

Dimetallaborane Analogues of the Octaboranes of the Type $\text{Cp}_2\text{M}_2\text{B}_6\text{H}_{10}$: Structural Variations with Changes in the Skeletal Electron Count

Adrian M. V. Brânzanic,¹ Alexandru Lupan,^{*1} and R. Bruce King^{*2}

¹*Department of Chemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, Cluj-Napoca, Romania*

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

Table 1. Initial $\text{Cp}_2\text{M}_2\text{B}_6\text{H}_{10}$ structures.

Table 2A. Distance table for the lowest-lying $\text{Cp}_2\text{Ta}_2\text{B}_6\text{H}_{10}$ structures.

Table 2B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Ta}_2\text{B}_6\text{H}_{10}$ structures.

Table 2C. Energy ranking for all of the $\text{Cp}_2\text{Ta}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 3A. Distance table for the lowest-lying $\text{Cp}_2\text{Mo}_2\text{B}_6\text{H}_{10}$ structures.

Table 3B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Mo}_2\text{B}_6\text{H}_{10}$ structures.

Table 3C. Energy ranking for all of the $\text{Cp}_2\text{Mo}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 4A. Distance table for the lowest-lying $\text{Cp}_2\text{W}_2\text{B}_6\text{H}_{10}$ structures.

Table 4B. Distance table for the lowest-lying $\text{Cp}^*_2\text{W}_2\text{B}_6\text{H}_{10}$ structures.

Table 4C. Energy ranking for all of the $\text{Cp}_2\text{W}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 5A. Distance table for the lowest-lying $\text{Cp}_2\text{Re}_2\text{B}_6\text{H}_{10}$ structures.

Table 5B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Re}_2\text{B}_6\text{H}_{10}$ structures.

Table 5C. Energy ranking for all of the $\text{Cp}_2\text{Re}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 6A. Distance table for the lowest-lying $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_{10}$ structures.

Table 6B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Ru}_2\text{B}_6\text{H}_{10}$ structures.

Table 6C. Energy ranking for all of the $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 7A. Distance table for the lowest-lying $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_{10}$ structures

Table 7B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Os}_2\text{B}_6\text{H}_{10}$ structures

Table 7C. Energy ranking for all of the $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 8A. Distance table for the lowest-lying $\text{Cp}_2\text{Rh}_2\text{B}_6\text{H}_{10}$ structures.

Table 8B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Rh}_2\text{B}_6\text{H}_{10}$ structures

Table 8C. Energy ranking for all of the $\text{Cp}_2\text{Rh}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 9A. Distance table for the lowest-lying $\text{Cp}_2\text{Ir}_2\text{B}_6\text{H}_{10}$ structures.

Table 9B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Ir}_2\text{B}_6\text{H}_{10}$ structures.

Table 10A. Distance table for the lowest-lying $\text{Cp}_2\text{Pd}_2\text{B}_6\text{H}_{10}$ structures.

Table 10B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Pd}_2\text{B}_6\text{H}_{10}$ structures.

Table 10C. Energy ranking for all of the $\text{Cp}_2\text{Pd}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 11A. Distance table for the lowest-lying $\text{Cp}_2\text{Pt}_2\text{B}_6\text{H}_{10}$ structures.

Table 11B. Distance table for the lowest-lying $\text{Cp}^*_2\text{Pt}_2\text{B}_6\text{H}_{10}$ structures.

Table 11C. Energy ranking for all of the $\text{Cp}_2\text{Pt}_2\text{B}_6\text{H}_{10}$ optimized structures.

Table 12. Orbital energies and HOMO-LUMO gaps

Complete Gaussian09 Reference (reference 26)

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 1. Initial $\text{Cp}_2\text{M}_2\text{B}_6\text{H}_{10}$ structures, a total of 187 structures.

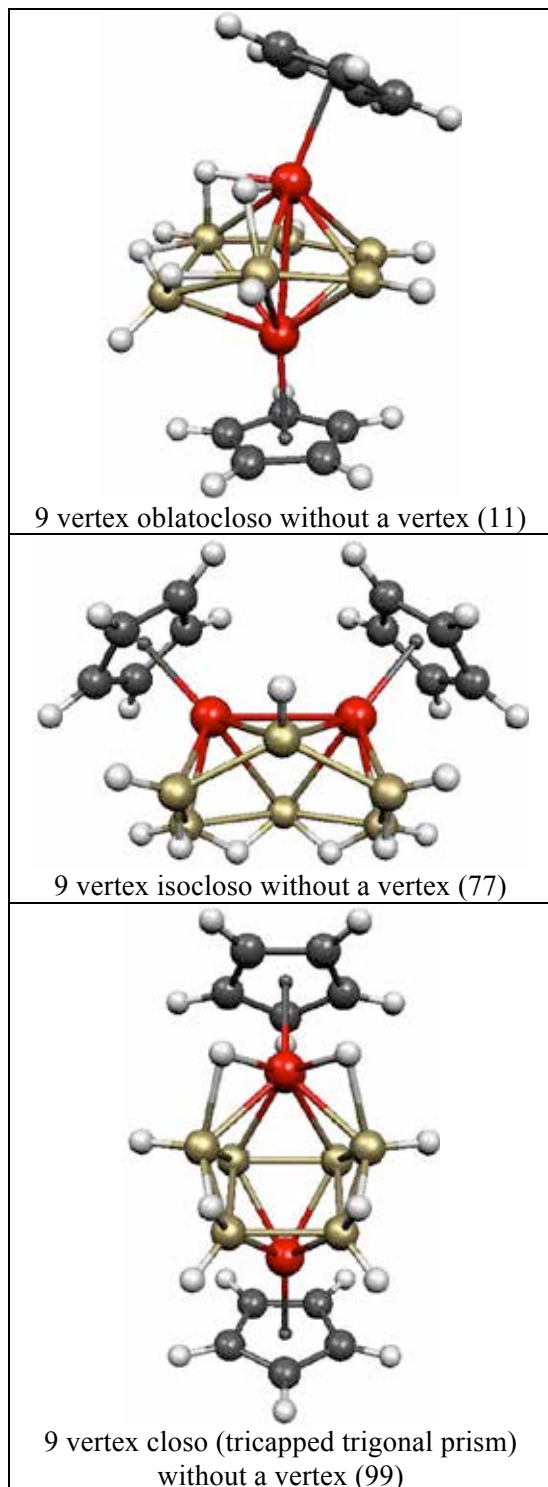
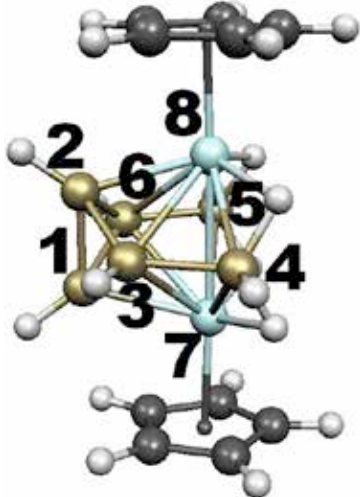
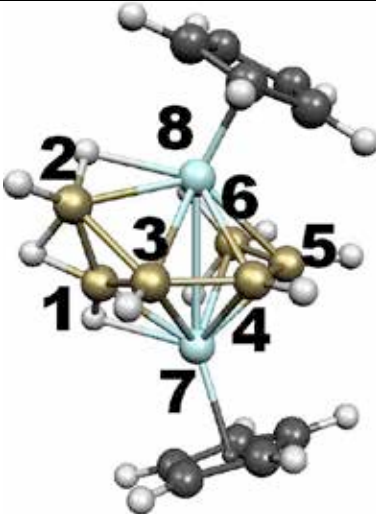
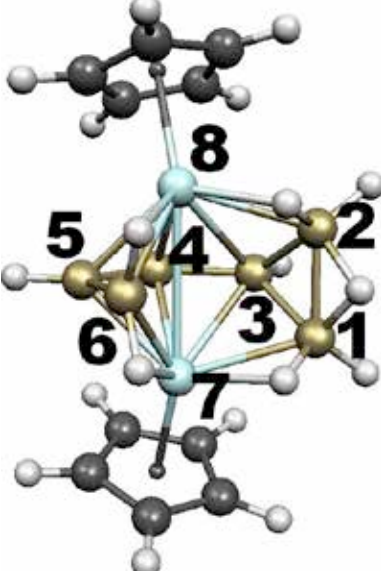
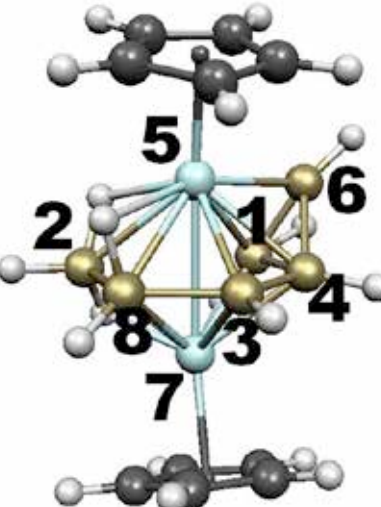
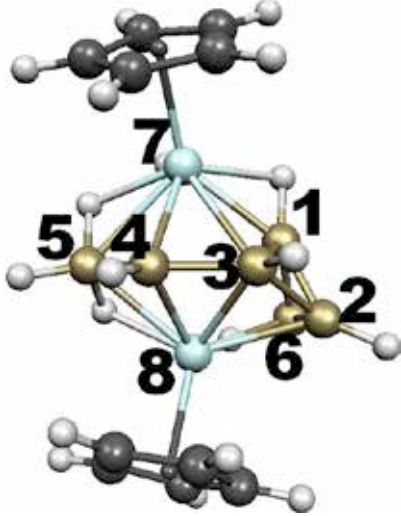
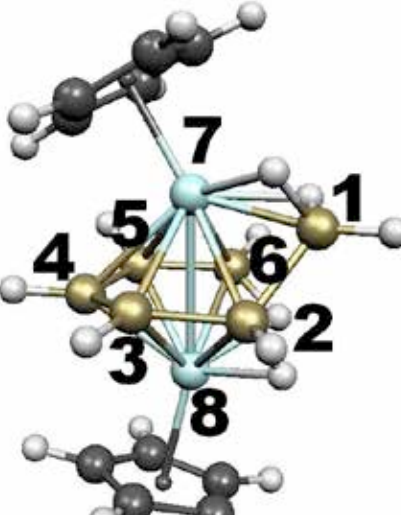
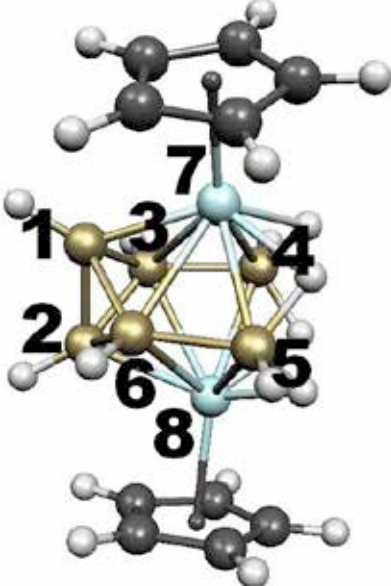
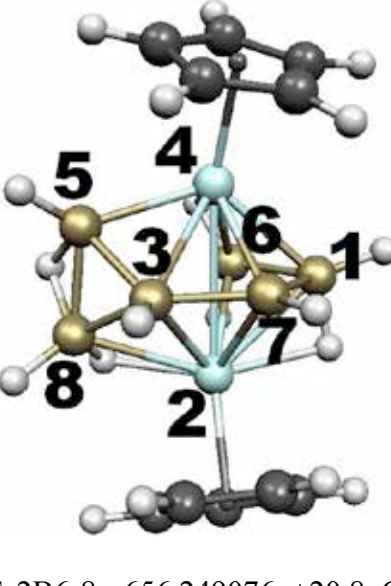


