 1.33 B5-H 1.32

 7. W2B3-7 -599.989155 +10.0 WBI 1.12	1 2 3 4 5 1 W 0.000000 2 B 2.353487 0.000000 3 B 2.316116 1.887034 0.000000 4 W 2.682470 2.223040 2.085339 0.000000 5 B 2.145509 3.512236 3.096793 2.153925 W1-H-B2 W1-H 1.90 B2-H 1.26 W1-H-B3 W1-H 1.79 B3-H 1.42 W1-H-B5 W1-H 1.84 B5-H 1.33 W4-H-B2 W4-H 1.87 B2-H 1.32
 8. W2B3-8 -599.980710 +15.3 WBI 1.83	1 2 3 4 5 1 W 0.000000 2 B 2.186047 0.000000 3 B 3.512015 1.851222 0.000000 4 W 2.441900 2.221990 2.204920 0.000000 5 B 2.146093 3.302901 3.518547 2.179670 W1-H-B2 W1-H 1.82 B2-H 1.40 W1-H-B4 W1-H 1.83 B4-H 1.35 W4-H-B3 W4-H 1.88 B3-H 1.32
 9. W2B3-9 -599.979786 +15.9 (Cs) WBI 1.28	1 2 3 4 5 1 W 0.000000 2 B 2.067257 0.000000 3 B 2.151617 1.715422 0.000000 4 B 3.636994 3.335011 1.719896 0.000000 5 W 2.654309 3.610881 2.154453 2.080656 W1-H-B2 W1-H 1.85 B2-H 1.29 W5-H-B4 W5-H 1.87 B4-H 1.30 B3-H-B4 B3-H 1.23 B4-H 1.55



10. W2B3-10 -599.976787
+17.8 C_{2v} WBI 1.20

	1	2	3	4	5
1 W	0.000000				
2 B	2.214319	0.000000			
3 W	2.916200	2.214319	0.000000		
4 B	2.214378	3.219400	2.214378	0.000000	
5 B	2.139576	1.969239	2.139576	1.969230	

W1-H-B2 W1-H 1.82 B2-H 1.36
W1-H-B4 W1-H 1.82 B4-H 1.36
W3-H-B2 W3-H 1.82 B2-H 1.36
W3-H-B4 W3-H 1.82 B4-H 1.36

Table S10B. Energy ranking for the B3LYP/6-31G(d) $Cp_2W_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	2_W_B.	-600.08859706	0.00
2	BPT-2	-600.08582081	1.74
3	BPT-1	-600.08161411	4.38
4	BPT-1-Mo__W	-600.08160992	4.38
5	1_W_Pentagon-1-Ca	-600.08037291	5.16
6	1_W_Pentagon-2-Cf	-600.07735235	7.06
7	1_W_Pentagon-1-Ce	-600.07661718	7.52
8	1_W_Pentagon-1-Bd	-600.07659767	7.53
9	1_W_Pentagon-1-Aa	-600.07565152	8.12
10	GES-mod2	-600.07213957	10.33
11	1_W_Pentagon-1-Bc	-600.07213403	10.33
12	GES-mod2-Mo_W	-600.07213237	10.33
13	1-Mo__W	-600.07212733	10.33
14	GES	-600.07195717	10.44
15	GES-mod1	-600.07195610	10.44
16	5v-Ta2B3-1__W	-600.07195581	10.44
17	1_W_Pentagon-1-Bd	-600.07151500	10.72
18	1_W_Pentagon-1-Be	-600.06894284	12.33
19	1_W_Pentagon-2-Bd	-600.06788822	13.00
20	1_W_Pentagon-2-Cb	-600.06788822	13.00