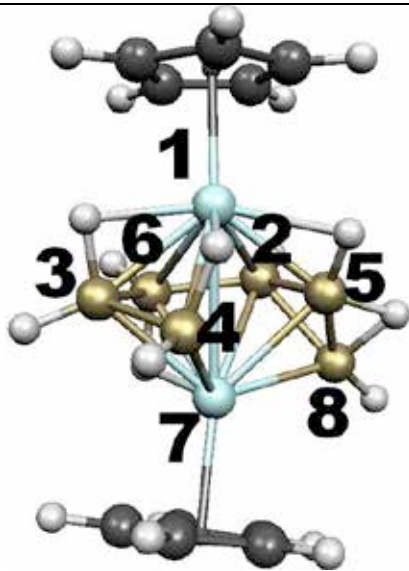
Table 2A. Distance table for the lowest-lying $\text{Cp}_2\text{Ta}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.704970</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.735147</td><td>1.735423</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.204740</td><td>3.204264</td><td>1.803970</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.204920</td><td>3.205085</td><td>3.615394</td><td>3.730209</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.736273</td><td>1.737028</td><td>2.634750</td><td>3.619864</td><td>1.806617</td></tr><tr><td>7 Ta</td><td>2.266155</td><td>3.170308</td><td>2.428033</td><td>2.374321</td><td>2.372335</td></tr><tr><td>8 Ta</td><td>3.175887</td><td>2.266964</td><td>2.433309</td><td>2.379681</td><td>2.377986</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ta</td><td>2.430765</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ta</td><td>2.435800</td><td>2.892289</td><td>0.000000</td><td></td><td></td></tr><tr><td colspan="6">Ta7-H-B4 Ta7-H 1.90 B4-H 1.27</td></tr><tr><td colspan="6">Ta7-H-B5 Ta7-H 1.90 B5-H 1.27</td></tr><tr><td colspan="6">Ta8-H-B4 Ta8-H 1.90 B4-H 1.28</td></tr><tr><td colspan="6">Ta8-H-B5 Ta8-H 1.90 B5-H 1.28</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.704970	0.000000				3 B	1.735147	1.735423	0.000000			4 B	3.204740	3.204264	1.803970	0.000000		5 B	3.204920	3.205085	3.615394	3.730209	0.000000	6 B	1.736273	1.737028	2.634750	3.619864	1.806617	7 Ta	2.266155	3.170308	2.428033	2.374321	2.372335	8 Ta	3.175887	2.266964	2.433309	2.379681	2.377986		6	7	8			6 B	0.000000					7 Ta	2.430765	0.000000				8 Ta	2.435800	2.892289	0.000000			Ta7-H-B4 Ta7-H 1.90 B4-H 1.27						Ta7-H-B5 Ta7-H 1.90 B5-H 1.27						Ta8-H-B4 Ta8-H 1.90 B4-H 1.28						Ta8-H-B5 Ta8-H 1.90 B5-H 1.28											
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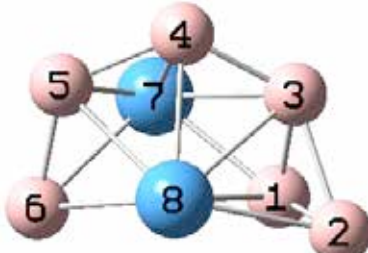
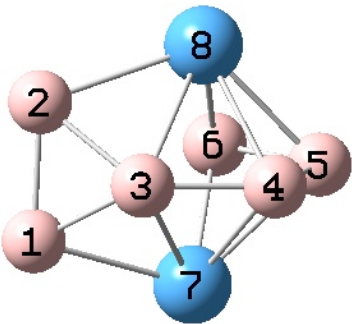
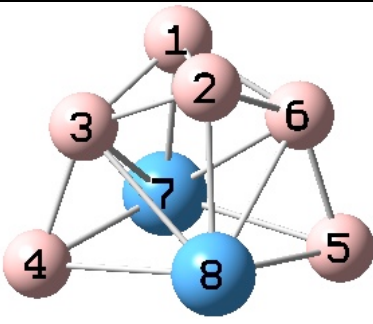
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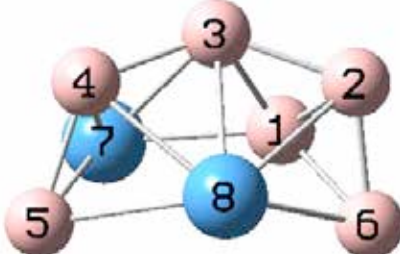
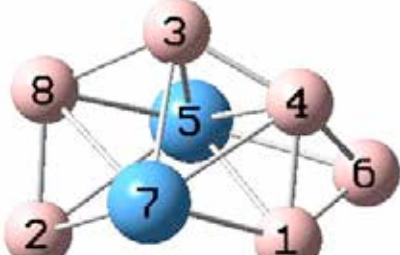
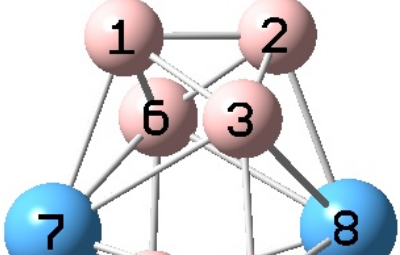


Ta2B6-9 -656.244505 +23.7 C₁
WBI 0.57

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5 B	2.221826	1.738735	3.507307	2.884920	0.000000
6 B	2.367965	1.801974	1.874310	3.184017	3.017317
7 Ta	2.978552	2.437645	2.386539	2.198016	2.356600
8 B	3.504147	1.858543	4.171710	3.836247	1.590706
	6	7	8		
6 B	0.000000				
7 Ta	2.283129	0.000000			
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Ta1-H-B3 Ta1-H 1.96 B3-H 1.25 Ta1-H-B4 Ta1-H 1.89 B4-H 1.33 Ta1-H-B5 Ta1-H 2.08 B5-H 1.25 B5-H-B8 B5-H 1.28 B8-H 1.35					

Table 2B. Distance table for the lowest-lying Cp*₂Ta₂B₆H₁₀ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Ta₂B₆H₁₀-1 = Ta₂B₆-2 -1049.243772 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.698377</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.690784</td><td>1.925668</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.878458</td><td>3.292544</td><td>1.731899</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.404871</td><td>4.107280</td><td>3.054773</td><td>1.734707</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.183784</td><td>4.048706</td><td>3.694694</td><td>3.096155</td><td>1.762852</td></tr><tr><td>7 Ta</td><td>2.159351</td><td>3.613271</td><td>2.444290</td><td>2.283867</td><td>2.202577</td></tr><tr><td>8 Ta</td><td>2.543997</td><td>2.315129</td><td>2.371828</td><td>2.250803</td><td>2.292617</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ta</td><td>2.398996</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ta</td><td>2.407907</td><td>3.081105</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.698377	0.000000				3 B	1.690784	1.925668	0.000000			4 B	2.878458	3.292544	1.731899	0.000000		5 B	3.404871	4.107280	3.054773	1.734707	0.000000	6 B	3.183784	4.048706	3.694694	3.096155	1.762852	7 Ta	2.159351	3.613271	2.444290	2.283867	2.202577	8 Ta	2.543997	2.315129	2.371828	2.250803	2.292617		6	7	8			6 B	0.000000					7 Ta	2.398996	0.000000				8 Ta	2.407907	3.081105	0.000000		
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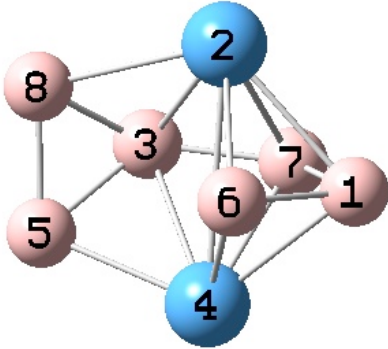
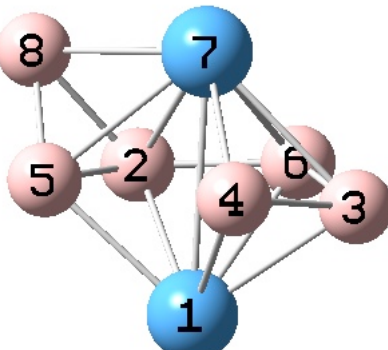
 Cp*Ta₂B₆H₁₀-8 = Ta₂B₆-8 -1049.207828 +22.6	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ta</td><td>2.337459</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.179548</td><td>2.348985</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ta</td><td>2.298078</td><td>3.138371</td><td>2.397738</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.981048</td><td>3.343259</td><td>1.758173</td><td>2.248901</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.832301</td><td>2.231151</td><td>3.262205</td><td>2.155118</td><td>3.327875</td></tr><tr><td>7 B</td><td>1.871870</td><td>2.253774</td><td>1.763181</td><td>2.226465</td><td>3.135695</td></tr><tr><td>8 B</td><td>4.080702</td><td>2.424741</td><td>1.758095</td><td>3.290942</td><td>1.770803</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.918945</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.379740</td><td>3.245515</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 Ta	2.337459	0.000000				3 B	3.179548	2.348985	0.000000			4 Ta	2.298078	3.138371	2.397738	0.000000		5 B	3.981048	3.343259	1.758173	2.248901	0.000000	6 B	1.832301	2.231151	3.262205	2.155118	3.327875	7 B	1.871870	2.253774	1.763181	2.226465	3.135695	8 B	4.080702	2.424741	1.758095	3.290942	1.770803		6	7	8			6 B	0.000000					7 B	2.918945	0.000000				8 B	3.379740	3.245515	0.000000		
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 Cp*Ta₂B₆H₁₀-9 = Ta₂B₆-9 -1049.203400 +25.3	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ta</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.291126</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.244105</td><td>3.167790</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.369299</td><td>3.562893</td><td>1.943160</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.224650</td><td>1.738032</td><td>3.518440</td><td>2.900241</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.361765</td><td>1.803843</td><td>1.874428</td><td>3.186987</td><td>3.021160</td></tr><tr><td>7 Ta</td><td>2.976660</td><td>2.440809</td><td>2.390957</td><td>2.197859</td><td>2.364024</td></tr><tr><td>8 B</td><td>3.507500</td><td>1.865679</td><td>4.173470</td><td>3.836434</td><td>1.594134</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ta</td><td>2.289779</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.214092</td><td>2.276852</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Ta	0.000000					2 B	2.291126	0.000000				3 B	2.244105	3.167790	0.000000			4 B	2.369299	3.562893	1.943160	0.000000		5 B	2.224650	1.738032	3.518440	2.900241	0.000000	6 B	2.361765	1.803843	1.874428	3.186987	3.021160	7 Ta	2.976660	2.440809	2.390957	2.197859	2.364024	8 B	3.507500	1.865679	4.173470	3.836434	1.594134		6	7	8			6 B	0.000000					7 Ta	2.289779	0.000000				8 B	3.214092	2.276852	0.000000		
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Table 2C. Energy ranking for all of the Cp₂Ta₂B₆H₁₀ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	008_B7Mo2-1F_c_Ta_B3LYP	-656.36021272	0.00
2	011_B7Mo2-1F_d_Ta_B3LYP	-656.36011056	0.06
3	007_B7Mo2-1F_b3-_Ta_B3LYP	-656.35885514	0.85
4	006_B7Mo2-1F_b3_Ta_B3LYP	-656.35885505	0.85
5	004_B7Mo2-1F_b2_Ta_B3LYP	-656.35762545	1.62
6	003_B7Mo2-1F_b1_Ta_B3LYP	-656.35761231	1.63
7	002_B7Mo2-1F_b1-_Ta_B3LYP	-656.35761188	1.63
8	005_B7Mo2-1F_b2-_Ta_B3LYP	-656.35761167	1.63
9	063_hexagonal-e05_Ta-B3LYP	-656.35368865	4.09
10	010_B7Mo2-1F_d_Ta_B3LYP	-656.33985935	12.77
11	091_closoTTP-A-a3_Ta-B3LYP	-656.33483482	15.92
12	059_hexagonal-e01_Ta-B3LYP	-656.33468140	16.02
13	026_hexagonal-b5_Ta-B3LYP	-656.33373108	16.62
14	009_B7Mo2-1F_c-_Ta_B3LYP	-656.32922479	19.45
15	149_closoTTP-A-l2_Ta-B3LYP	-656.32805416	20.18
16	171_closoTTP-A-o2_Ta-B3LYP	-656.32695269	20.87
17	185_closoTTP-B-h_Ta-B3LYP-i112	-656.32695223	20.87
18	185_closoTTP-B-h_Ta-B3LYP-i12	-656.32695200	20.87
19	001_B7Mo2-1F_a_Ta-B3LYP	-656.31936665	25.63
20	069_hexagonal-e11_Ta-B3LYPCC	-656.31602196	27.73
21	113_closoTTP-A-f-1_Ta-B3LYP	-656.31586056	27.83
22	068_hexagonal-e10_Ta-B3LYPCC	-656.31521354	28.24
23	116_closoTTP-A-f3_Ta-B3LYP	-656.31397400	29.02
24	114_closoTTP-A-f2_Ta-B3LYP	-656.31397349	29.02
25	115_closoTTP-A-f-2_Ta-B3LYP	-656.31397349	29.02
26	184_closoTTP-B-g_Ta-B3LYP	-656.31200655	30.25
27	118_closoTTP-A-f4_Ta-B3LYP	-656.31200641	30.25
28	168_closoTTP-A-n5_Ta-B3LYP	-656.31133813	30.67
29	177_closoTTP-A-p3_Ta-B3LYP	-656.31014060	31.42
30	172_closoTTP-A-o3_Ta-B3LYP	-656.30901387	32.13
31	012_hexagonal-a1_Ta-B3LYP-i19	-656.30868677	32.33
32	148_closoTTP-A-l-1_Ta-B3LYP	-656.30796591	32.79
33	138_closoTTP-A-j2_Ta-B3LYP	-656.30757154	33.03
34	117_closoTTP-A-f-3_Ta-B3LYP	-656.30756005	33.04
35	186_closoTTP-B-i_Ta-B3LYP	-656.30696754	33.41
36	086_hexagonal-f13_Ta-B3LYP	-656.30643607	33.75
37	084_hexagonal-f11_Ta-B3LYP	-656.30643606	33.75
38	077_hexagonal-f04_Ta-B3LYP	-656.30308354	35.85