21	1_W_Pentagon-2-Be	-600.06771600	13.10
22	1_W_Pentagon-1-Cc	-600.06723582	13.40
23	1_W_Pentagon-1-Cb	-600.06687091	13.63
24	1_W_Pentagon-1-Ba	-600.06412075	15.36
25	1_W_Pentagon-2-Cd	-600.06294844	16.09
26	1_W_Pentagon-1-Bc	-600.06292748	16.11
27	1_W_Pentagon-1-Bb	-600.06163413	16.92
28	5-Mo__W	-600.06152063	16.99
29	1_W_Pentagon-2-Cf	-600.06090940	17.37
30	3-Mo__W	-600.06065436	17.53
31	GES-mod3	-600.06065436	17.53
32	1_Mo_Pentagon-2-Bd	-600.05945579	18.29
33	1_W_Pentagon-1-Ce	-600.05920950	18.44
34	4-Mo__W	-600.05709110	19.77
35	1_W_Pentagon-2-Cd	-600.05515981	20.98
36	6-Mo__W	-600.05208420	22.91
37	1_W_Pentagon-1-Cc	-600.05063508	23.82
38	1_W_Pentagon-2-Aa	-600.04913353	24.76
39	1_W_Pentagon-1-Be	-600.04872443	25.02
40	7-Mo__W	-600.04707697	26.05
41	2_W_A.	-600.04488204	27.43
42	2_W_A1-M06L	-600.04320151	28.49
43	1_W_Pentagon-1-Ac	-600.04106359	29.83
44	1_W_Pentagon-1-Ac	-600.04106358	29.83
45	1_W_Pentagon-2-Ad	-600.03782766	31.86
46	2_W_C.	-600.03765452	31.97
47	1_W_Pentagon-1-Ab	-600.03512430	33.55
48	1_W_Pentagon-1-Cd	-600.03327538	34.71
49	1_W_Pentagon-2-Ch	-600.02898027	37.41
50	1_W_Pentagon-2-Cg.	-600.02857915	37.66
51	1_W_Pentagon-2-Cc	-600.02453503	40.20
52	1_W_Pentagon-2-Ca	-600.02067338	42.62
53	1_W_Pentagon-2-Bb	-600.01862603	43.91
54	2_W_A2-M06L	-600.01666047	45.14
55	1_W_Pentagon-2-Ba	-600.01065303	48.91
56	1_W_Pentagon-2-Ce	-600.01064235	48.92
57	1_W_Pentagon-2-Ac	-600.01007957	49.27
58	1_W_Pentagon-2-Ab	-600.01007956	49.27
59	1_W_Pentagon-2-Bc	-600.00350973	53.39
60	1_W_Pentagon-2-Ae	-599.95766320	82.16

Table S11A. Distance table for the lowest-lying $Cp_2Ta_2B_3H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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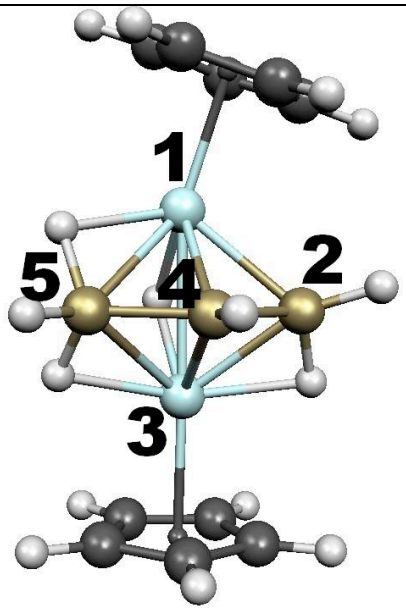
<td> 

1. Ta2B3-1 -579.846313 a.u.
0.0 kcal/mol WBI 1.11</td>
<td>1 2 3 4 5
1 Ta 0.000000
2 B 2.300990 0.000000
3 Ta 2.737824 2.219098 0.000000
4 B 2.303440 1.758072 2.255441 0.000000
5 B 2.352154 3.108042 2.331263 1.756317

Ta1-H-Ta3 Ta1-H 1.97 Ta3-H 1.95
Ta1-H-B5 Ta1-H 1.89 B5-H 1.34
Ta3-H-B2 Ta3-H 1.91 B2-H 1.26
Ta3-H-B5 Ta3-H 1.94 B5-H 1.28</td>
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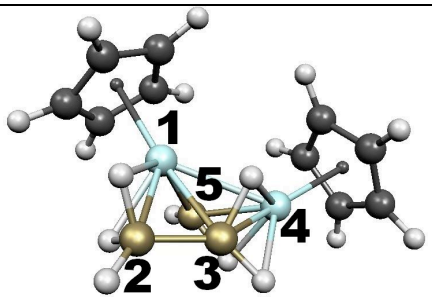
<td> 

2. Ta2B3-2 -579.807993 +24.1
WBI 1.23</td>
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1 Ta 0.000000
2 B 2.265293 0.000000
3 B 2.250464 1.707198 0.000000
4 Ta 2.710531 3.679671 2.188535 0.000000
5 B 2.280465 3.615177 2.975894 2.186436