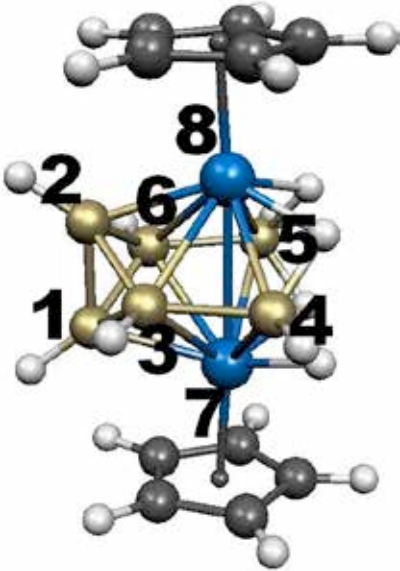
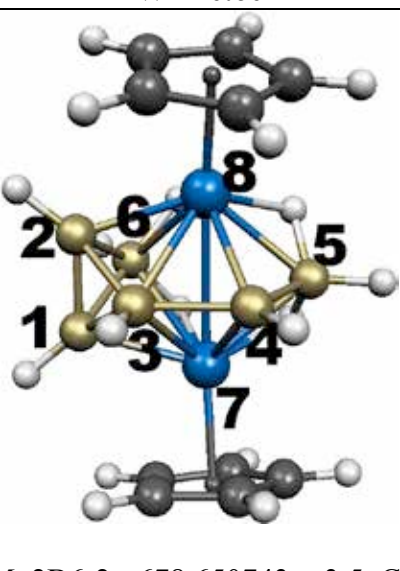
39	154_closoTTP-A-l-4 Ta-B3LYP	-656.30209896	36.47
40	023_hexagonal-b3- Ta-B3LYP-i228	-656.30199044	36.54
41	110_closoTTP-A-e4 Ta-B3LYP	-656.29974002	37.95
42	179_closoTTP-B-b Ta-B3LYP	-656.29869951	38.60
43	151_closoTTP-A-l3 Ta-B3LYP	-656.29751261	39.34
44	156_closoTTP-A-l-5 Ta-B3LYP	-656.29706423	39.63
45	152_closoTTP-A-l-3 Ta-B3LYP	-656.29686308	39.75
46	141_closoTTP-A-j5-Ta-B3LYP	-656.29664875	39.89
47	139_closoTTP-A-j3 Ta-B3LYP	-656.29656398	39.94
48	176_closoTTP-A-p2 Ta-B3LYP	-656.29514635	40.83
49	036_hexagonal-c07 Ta-B3LYP	-656.29511467	40.85
50	170_closoTTP-A-o1 Ta-B3LYP	-656.29509654	40.86
51	035_hexagonal-c06 Ta-B3LYP	-656.29488546	40.99
52	037_hexagonal-c08 Ta-B3LYP	-656.29318325	42.06
53	135_closoTTP-A-i4 Ta-B3LYP	-656.29245426	42.52
54	136_closoTTP-A-i5 Ta-B3LYP	-656.29116565	43.33
55	119_closoTTP-A-f-4 Ta-B3LYP	-656.29096170	43.46
56	178_closoTTP-B-a Ta-B3LYP	-656.29001667	44.05
57	028_hexagonal-b6 Ta-B3LYP	-656.28936261	44.46
58	028_hexagonal-b6 Ta-B3LYP	-656.28936261	44.46
59	078_hexagonal-f05 Ta-B3LYP	-656.28911105	44.62
60	101_closoTTP-A-c5 Ta-B3LYP	-656.28911102	44.62
61	134_closoTTP-A-i3 Ta-B3LYP	-656.28885767	44.78
62	097_closoTTP-A-c1 Ta-B3LYP	-656.28857990	44.95
63	039_hexagonal-c10 Ta-B3LYP	-656.28844059	45.04
64	173_closoTTP-A-o4 Ta-B3LYP	-656.28786610	45.40
65	108_closoTTP-A-e2 Ta-B3LYP	-656.28786606	45.40
66	109_closoTTP-A-e3 Ta-B3LYP	-656.28778887	45.45
67	023_hexagonal-b3- Ta-B3LYP-i676	-656.28692267	45.99
68	111_closoTTP-A-e5 Ta-B3LYP	-656.28669400	46.13
69	083_hexagonal-f10 Ta-B3LYP	-656.28669381	46.13
70	120_closoTTP-A-f5 Ta-B3LYP	-656.28613934	46.48
71	112_closoTTP-A-f1 Ta-B3LYP	-656.28613873	46.48
72	157_closoTTP-A-m1 Ta-B3LYP-i419	-656.28589497	46.64
73	157_closoTTP-A-m1 Ta-B3LYP-i50	-656.28589494	46.64
74	040_hexagonal-c11 Ta-B3LYP	-656.28443236	47.55
75	174_closoTTP-A-o5 Ta-B3LYP	-656.28426021	47.66
76	031_hexagonal-c02 Ta-B3LYP	-656.28403778	47.80
77	122_closoTTP-A-g1 Ta-B3LYP	-656.28297896	48.46
78	123_closoTTP-A-g2 Ta-B3LYP	-656.28292429	48.50
79	169_closoTTP-A-n-5 Ta-B3LYP	-656.28234303	48.86

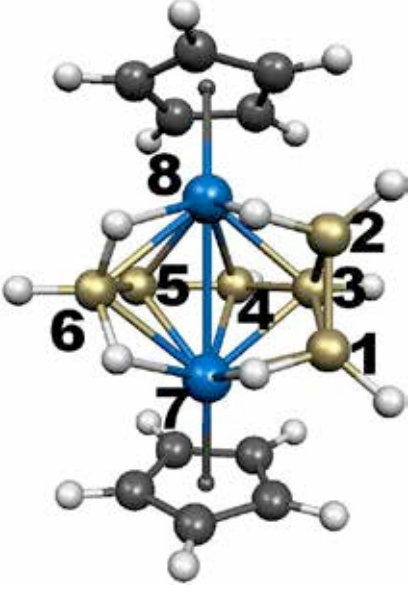
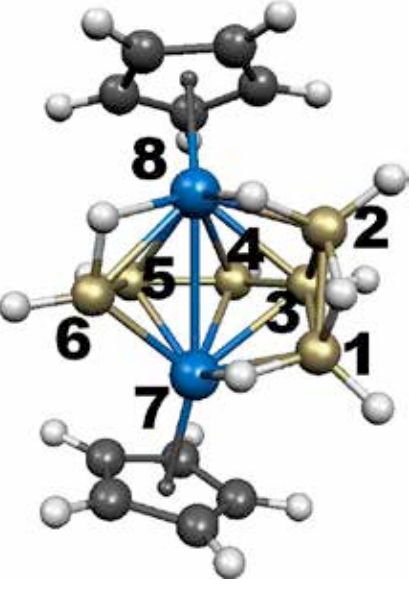
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81	145_closoTTP-A-k4_Ta-B3LYP	-656.28223116	48.93
82	124_closoTTP-A-g3_Ta-B3LYP	-656.28217789	48.97
83	079_hexagonal-f06_Ta-B3LYP	-656.28213603	48.99
84	150_closoTTP-A-l2_Ta-B3LYP	-656.28166466	49.29
85	042_hexagonal-c13_Ta-B3LYP	-656.28157413	49.35
86	187_closoTTP-B-j_Ta-B3LYP-i80	-656.28038837	50.09
87	085_hexagonal-f12_Ta-B3LYP	-656.27999542	50.34
88	074_hexagonal-f01_Ta-B3LYP	-656.27899142	50.97
89	067_hexagonal-e09_Ta-B3LYP	-656.27852497	51.26
90	058_hexagonal-d15_Ta-B3LYP	-656.27846824	51.30
91	133_closoTTP-A-i2_Ta-B3LYP	-656.27843837	51.31
92	076_hexagonal-f03_Ta-B3LYP	-656.27794558	51.62
93	088_hexagonal-f15_Ta-B3LYP	-656.27790167	51.65
94	121_closoTTP-A-f-5_Ta-B3LYP	-656.27787423	51.67
95	147_closoTTP-A-l1_Ta-B3LYP	-656.27707656	52.17
96	155_closoTTP-A-l5_Ta-B3LYP	-656.27637600	52.61
97	153_closoTTP-A-l4_Ta-B3LYP	-656.27637142	52.61
98	041_hexagonal-c12_Ta-B3LYP	-656.27625071	52.69
99	032_hexagonal-c03_Ta-B3LYP	-656.27593051	52.89
100	070_hexagonal-e12_Ta-B3LYP	-656.27542032	53.21
101	075_hexagonal-f02_Ta-B3LYP	-656.27442511	53.83
102	100_closoTTP-A-c4_Ta-B3LYP	-656.27420866	53.97
103	125_closoTTP-A-g4_Ta-B3LYP	-656.27391248	54.15
104	020_hexagonal-b2_Ta-B3LYP	-656.27369314	54.29
105	132_closoTTP-A-i1_Ta-B3LYP	-656.27286682	54.81
106	127_closoTTP-A-h1_Ta-B3LYP	-656.27185198	55.45
107	054_hexagonal-d11_Ta-B3LYP	-656.27160838	55.60
108	056_hexagonal-d13_Ta-B3LYP	-656.27154865	55.64
109	047_hexagonal-d04_Ta-B3LYP	-656.27044186	56.33
110	016_hexagonal-a5_Ta-B3LYP	-656.26957246	56.88
111	061_hexagonal-e03_Ta-B3LYP	-656.26913040	57.16
112	094_closoTTP-A-b3_Ta-B3LYP	-656.26871529	57.42
113	025_hexagonal-b4-_Ta-B3LYP-i90	-656.26802911	57.85
114	027_hexagonal-b5-_Ta-B3LYP	-656.26802892	57.85
115	024_hexagonal-b4_Ta-B3LYP-i93	-656.26578432	59.25
116	013_hexagonal-a2_Ta-B3LYP	-656.26544589	59.47
117	071_hexagonal-e13_Ta-B3LYP	-656.26528057	59.57
118	066_hexagonal-e08_Ta-B3LYP	-656.26525061	59.59
119	087_hexagonal-f14_Ta-B3LYP-i71	-656.26473936	59.91
120	146_closoTTP-A-k5_Ta-B3LYP	-656.26467057	59.95