Ta1-H’-B2 Ta1-H’ 2.05 B2-H 1.27
Ta1-H’’-B2 Ta1-H’’ 1.99 B2-H 1.31
Ta1-Ta4-B3-H Ta1-H 2.18 Ta4-H 1.99 B3-H 1.34
Ta4-H-B5 Ta4-H 1.93 B5-H 1.32</td>
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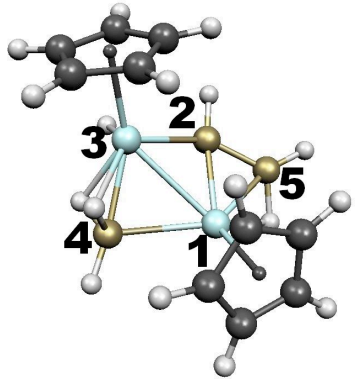
<td> 

3. Ta2B3-3 -579.807752 +24.2
WBI 1.07</td>
<td>1 2 3 4 5
1 Ta 0.000000
2 B 2.201646 0.000000
3 Ta 2.807883 2.240443 0.000000
4 B 2.482109 3.393499 2.167397 0.000000
5 B 2.176156 1.655253 3.713330 4.294884

Ta1-H-B5 Ta1-H 1.91 B5-H 1.28
Ta3-H’-B4 Ta3-H’ 1.97 B4-H’1.28
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Ta3-H 1.78</td>
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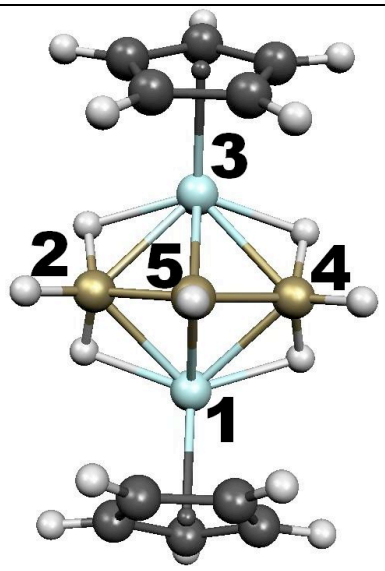
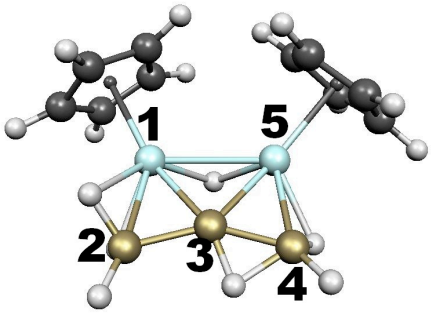


4. Ta2B3-4 -579.807450 +24.4 C_{2v} WBI 0.94

	1	2	3	4	5
1	Ta	0.000000			
2	B	2.295775	0.000000		
3	Ta	3.172800	2.295775	0.000000	
4	B	2.295823	3.131400	2.295823	0.000000
5	B	2.193602	1.839196	2.193602	1.839091

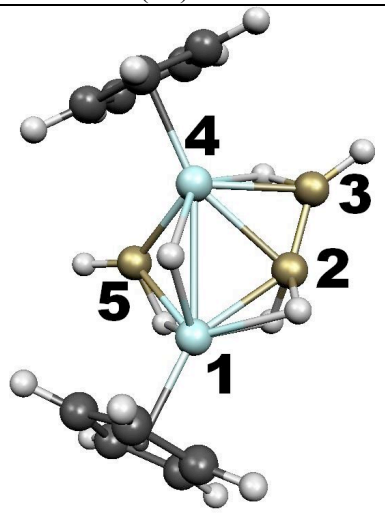
Ta1-H-B4 Ta1-H 1.88 B4-H 1.35
Ta1-H-B2 Ta1-H 1.88 B2-H 1.35
Ta3-H-B4 Ta3-H 1.88 B4-H 1.35
Ta3-H-B2 Ta3-H 1.88 B2-H 1.35



5. Ta2B3-5 -579.807176 +24.6 (Cs) WBI 1.74

	1	2	3	4	5
1	Ta	0.000000			
2	B	2.217593	0.000000		
3	B	2.244243	1.753143	0.000000	
4	B	3.693814	3.326241	1.679666	0.000000
5	Ta	2.661799	3.713217	2.204865	2.192724

Ta1-H-Ta5 Ta1-H 1.93 Ta5-H 1.98
Ta1-H'-B2 Ta1-H' 2.01 B2-H' 1.26
Ta1-H''-B2 Ta1-H'' 2.01 B2-H' 1.31
Ta5-H-B4 Ta5-H 1.95 B4-H 1.29
B3-H-B4 B3-H 1.28 B4-H 1.39