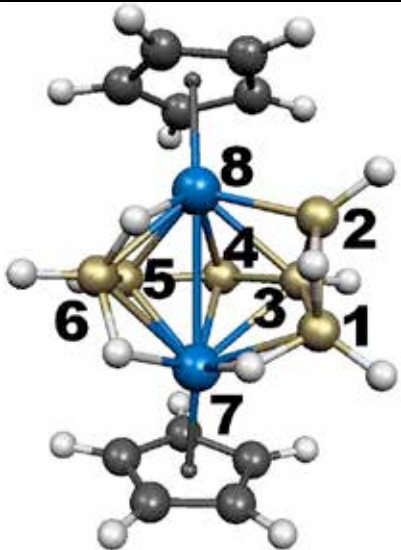
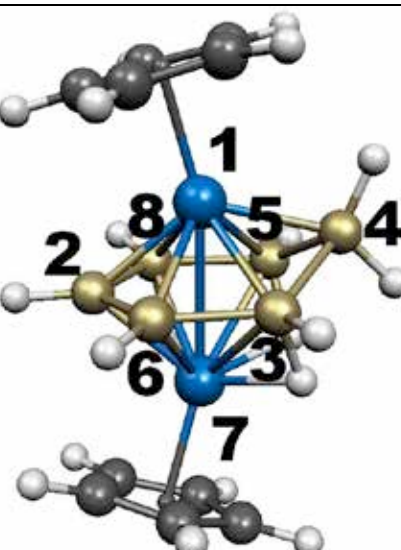
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123	157_closoTTP-A-m1_Ta-B3LYP-i71	-656.26411091	60.30
124	030_hexagonal-c01_Ta-B3LYP	-656.26403400	60.35
125	098_closoTTP-A-c2_Ta-B3LYP	-656.26392742	60.42
126	065_hexagonal-e07_Ta-B3LYP	-656.26363043	60.61
127	130_closoTTP-A-h4_Ta-B3LYP	-656.26339722	60.75
128	049_hexagonal-d06_Ta-B3LYP	-656.26339696	60.75
129	129_closoTTP-A-h3_Ta-B3LYP	-656.26339673	60.75
130	131_closoTTP-A-h5_Ta-B3LYP	-656.26339670	60.75
131	064_hexagonal-e06_Ta-B3LYP	-656.26336731	60.77
132	144_closoTTP-A-k3_Ta-B3LYP	-656.26250325	61.31
133	018_hexagonal-b1_Ta-B3LYP	-656.26212297	61.55
134	089_closoTTP-A-a1_Ta-B3LYP-i36	-656.26212281	61.55
135	126_closoTTP-A-g5_Ta-B3LYP	-656.26137666	62.02
136	087_hexagonal-f14_Ta-B3LYP-i12	-656.26060350	62.51
137	099_closoTTP-A-c3_Ta-B3LYP	-656.26033651	62.67
138	021_hexagonal-b2-_Ta-B3LYP	-656.25980008	63.01
139	038_hexagonal-c09_Ta-B3LYP	-656.25831262	63.94
140	051_hexagonal-d08_Ta-B3LYP	-656.25703985	64.74
141	128_closoTTP-A-h2_Ta-B3LYP	-656.25688205	64.84
142	183_closoTTP-B-f_Ta-B3LYP	-656.25682620	64.88
143	014_hexagonal-a3_Ta-B3LYP	-656.25660026	65.02
144	033_hexagonal-c04_Ta-B3LYP	-656.25604630	65.37
145	015_hexagonal-a4_Ta-B3LYP-65	-656.25486405	66.11
146	015_hexagonal-a4_Ta-B3LYP-i14	-656.25486399	66.11
147	082_hexagonal-f09_Ta-B3LYP	-656.25485550	66.11
148	137_closoTTP-A-j1_Ta-B3LYP	-656.25367490	66.85
149	096_closoTTP-A-b5_Ta-B3LYP	-656.25317887	67.16
150	015_hexagonal-a4_Ta-B3LYP-i68	-656.25204478	67.88
151	181_closoTTP-B-d_Ta-B3LYP	-656.25156208	68.18
152	043_hexagonal-c14_Ta-B3LYP	-656.25099262	68.54
153	180_closoTTP-B-c_Ta-B3LYP	-656.25094301	68.57
154	019_hexagonal-b1-_Ta-B3LYP-i33	-656.25031269	68.96
155	104_closoTTP-A-d3_Ta-B3LYP	-656.25007394	69.11
156	081_hexagonal-f08_Ta-B3LYP	-656.24974052	69.32
157	048_hexagonal-d05_Ta-B3LYP	-656.24798210	70.43
158	073_hexagonal-e15_Ta-B3LYP	-656.24634934	71.45
159	053_hexagonal-d10_Ta-B3LYP	-656.24470438	72.48
160	050_hexagonal-d07_Ta-B3LYP	-656.24470368	72.48
161	046_hexagonal-d03_Ta-B3LYP	-656.24470365	72.48

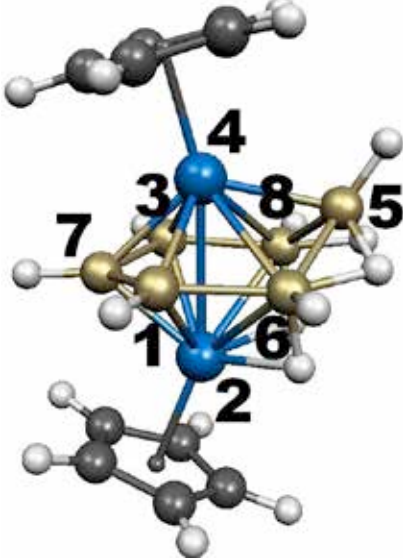
162	052_hexagonal-d09_Ta-B3LYP	-656.24434327	72.71
163	045_hexagonal-d02_Ta-B3LYP	-656.24420754	72.79
164	107_closoTTP-A-e1_Ta-B3LYP	-656.24154691	74.46
165	029_hexagonal-b6-_Ta-B3LYP	-656.24042791	75.17
166	034_hexagonal-c05_Ta-B3LYP	-656.23900240	76.06
167	103_closoTTP-A-d2_Ta-B3LYP	-656.23898015	76.07
168	090_closoTTP-A-a2_Ta-B3LYP	-656.23882435	76.17
169	095_closoTTP-A-b4_Ta-B3LYP	-656.23543101	78.30
170	062_hexagonal-e04_Ta-B3LYP-i26	-656.23531893	78.37
171	055_hexagonal-d12_Ta-B3LYP	-656.23449822	78.89
172	044_hexagonal-d01_Ta-B3LYP	-656.23412981	79.12
173	102_closoTTP-A-d1_Ta-B3LYP	-656.23387029	79.28
174	182_closoTTP-B-e_Ta-B3LYP	-656.23267645	80.03
175	022_hexagonal-b3_Ta-B3LYP	-656.23134905	80.86
176	143_closoTTP-A-k2_Ta-B3LYP	-656.22984053	81.81
177	092_closoTTP-A-b1_Ta-B3LYP	-656.22721437	83.46
178	142_closoTTP-A-k1_Ta-B3LYP	-656.22703143	83.57
179	175_closoTTP-A-p1_Ta-B3LYP-i42	-656.22624778	84.06
180	060_hexagonal-e02_Ta-B3LYP	-656.22204132	86.70
181	140_closoTTP-A-j4_Ta-B3LYP	-656.21853065	88.91
182	105_closoTTP-A-d4_Ta-B3LYP	-656.21090480	93.69
183	072_hexagonal-e14_Ta-B3LYP	-656.26913017	57.16
184	017_hexagonal-a6_Ta-B3LYP-i61-i14	-656.13304388	142.55
185	093_closoTTP-A-b2_Ta-B3LYP	-656.27370541	54.28
186	158_closoTTP-A-m2_Ta-B3LYP-i19	-656.26343579	60.73
187	163_closoTTP-A-n-2_Ta-B3LYP	-656.29617995	40.18

Table 3A. Distance table for the lowest-lying $\text{Cp}_2\text{Mo}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.672086</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.776439</td><td>1.776439</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.211782</td><td>3.211782</td><td>1.803332</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.211782</td><td>3.211782</td><td>3.457237</td><td>3.306792</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.776439</td><td>1.776439</td><td>2.631094</td><td>3.457237</td><td>1.803332</td></tr><tr><td>7 Mo</td><td>2.153890</td><td>3.091205</td><td>2.312384</td><td>2.283475</td><td>2.283475</td></tr><tr><td>8 Mo</td><td>3.091205</td><td>2.153890</td><td>2.312384</td><td>2.283475</td><td>2.283475</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.312384</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Mo</td><td>2.312384</td><td>2.940224</td><td>0.000000</td><td></td><td></td></tr><tr><td colspan="6">Mo7-H-B4 Mo7-H 1.80 B4-H 1.32</td></tr><tr><td colspan="6">Mo7-H-B5 Mo7-H 1.80 B5-H 1.32</td></tr><tr><td colspan="6">Mo8-H-B4 Mo8-H 1.80 B4-H 1.32</td></tr><tr><td colspan="6">Mo8-H-B5 Mo8-H 1.80 B5-H 1.32</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.672086	0.000000				3 B	1.776439	1.776439	0.000000			4 B	3.211782	3.211782	1.803332	0.000000		5 B	3.211782	3.211782	3.457237	3.306792	0.000000	6 B	1.776439	1.776439	2.631094	3.457237	1.803332	7 Mo	2.153890	3.091205	2.312384	2.283475	2.283475	8 Mo	3.091205	2.153890	2.312384	2.283475	2.283475		6	7	8			6 B	0.000000					7 Mo	2.312384	0.000000				8 Mo	2.312384	2.940224	0.000000			Mo7-H-B4 Mo7-H 1.80 B4-H 1.32						Mo7-H-B5 Mo7-H 1.80 B5-H 1.32						Mo8-H-B4 Mo8-H 1.80 B4-H 1.32						Mo8-H-B5 Mo8-H 1.80 B5-H 1.32					
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7 Mo	2.345438	3.253954	2.282446	2.188104	2.165167																																																																		
8 Mo	3.167225	2.199710	2.323254	2.143793	2.170162																																																																		
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7 Mo	2.330170	0.000000																																																																					
8 Mo	2.244137	2.931617	0.000000																																																																				
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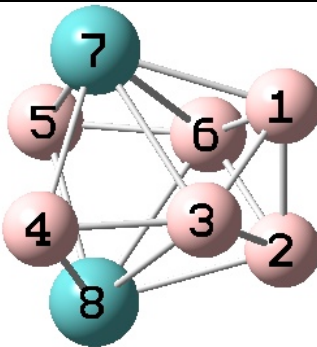
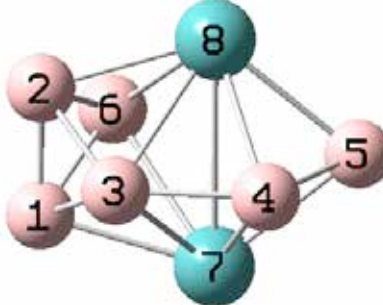
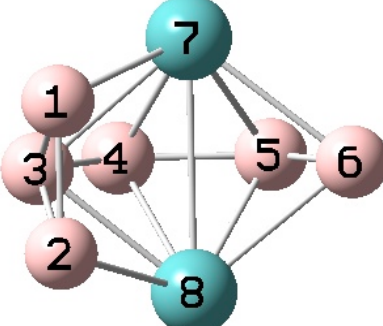


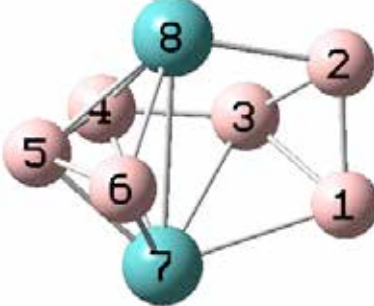
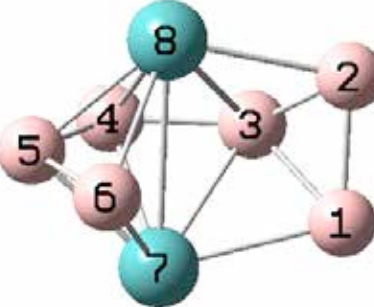
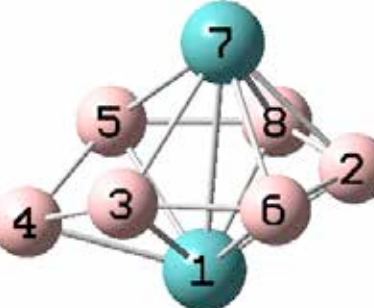
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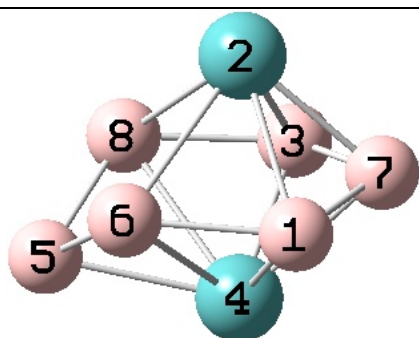
	1	2	3	4	5
1 B	0.000000				
2 Mo	2.262391	0.000000			
3 B	3.046203	2.262336	0.000000		
4 Mo	2.098773	2.877141	2.098785	0.000000	
5 B	3.261356	3.240054	3.261360	2.204981	0.000000
6 B	1.905277	2.386807	3.451369	2.347929	1.865976
7 B	1.814621	2.088975	1.814635	2.166323	3.865299
8 B	3.451380	2.386784	1.905266	2.347930	1.865986
	6	7	8		
6 B	0.000000				
7 B	3.172970	0.000000			
8 B	2.718771	3.172978	0.000000		

Mo2-H-B6	Mo2-H	1.87	B6-H	1.28
Mo2-H-B8	Mo2-H	1.87	B8-H	1.28
B5-H-B6	B5-H	1.27	B6-H	1.40
B5-H-B8	B5-H	1.27	B8-H	1.40

Table 3B. Distance table for the lowest-lying $\text{Cp}^*\text{Mo}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Mo2B6H10-1 = Mo2B6-1 -1071.620508 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.675849</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.776912</td><td>1.776872</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.204485</td><td>3.204517</td><td>1.804622</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.202534</td><td>3.202415</td><td>3.467733</td><td>3.314603</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.777447</td><td>1.777417</td><td>2.650945</td><td>3.473199</td><td>1.804984</td></tr><tr><td>7 Mo</td><td>2.141767</td><td>3.083895</td><td>2.317763</td><td>2.285424</td><td>2.284962</td></tr><tr><td>8 Mo</td><td>3.083994</td><td>2.141749</td><td>2.317695</td><td>2.285527</td><td>2.284947</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.321134</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Mo</td><td>2.321281</td><td>2.937966</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.675849	0.000000				3 B	1.776912	1.776872	0.000000			4 B	3.204485	3.204517	1.804622	0.000000		5 B	3.202534	3.202415	3.467733	3.314603	0.000000	6 B	1.777447	1.777417	2.650945	3.473199	1.804984	7 Mo	2.141767	3.083895	2.317763	2.285424	2.284962	8 Mo	3.083994	2.141749	2.317695	2.285527	2.284947		6	7	8			6 B	0.000000					7 Mo	2.321134	0.000000				8 Mo	2.321281	2.937966	0.000000		
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 Cp*Mo2B6H10-2 = Mo2B6-2 -1071.614094 4.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.642760</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.765259</td><td>1.765183</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.186772</td><td>3.186799</td><td>1.819265</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.906101</td><td>3.906059</td><td>3.178382</td><td>1.819935</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.850434</td><td>1.850421</td><td>2.694917</td><td>3.422197</td><td>3.288473</td></tr><tr><td>7 Mo</td><td>2.189600</td><td>3.100705</td><td>2.276313</td><td>2.155034</td><td>2.265690</td></tr><tr><td>8 Mo</td><td>3.100704</td><td>2.189593</td><td>2.276189</td><td>2.155091</td><td>2.265572</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.388474</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Mo</td><td>2.388474</td><td>2.934107</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.642760	0.000000				3 B	1.765259	1.765183	0.000000			4 B	3.186772	3.186799	1.819265	0.000000		5 B	3.906101	3.906059	3.178382	1.819935	0.000000	6 B	1.850434	1.850421	2.694917	3.422197	3.288473	7 Mo	2.189600	3.100705	2.276313	2.155034	2.265690	8 Mo	3.100704	2.189593	2.276189	2.155091	2.265572		6	7	8			6 B	0.000000					7 Mo	2.388474	0.000000				8 Mo	2.388474	2.934107	0.000000		
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8 Mo	2.388474	2.934107	0.000000																																																																												
 Cp*Mo2B6H10-3 = Mo2B6-3 -1071.611025 6.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.737360</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.754883</td><td>1.754880</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.192877</td><td>3.192869</td><td>1.750570</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.942551</td><td>3.942556</td><td>3.038236</td><td>1.727752</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.757879</td><td>3.757890</td><td>3.557969</td><td>3.017913</td><td>1.726220</td></tr><tr><td>7 Mo</td><td>2.277948</td><td>3.198679</td><td>2.269105</td><td>2.169110</td><td>2.203141</td></tr><tr><td>8 Mo</td><td>3.198670</td><td>2.277949</td><td>2.269112</td><td>2.169103</td><td>2.203143</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.326330</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Mo</td><td>2.326324</td><td>2.902375</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.737360	0.000000				3 B	1.754883	1.754880	0.000000			4 B	3.192877	3.192869	1.750570	0.000000		5 B	3.942551	3.942556	3.038236	1.727752	0.000000	6 B	3.757879	3.757890	3.557969	3.017913	1.726220	7 Mo	2.277948	3.198679	2.269105	2.169110	2.203141	8 Mo	3.198670	2.277949	2.269112	2.169103	2.203143		6	7	8			6 B	0.000000					7 Mo	2.326330	0.000000				8 Mo	2.326324	2.902375	0.000000		
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 Cp*Mo2B6H10-5 = Mo2B6-4 -1071.600244 12.7	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.821356</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.776611</td><td>1.758960</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.184958</td><td>3.184547</td><td>1.725642</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.916448</td><td>3.960862</td><td>3.029274</td><td>1.763492</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.559390</td><td>3.690709</td><td>3.471367</td><td>3.059277</td><td>1.824145</td></tr><tr><td>7 Mo</td><td>2.300017</td><td>3.272710</td><td>2.296847</td><td>2.172207</td><td>2.130755</td></tr><tr><td>8 Mo</td><td>3.242024</td><td>2.340789</td><td>2.326409</td><td>2.201533</td><td>2.163712</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.139821</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Mo</td><td>2.287862</td><td>2.873959</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.821356	0.000000				3 B	1.776611	1.758960	0.000000			4 B	3.184958	3.184547	1.725642	0.000000		5 B	3.916448	3.960862	3.029274	1.763492	0.000000	6 B	3.559390	3.690709	3.471367	3.059277	1.824145	7 Mo	2.300017	3.272710	2.296847	2.172207	2.130755	8 Mo	3.242024	2.340789	2.326409	2.201533	2.163712		6	7	8			6 B	0.000000					7 Mo	2.139821	0.000000				8 Mo	2.287862	2.873959	0.000000		
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 Cp*Mo2B6H10-6 = Mo2B6-6 -1071.590089 19.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Mo</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.159265</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.211384</td><td>3.045983</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.167871</td><td>3.867954</td><td>1.908128</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.198982</td><td>3.157002</td><td>2.820963</td><td>1.896684</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.156731</td><td>1.727974</td><td>1.781493</td><td>3.292760</td><td>3.446455</td></tr><tr><td>7 Mo</td><td>2.841329</td><td>2.182597</td><td>2.362731</td><td>3.174069</td><td>2.412440</td></tr><tr><td>8 B</td><td>2.166606</td><td>1.812842</td><td>3.492119</td><td>3.402841</td><td>1.940582</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Mo</td><td>2.217660</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.041124</td><td>2.291864</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Mo	0.000000					2 B	2.159265	0.000000				3 B	2.211384	3.045983	0.000000			4 B	2.167871	3.867954	1.908128	0.000000		5 B	2.198982	3.157002	2.820963	1.896684	0.000000	6 B	2.156731	1.727974	1.781493	3.292760	3.446455	7 Mo	2.841329	2.182597	2.362731	3.174069	2.412440	8 B	2.166606	1.812842	3.492119	3.402841	1.940582		6	7	8			6 B	0.000000					7 Mo	2.217660	0.000000				8 B	3.041124	2.291864	0.000000		
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8 B	3.041124	2.291864	0.000000																																																																												



Cp*Mo₂B₆H₁₀₋₇ = Mo₂B₆₋₇
 -1071.575781 28.1

		1	2	3	4	5
1	B	0.000000				
2	Mo	2.259103	0.000000			
3	B	3.042181	2.258725	0.000000		
4	Mo	2.102296	2.874953	2.102385	0.000000	
5	B	3.270694	3.236757	3.270613	2.210328	0.000000
6	B	1.911194	2.386518	3.460917	2.355328	1.874926
7	B	1.809342	2.083552	1.809427	2.172309	3.870877
8	B	3.460976	2.386176	1.910825	2.355386	1.875179
		6	7	8		
6	B	0.000000				
7	B	3.176406	0.000000			
8	B	2.736916	3.176266	0.000000		