6. Ta2B3-6 -579.801970 +27.8 WBI 0.98

	1	2	3	4	5
1	Ta	0.000000			
2	B	2.159854	0.000000		
3	B	3.565300	1.618323	0.000000	
4	Ta	2.798648	2.367241	2.236524	0.000000
5	B	2.279271	3.119158	3.702142	2.196584

Ta1-H-Ta4 Ta1-H 1.89 Ta4-H 1.97
Ta1-H'-B2 Ta1-H' 2.02 B2-H' 1.28
Ta1-H''-B2 Ta1-H'' 1.91 B2-H'' 1.33
Ta1-H-B5 Ta1-H 1.86 B5-H 1.36
Ta4-H-B3 Ta4-H 1.95 B3-H 1.31

Table S11B. Energy ranking for the B3LYP/6-31G(d) $Cp_2Ta_2B_3H_7$ optimized structures.

Nr.	Name	Energy (a.u.)	ΔE(kcal/mol)
1	BPT-1	-579.95879960	0.00
2	BPT-2	-579.95878953	0.01
3	GES-mod1	-579.95846185	0.21
4	GESTAA-Ta	-579.95846123	0.21
5	GES-mod3	-579.91982654	24.46
6	4_Ta_Pentagon-1-Ac	-579.91980218	24.47
7	4_Ta_Pentagon-1-Ac	-579.91695170	26.26
8	4_Ta_Pentagon-2-Be	-579.91327901	28.56
9	4_Ta_Pentagon-1-Ac	-579.90805879	31.84
10	4_Ta_Pentagon-1-Bd	-579.90794575	31.91
11	4_Ta_Pentagon-1-Aa	-579.90141300	36.01
12	4_Ta_Pentagon-1-Ce	-579.89975520	37.05
13	4_Ta_Pentagon-2-Cb	-579.89963450	37.13
14	4_Ta_Pentagon-2-Bd	-579.89963420	37.13
15	4_Ta_Pentagon-2-Ba	-579.89963420	37.13
16	4_Ta_Pentagon-2-Cf	-579.89963420	37.13
17	4_Ta_Pentagon-1-Be	-579.89850230	37.84
18	4_Ta_Pentagon-1-Ca	-579.89834740	37.93
19	4_Ta_Pentagon-1-Bd	-579.89823320	38.01
20	4_Ta_Pentagon-1-Cb	-579.89823320	38.01
21	4_Ta_Pentagon-1-Bc	-579.89800880	38.15
22	4_Ta_Pentagon-2-Be	-579.89757600	38.42
23	4_Ta_Pentagon-1-Ac	-579.89545890	39.75
24	4_Ta_Pentagon-1-Cc	-579.89504190	40.01
25	4_Ta_Pentagon-2-Ad	-579.89075880	42.70
26	4_Ta_A2	-579.88744890	44.77
27	4_Ta_C._B3LYP_CC	-579.88671560	45.23
28	4_Ta_B.	-579.88564040	45.91
29	4_Ta_Pentagon-2-Ch	-579.88263970	47.79
30	4_Ta_Pentagon-1-Ba	-579.88025320	49.29
31	4_Ta_A1	-579.87713869	51.24
32	4_Ta_Pentagon-2-Ca	-579.87712620	51.25
33	4_Ta_Pentagon-1-Ab	-579.87537390	52.35
34	4_Ta_Pentagon-1-Cd	-579.87355480	53.49
35	4_Ta_Pentagon-2-Ac	-579.86736220	57.38
36	4_Ta_Pentagon-2-Aa	-579.86736220	57.38
37	4_Ta_Pentagon-2-Ae	-579.86736220	57.38
38	4_Ta_Pentagon-2-Cg	-579.86671530	57.78

39	4_Ta_Pentagon-2-Ce	-579.86273450	60.28
40	4_Ta_Pentagon-2-Bb	-579.86209280	60.68
41	4_Ta_Pentagon-2-Cd	-579.85936650	62.39
42	4_Ta_Pentagon-2-Ab	-579.85819290	63.13
43	4_Ta_Pentagon-1-Bb	-579.85682740	63.99
44	4_Ta_A.	-579.85643080	64.24
45	4_Ta_Pentagon-2-Cc	-579.85272660	66.56
46	4_Ta_Pentagon-2-Bc	-579.83365430	78.53