Table 3C. Energy ranking for all of the $\text{Cp}_2\text{Mo}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	010_B7Mo2-1F_d_Mo_B3LYP	-678.7433353	0.00
2	011_B7Mo2-1F_d_Mo_B3LYP	-678.7433352	0.00
3	004_B7Mo2-1F_b2_Mo_B3LYP	-678.7347606	5.38
4	005_B7Mo2-1F_b2-_Mo_B3LYP	-678.7347594	5.38
5	009_B7Mo2-1F_c-_Mo_B3LYP	-678.7347564	5.38
6	008_B7Mo2-1F_c_Mo_B3LYP-i20	-678.7346566	5.45
7	008_B7Mo2-1F_c_Mo_B3LYP-i19	-678.7345613	5.51
8	006_B7Mo2-1F_b3_Mo_B3LYP	-678.7302115	8.24
9	149_closoTTP-A-l2_Mo-B3LYP	-678.7302112	8.24
10	007_B7Mo2-1F_b3-_Mo_B3LYP	-678.7302111	8.24
11	003_B7Mo2-1F_b1_Mo_B3LYP	-678.729763	8.52
12	002_B7Mo2-1F_b1-_Mo_B3LYP	-678.7297334	8.54
13	109_closoTTP-A-e3_Mo-B3LYP	-678.7143169	18.21
14	159_closoTTP-A-m3_Mo-B3LYP	-678.7143036	18.22
15	187_closoTTP-B-j_Mo-B3LYP-i473	-678.7143008	18.22
16	147_closoTTP-A-l1_Mo-B3LYP	-678.7037473	24.84
17	063_hexagonal-e05_Mo-B3LYP	-678.7037473	24.84
18	059_hexagonal-e01_Mo-B3LYP	-678.7037473	24.84
19	067_hexagonal-e09_Mo-B3LYP	-678.7037473	24.84
20	001_B7Mo2-1F_a_Mo-B3LYP	-678.703744	24.84
21	186_closoTTP-B-i_Mo-B3LYP	-678.6906533	33.06
22	162_closoTTP-A-n2_Mo-B3LYP	-678.6906522	33.06
23	161_closoTTP-A-n-1_Mo-B3LYP	-678.6897231	33.64
24	160_closoTTP-A-n1_Mo-B3LYP	-678.6897225	33.64
25	148_closoTTP-A-l-1_Mo-B3LYP	-678.6890808	34.05
26	026_hexagonal-b5_Mo-B3LYP	-678.6868969	35.42
27	119_closoTTP-A-f-4_Mo-B3LYP	-678.684449	36.95
28	121_closoTTP-A-f-5_Mo-B3LYP	-678.6844488	36.95
29	168_closoTTP-A-n5_Mo-B3LYP	-678.6836567	37.45
30	169_closoTTP-A-n-5_Mo-B3LYP	-678.6808396	39.22
31	177_closoTTP-A-p3_Mo-B3LYP	-678.6806838	39.31
32	120_closoTTP-A-f5_Mo-B3LYP	-678.6800796	39.69
33	115_closoTTP-A-f-2_Mo-B3LYP	-678.6800795	39.69
34	124_closoTTP-A-g3_Mo-B3LYP	-678.6800415	39.72
35	039_hexagonal-c10_Mo-B3LYP	-678.6800407	39.72
36	125_closoTTP-A-g4_Mo-B3LYP	-678.6800403	39.72
37	113_closoTTP-A-f-1_Mo-B3LYP	-678.6767056	41.81
38	163_closoTTP-A-n-2_Mo-B3LYP	-678.6767028	41.81

39	170_closoTTP-A-o1_Mo-B3LYP	-678.675631	42.49
40	172_closoTTP-A-o3_Mo-B3LYP	-678.6756309	42.49
41	185_closoTTP-B-h_Mo-B3LYP	-678.675469	42.59
42	114_closoTTP-A-f2_Mo-B3LYP	-678.6746908	43.08
43	089_closoTTP-A-a1_Mo-B3LYP-i212	-678.6746103	43.13
44	042_hexagonal-c13_Mo-B3LYP	-678.6743284	43.30
45	123_closoTTP-A-g2_Mo-B3LYP	-678.6734414	43.86
46	099_closoTTP-A-c3_Mo-B3LYP	-678.6734414	43.86
47	135_closoTTP-A-i4_Mo-B3LYP	-678.6732646	43.97
48	052_hexagonal-d09_Mo-B3LYP	-678.6732646	43.97
49	127_closoTTP-A-h1_Mo-B3LYP	-678.6732645	43.97
50	133_closoTTP-A-i2_Mo-B3LYP	-678.6732645	43.97
51	180_closoTTP-B-c_Mo-B3LYP-i32	-678.6732643	43.97
52	134_closoTTP-A-i3_Mo-B3LYP	-678.6732642	43.97
53	040_hexagonal-c11_Mo-B3LYP	-678.6718348	44.87
54	116_closoTTP-A-f3_Mo-B3LYP	-678.6712892	45.21
55	165_closoTTP-A-n-3_Mo-B3LYP	-678.6690357	46.62
56	171_closoTTP-A-o2_Mo-B3LYP	-678.6689637	46.67
57	068_hexagonal-e10_Mo-B3LYP	-678.6688871	46.72
58	060_hexagonal-e02_Mo-B3LYP	-678.6681216	47.20
59	150_closoTTP-A-l-2_Mo-B3LYP	-678.6673791	47.66
60	152_closoTTP-A-l-3_Mo-B3LYP	-678.6673052	47.71
61	154_closoTTP-A-l-4_Mo-B3LYP	-678.6666603	48.11
62	108_closoTTP-A-e2_Mo-B3LYP	-678.666488	48.22
63	158_closoTTP-A-m2_Mo-B3LYP	-678.6664875	48.22
64	088_hexagonal-f15_Mo-B3LYP	-678.6664038	48.28
65	076_hexagonal-f03_Mo-B3LYP	-678.6664032	48.28
66	082_hexagonal-f09_Mo-B3LYP	-678.6664029	48.28
67	075_hexagonal-f02_Mo-B3LYP	-678.6664029	48.28
68	077_hexagonal-f04_Mo-B3LYP	-678.6664029	48.28
69	085_hexagonal-f12_Mo-B3LYP	-678.6664028	48.28
70	087_hexagonal-f14_Mo-B3LYP	-678.6664026	48.28
71	074_hexagonal-f01_Mo-B3LYP	-678.6664024	48.28
72	100_closoTTP-A-c4_Mo-B3LYP	-678.6664018	48.28
73	027_hexagonal-b5-_Mo-B3LYP	-678.6659763	48.54
74	136_closoTTP-A-i5_Mo-B3LYP	-678.6644848	49.48
75	041_hexagonal-c12_Mo-B3LYP	-678.6644417	49.51
76	122_closoTTP-A-g1_Mo-B3LYP	-678.6644225	49.52
77	038_hexagonal-c09_Mo-B3LYP	-678.6644222	49.52
78	179_closoTTP-B-b_Mo-B3LYP	-678.6644177	49.52
79	032_hexagonal-c03_Mo-B3LYP	-678.6643107	49.59

80	126_closoTTP-A-g5_Mo-B3LYP	-678.6643105	49.59
81	031_hexagonal-c02_Mo-B3LYP	-678.6643103	49.59
82	167_closoTTP-A-n-4_Mo-B3LYP	-678.6641993	49.66
83	117_closoTTP-A-f-3_Mo-B3LYP	-678.663117	50.34
84	018_hexagonal-b1_Mo-B3LYP	-678.6613579	51.44
85	175_closoTTP-A-p1_Mo-B3LYP-i14	-678.6607339	51.83
86	098_closoTTP-A-c2_Mo-B3LYP	-678.6601718	52.19
87	157_closoTTP-A-m1_Mo-B3LYP-i529	-678.659801	52.42
88	157_closoTTP-A-m1_Mo-B3LYP-i246	-678.6597303	52.46
89	036_hexagonal-c07_Mo-B3LYP	-678.6596354	52.52
90	024_hexagonal-b4_Mo-B3LYP-i132	-678.659278	52.75
91	037_hexagonal-c08_Mo-B3LYP	-678.6590266	52.90
92	035_hexagonal-c06_Mo-B3LYP	-678.6574177	53.91
93	090_closoTTP-A-a2_Mo-B3LYP	-678.6568362	54.28
94	062_hexagonal-e04_Mo-B3LYP	-678.656836	54.28
95	111_closoTTP-A-e5_Mo-B3LYP	-678.6564319	54.53
96	083_hexagonal-f10_Mo-B3LYP	-678.6564318	54.53
97	110_closoTTP-A-e4_Mo-B3LYP	-678.6564316	54.53
98	106_closoTTP-A-d5_Mo-B3LYP	-678.6562699	54.63
99	079_hexagonal-f06_Mo-B3LYP	-678.6560836	54.75
100	080_hexagonal-f07_Mo-B3LYP	-678.6560832	54.75
101	081_hexagonal-f08_Mo-B3LYP	-678.6560832	54.75
102	166_closoTTP-A-n4_Mo-B3LYP	-678.6559592	54.83
103	155_closoTTP-A-l5_Mo-B3LYP	-678.6548385	55.53
104	033_hexagonal-c04_Mo-B3LYP	-678.6529527	56.72
105	069_hexagonal-e11_Mo-B3LYP	-678.6513389	57.73
106	070_hexagonal-e12_Mo-B3LYP	-678.6513382	57.73
107	058_hexagonal-d15_Mo-B3LYP	-678.6511726	57.83
108	101_closoTTP-A-c5_Mo-B3LYP	-678.650794	58.07
109	029_hexagonal-b6-_Mo-B3LYP	-678.6505601	58.22
110	028_hexagonal-b6_Mo-B3LYP	-678.65056	58.22
111	020_hexagonal-b2_Mo-B3LYP	-678.6505599	58.22
112	174_closoTTP-A-o5_Mo-B3LYP	-678.6499221	58.62
113	014_hexagonal-a3_Mo-B3LYP	-678.6494938	58.89
114	140_closoTTP-A-j4_Mo-B3LYP-i19	-678.6494662	58.90
115	137_closoTTP-A-j1_Mo-B3LYP	-678.649464	58.91
116	013_hexagonal-a2_Mo-B3LYP	-678.6494636	58.91
117	138_closoTTP-A-j2_Mo-B3LYP	-678.6494613	58.91
118	016_hexagonal-a5_Mo-B3LYP	-678.6490673	59.15
119	178_closoTTP-B-a_Mo-B3LYP	-678.6490645	59.16
120	015_hexagonal-a4_Mo-B3LYP	-678.6490065	59.19

121	072_hexagonal-e14_Mo-B3LYP	-678.6486623	59.41
122	092_closoTTP-A-b1_Mo-B3LYP	-678.6480132	59.82
123	086_hexagonal-f13_Mo-B3LYP	-678.6473172	60.25
124	128_closoTTP-A-h2_Mo-B3LYP	-678.6454592	61.42
125	129_closoTTP-A-h3_Mo-B3LYP	-678.645459	61.42
126	023_hexagonal-b3-_Mo-B3LYP	-678.6454008	61.45
127	112_closoTTP-A-f1_Mo-B3LYP	-678.6454005	61.46
128	022_hexagonal-b3_Mo-B3LYP	-678.6453983	61.46
129	021_hexagonal-b2-_Mo-B3LYP	-678.6448752	61.78
130	061_hexagonal-e03_Mo-B3LYP	-678.6438104	62.45
131	053_hexagonal-d10_Mo-B3LYP	-678.6434494	62.68
132	054_hexagonal-d11_Mo-B3LYP	-678.643449	62.68
133	056_hexagonal-d13_Mo-B3LYP	-678.643449	62.68
134	094_closoTTP-A-b3_Mo-B3LYP	-678.6430955	62.90
135	153_closoTTP-A-l4_Mo-B3LYP	-678.6430837	62.91
136	084_hexagonal-f11_Mo-B3LYP-i33	-678.6416786	63.79
137	055_hexagonal-d12_Mo-B3LYP	-678.640549	64.50
138	095_closoTTP-A-b4_Mo-B3LYP	-678.6401914	64.72
139	045_hexagonal-d02_Mo-B3LYP	-678.6397854	64.98
140	051_hexagonal-d08_Mo-B3LYP	-678.6393986	65.22
141	118_closoTTP-A-f4_Mo-B3LYP	-678.6388899	65.54
142	065_hexagonal-e07_Mo-B3LYP	-678.6387379	65.64
143	132_closoTTP-A-i1_Mo-B3LYP	-678.6384411	65.82
144	156_closoTTP-A-l-5_Mo-B3LYP	-678.638137	66.01
145	066_hexagonal-e08_Mo-B3LYP	-678.6369396	66.76
146	173_closoTTP-A-o4_Mo-B3LYP	-678.6354454	67.70
147	043_hexagonal-c14_Mo-B3LYP	-678.6343946	68.36
148	073_hexagonal-e15_Mo-B3LYP	-678.6343209	68.41
149	019_hexagonal-b1-_Mo-B3LYP	-678.633393	68.99
150	131_closoTTP-A-h5_Mo-B3LYP	-678.632955	69.26
151	130_closoTTP-A-h4_Mo-B3LYP	-678.6329549	69.26
152	049_hexagonal-d06_Mo-B3LYP	-678.6329548	69.26
153	184_closoTTP-B-g_Mo-B3LYP	-678.6303747	70.88
154	047_hexagonal-d04_Mo-B3LYP	-678.6299521	71.15
155	048_hexagonal-d05_Mo-B3LYP	-678.6299492	71.15
156	030_hexagonal-c01_Mo-B3LYP	-678.6295108	71.43
157	142_closoTTP-A-k1_Mo-B3LYP	-678.6292994	71.56
158	181_closoTTP-B-d_Mo-B3LYP	-678.6275286	72.67
159	044_hexagonal-d01_Mo-B3LYP	-678.6268615	73.09
160	093_closoTTP-A-b2_Mo-B3LYP	-678.6267903	73.13
161	096_closoTTP-A-b5_Mo-B3LYP	-678.6247826	74.39

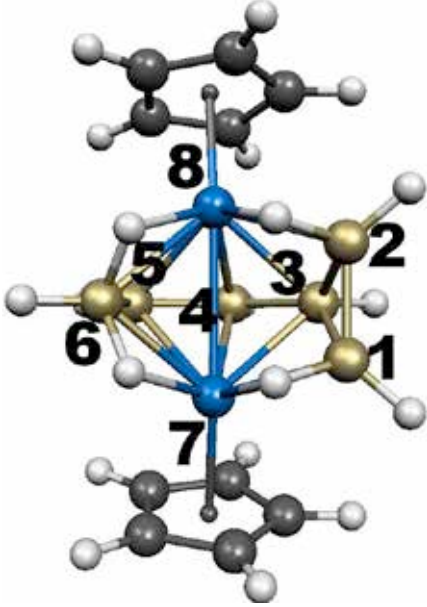
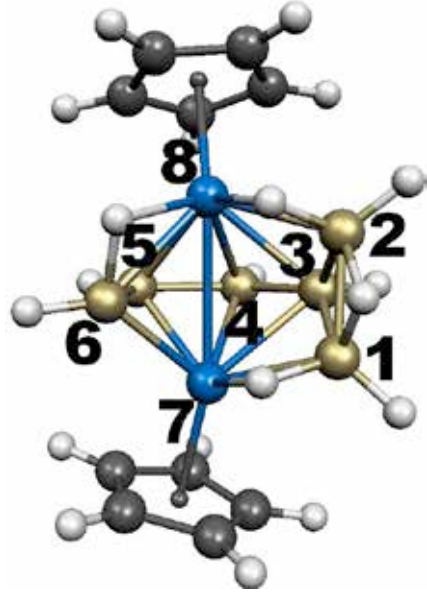
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163	012_hexagonal-a1_Mo-B3LYP-i525	-678.6208883	76.84
164	012_hexagonal-a1_Mo-B3LYP-i20	-678.6208871	76.84
165	071_hexagonal-e13_Mo-B3LYP	-678.6206083	77.01
166	139_closoTTP-A-j3_Mo-B3LYP	-678.6197869	77.53
167	141_closoTTP-A-j5_Mo-B3LYP	-678.6197856	77.53
168	107_closoTTP-A-e1_Mo-B3LYP	-678.6180251	78.63
169	064_hexagonal-e06_Mo-B3LYP	-678.617206	79.15
170	097_closoTTP-A-c1_Mo-B3LYP	-678.6167127	79.46
171	078_hexagonal-f05_Mo-B3LYP	-678.61671	79.46
172	050_hexagonal-d07_Mo-B3LYP	-678.6164017	79.65
173	046_hexagonal-d03_Mo-B3LYP	-678.6164012	79.65
174	164_closoTTP-A-n3_Mo-B3LYP	-678.6163594	79.68
175	151_closoTTP-A-l3_Mo-B3LYP	-678.6160133	79.90
176	176_closoTTP-A-p2_Mo-B3LYP	-678.614872	80.61
177	102_closoTTP-A-d1_Mo-B3LYP	-678.6148545	80.62
178	017_hexagonal-a6_Mo-B3LYP	-678.6088076	84.42
179	091_closoTTP-A-a3_Mo-B3LYP	-678.6079754	84.94
180	025_hexagonal-b4-_Mo-B3LYP-i7	-678.6061937	86.06
181	182_closoTTP-B-e_Mo-B3LYP	-678.6060317	86.16
182	057_hexagonal-d14_Mo-B3LYP	-678.6057442	86.34
183	034_hexagonal-c05_Mo-B3LYP	-678.6044835	87.13
184	103_closoTTP-A-d2_Mo-B3LYP	-678.6024129	88.43
185	183_closoTTP-B-f_Mo-B3LYP	-678.6018951	88.76
186	175_closoTTP-A-p1_Mo-B3LYP-i90	-678.6008625	89.40
187	145_closoTTP-A-k4_Mo-B3LYP	-678.5971098	91.76
188	144_closoTTP-A-k3_Mo-B3LYP	-678.5959071	92.51
189	104_closoTTP-A-d3_Mo-B3LYP	-678.5958277	92.56
190	105_closoTTP-A-d4_Mo-B3LYP	-678.5870367	98.08
191	146_closoTTP-A-k5_Mo-B3LYP	-678.5860946	98.67

Table 4A. Distance table for the lowest-lying $\text{Cp}_2\text{W}_2\text{B}_6\text{H}_{10}$ 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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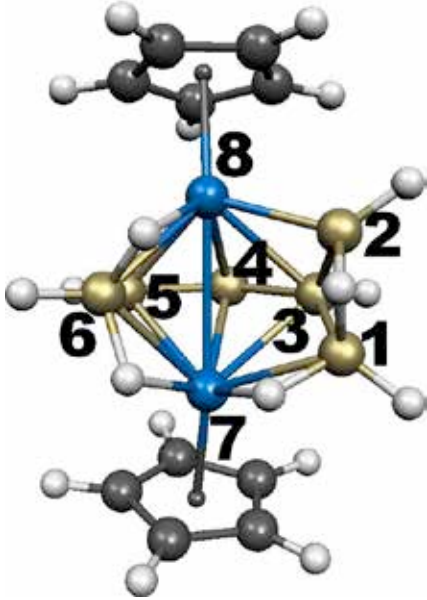
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W2B6-2 -676.462405 +3.4 C_s
WBI 0.63

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7 W	2.137434	0.000000																																																																													
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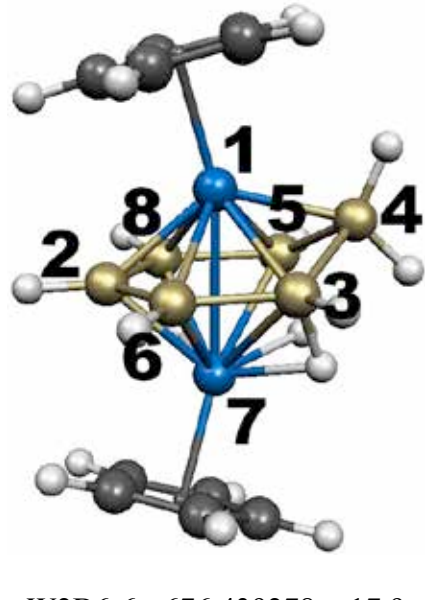
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	6	7	8		
6 B	0.000000				
7 W	2.326197	0.000000			
8 W	2.250325	2.964911	0.000000		

W7-H-B1 W7-H 1.86 B1-H 1.30
W7-H-B6 W7-H 1.82 B6-H 1.35
W8-H-B6 W8-H 1.86 B6-H 1.31
B1-H-B2 B1-H 1.34 B2-H 1.29



W2B6-6 -676.439278 +17.9
(Cs)
WBI 0.60

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4 B	2.172640	3.881327	1.922756	0.000000	
5 B	2.201020	3.139598	2.801857	1.899014	0.000000
6 B	2.170491	1.735464	1.781970	3.311618	3.434308
7 W	2.891065	2.199925	2.368461	3.214048	2.425640
8 B	2.178582	1.803690	3.475817	3.402223	1.924428
	6	7	8		
6 B	0.000000				
7 W	2.230204	0.000000			
8 B	3.036641	2.311726	0.000000		

W7-H-B8 W7-H 1.83 B8-H 1.34
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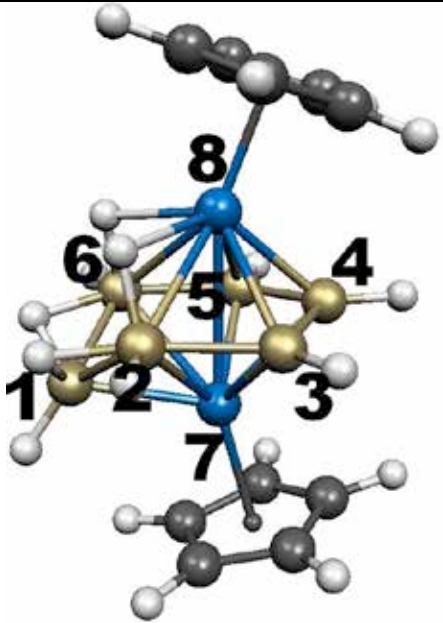
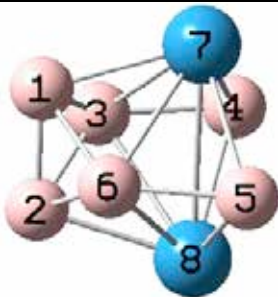
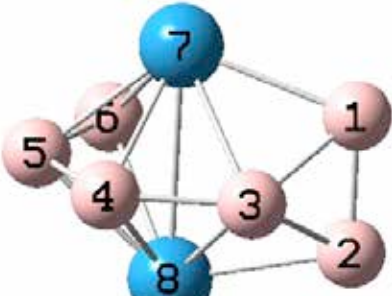
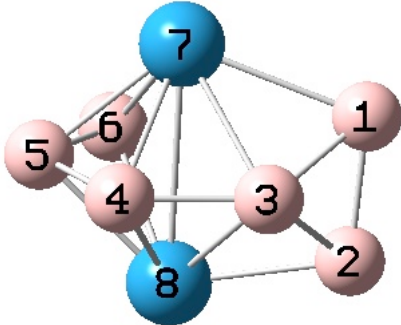
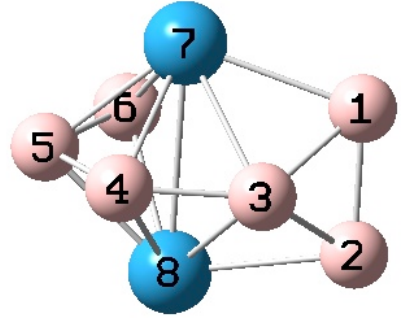
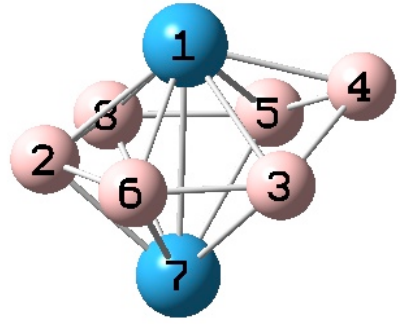
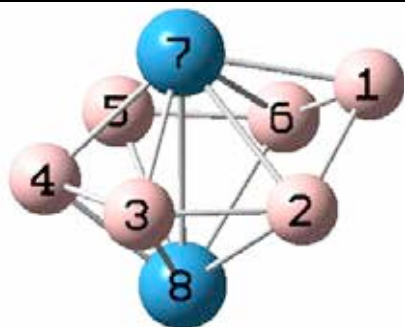
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	5 B	3.284239	3.452267	3.057300	1.816862	0.000000
	6 B	1.880939	2.716400	3.452299	3.166476	1.900940
	7 W	2.218037	2.353631	2.123447	2.180884	2.123514
	8 W	3.266404	2.389133	2.274090	2.108820	2.273914
		6	7	8		
	6 B	0.000000				
	7 W	2.353633	0.000000			
	8 W	2.389118	2.914892	0.000000		
	W8-H-B2	W8-H 1.87	B2-H 1.29			
	W8-H-B6	W8-H 1.87	B6-H 1.29			
	B1-H-B2	B1-H 1.26	B2-H 1.41			
	B1-H-B6	B1-H 1.26	B6-H 1.41			

Table 4B. Distance table for the lowest-lying $\text{Cp}^*\text{W}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*W2B6H10-1 = W2B6-1 -1069.430638 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.673391</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.782393</td><td>1.783764</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.203434</td><td>3.204982</td><td>1.806574</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.204870</td><td>3.200478</td><td>3.472392</td><td>3.300132</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.783314</td><td>1.780433</td><td>2.665010</td><td>3.471824</td><td>1.804889</td></tr><tr><td>7 W</td><td>2.152163</td><td>3.097187</td><td>2.335997</td><td>2.288880</td><td>2.291015</td></tr><tr><td>8 W</td><td>3.098699</td><td>2.150399</td><td>2.335524</td><td>2.292115</td><td>2.288991</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 W</td><td>2.334055</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 W</td><td>2.335335</td><td>2.969573</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.673391	0.000000				3 B	1.782393	1.783764	0.000000			4 B	3.203434	3.204982	1.806574	0.000000		5 B	3.204870	3.200478	3.472392	3.300132	0.000000	6 B	1.783314	1.780433	2.665010	3.471824	1.804889	7 W	2.152163	3.097187	2.335997	2.288880	2.291015	8 W	3.098699	2.150399	2.335524	2.292115	2.288991		6	7	8			6 B	0.000000					7 W	2.334055	0.000000				8 W	2.335335	2.969573	0.000000		
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 Cp*W2B6H10-2 = W2B6-2 -1069.427275 +2.1	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.647157</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.775542</td><td>1.775595</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.200541</td><td>3.200670</td><td>1.819666</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.910557</td><td>3.910645</td><td>3.164876</td><td>1.804016</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.839762</td><td>1.840009</td><td>2.667137</td><td>3.392530</td><td>3.262542</td></tr><tr><td>7 W</td><td>2.203039</td><td>3.122358</td><td>2.292484</td><td>2.176857</td><td>2.274476</td></tr><tr><td>8 W</td><td>3.122028</td><td>2.202989</td><td>2.292398</td><td>2.176947</td><td>2.274293</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 W</td><td>2.368518</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 W</td><td>2.368432</td><td>2.971678</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.647157	0.000000				3 B	1.775542	1.775595	0.000000			4 B	3.200541	3.200670	1.819666	0.000000		5 B	3.910557	3.910645	3.164876	1.804016	0.000000	6 B	1.839762	1.840009	2.667137	3.392530	3.262542	7 W	2.203039	3.122358	2.292484	2.176857	2.274476	8 W	3.122028	2.202989	2.292398	2.176947	2.274293		6	7	8			6 B	0.000000					7 W	2.368518	0.000000				8 W	2.368432	2.971678	0.000000		
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 Cp*W2B6H10-3 = W2B6-3 -1069.425678 +3.1	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.726384</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.761364</td><td>1.761396</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.209853</td><td>3.209848</td><td>1.758580</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.959458</td><td>3.959475</td><td>3.043900</td><td>1.724985</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.751593</td><td>3.751574</td><td>3.542929</td><td>3.003301</td><td>1.723291</td></tr><tr><td>7 W</td><td>2.288890</td><td>3.208339</td><td>2.279332</td><td>2.186893</td><td>2.221630</td></tr><tr><td>8 W</td><td>3.208323</td><td>2.288875</td><td>2.279354</td><td>2.186868</td><td>2.221684</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 W</td><td>2.319757</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 W</td><td>2.319714</td><td>2.927739</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.726384	0.000000				3 B	1.761364	1.761396	0.000000			4 B	3.209853	3.209848	1.758580	0.000000		5 B	3.959458	3.959475	3.043900	1.724985	0.000000	6 B	3.751593	3.751574	3.542929	3.003301	1.723291	7 W	2.288890	3.208339	2.279332	2.186893	2.221630	8 W	3.208323	2.288875	2.279354	2.186868	2.221684		6	7	8			6 B	0.000000					7 W	2.319757	0.000000				8 W	2.319714	2.927739	0.000000		
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Cp*W2B6H10-7 = W2B6-7
-1069.382439 +30.2

		1	2	3	4	5
1	B	0.000000				
2	B	1.890300	0.000000			
3	B	3.293035	1.903729	0.000000		
4	B	3.887134	3.168959	1.812912	0.000000	
5	B	3.293129	3.460281	3.054842	1.812964	0.000000
6	B	1.890167	2.732945	3.460213	3.169077	1.903943
7	W	2.223343	2.360572	2.129075	2.184201	2.128999
8	W	3.263852	2.387866	2.268954	2.107004	2.268949
		6	7	8		
6	B	0.000000				
7	W	2.360457	0.000000			
8	W	2.387890	2.913454	0.000000		

Table 4C. Energy ranking for all of the $\text{Cp}_2\text{W}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	B7Mo2-1F_d_W	-676.75616394	0.00
2	B7Mo2-1F_d- 1_W	-676.75616388	0.00
3	B7Mo2-1F_c- W	-676.74814313	5.03
4	B7Mo2-1F_c_W	-676.74814306	5.03
5	B7Mo2-1F_b2- W	-676.74443954	7.36
6	B7Mo2-1F_b2_W	-676.74443849	7.36
7	hexagonal-b1- W	-676.73303917	14.51
8	hexagonal-b1_W ca-	-676.73293198	14.58
9	B7Mo2-1F_b1- W	-676.73292365	14.58
10	149_closoTTP-A-l2_W	-676.73268901	14.73
11	B7Mo2-1F_b3- W	-676.73268885	14.73
12	B7Mo2-1F_b3_W	-676.73268874	14.73
13	152_closoTTP-A-l3_W	-676.72487535	19.63
14	151_closoTTP-A-l3_W	-676.72471299	19.74
15	hexagonal-e09_W	-676.72463124	19.79
16	hexagonal-e05_W	-676.72463062	19.79
17	142_closoTTP-A-k1_W	-676.70950207	29.28
18	B7Mo2-1F_a_W.log	-676.70610178	31.41
19	hexagonal-e01_W	-676.70610159	31.41
20	hexagonal-e08_W	-676.70272043	33.54
21	155_closoTTP-A-l5_W	-676.70272027	33.54
22	187_closoTTP-B-j_W_r-348	-676.70112698	34.54
23	159_closoTTP-A-m3_W	-676.70112597	34.54
24	187_closoTTP-B-j_W i-348	-676.69978788	35.38
25	161_closoTTP-A-n-1_W	-676.69724534	36.97
26	144_closoTTP-A-k3_W	-676.69636867	37.52
27	118_closoTTP-A-f4_W	-676.69170552	40.45
28	115_closoTTP-A-f-2_W	-676.69170531	40.45
29	167_closoTTP-A-n-4_W	-676.68965474	41.73
30	109_closoTTP-A-e3_W	-676.68868413	42.34
31	148_closoTTP-A-l-1_W	-676.68800006	42.77
32	147_closoTTP-A-l1_W	-676.68758178	43.04
33	hexagonal-e06_W	-676.68755295	43.05
34	117_closoTTP-A-f-3_W	-676.68666626	43.61
35	120_closoTTP-A-f5_W	-676.68666613	43.61
36	172_closoTTP-A-o3_W	-676.68665606	43.62
37	169_closoTTP-A-n-5_W	-676.68658577	43.66
38	121_closoTTP-A-f-5_W	-676.68652213	43.70
39	119_closoTTP-A-f-4_W	-676.68652187	43.70
40	163_closoTTP-A-n-2_W	-676.68266447	46.12

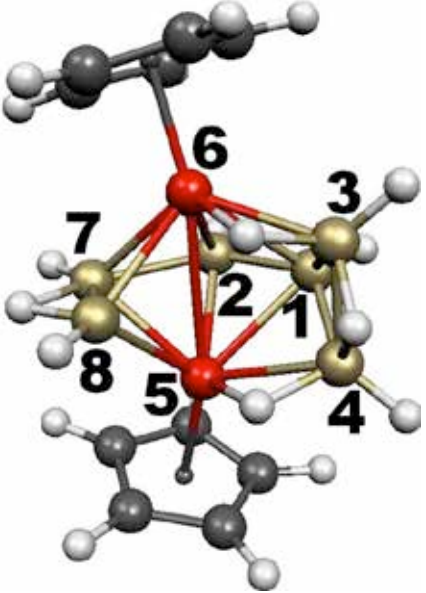
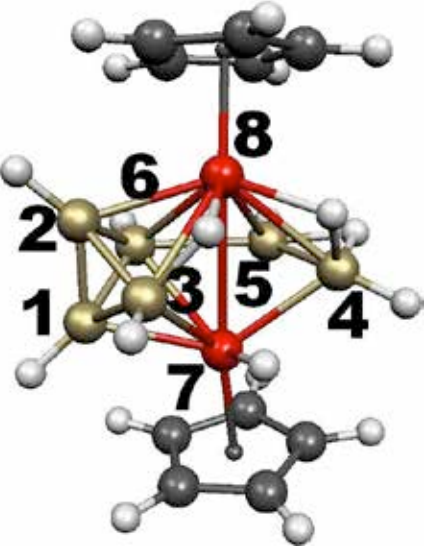
41	165_closoTTP-A-n-3_W	-676.68261748	46.15
42	186_closoTTP-B-i_W	-676.68223775	46.39
43	116_closoTTP-A-f3_W	-676.68015272	47.70
44	171_closoTTP-A-o2_W	-676.67633923	50.09
45	184_closoTTP-B-g_W	-676.67478109	51.07
46	168_closoTTP-A-n5_W	-676.67410413	51.49
47	162_closoTTP-A-n2_W	-676.67384376	51.66
48	114_closoTTP-A-f2_W	-676.67270268	52.37
49	hexagonal-b5- W	-676.67251608	52.49
50	hexagonal-b4- W_r-271	-676.67251602	52.49
51	176_closoTTP-A-p2_W	-676.67141038	53.18
52	177_closoTTP-A-p3_W	-676.67131798	53.24
53	hexagonal-b5_W-caxqc	-676.67102187	53.43
54	185_closoTTP-B-h_W_r-57	-676.67041599	53.81
55	185_closoTTP-B-h_W	-676.67032547	53.86
56	170_closoTTP-A-o1_W	-676.67019910	53.94
57	173_closoTTP-A-o4_W	-676.67017157	53.96
58	154_closoTTP-A-l-4_W	-676.66903069	54.68
59	hexagonal-b6- W-caxqc	-676.66883576	54.80
60	hexagonal-b2_W	-676.66880793	54.82
61	113_closoTTP-A-f-1_W	-676.66874357	54.86
62	156_closoTTP-A-l-5_W	-676.66691944	56.00
63	164_closoTTP-A-n3_W	-676.66688023	56.03
64	143_closoTTP-A-k2_W	-676.66687997	56.03
65	160_closoTTP-A-n1_W	-676.66543471	56.93
66	175_closoTTP-A-p1_W	-676.66475063	57.36
67	166_closoTTP-A-n4_W	-676.66341611	58.20
68	124_closoTTP-A-g3_W	-676.66125309	59.56
69	125_closoTTP-A-g4_W	-676.66075583	59.87
70	hexagonal-c10_W	-676.66068761	59.91
71	B7Mo2-1F_b1_W.log	-676.66001071	60.34
72	112_closoTTP-A-f1_W	-676.65962097	60.58
73	179_closoTTP-B-b_W-cont	-676.65825113	61.44
74	122_closoTTP-A-g1_W	-676.65824858	61.44
75	099_closoTTP-A-c3_W	-676.65824689	61.44
76	123_closoTTP-A-g2_W	-676.65750802	61.91
77	150_closoTTP-A-l-2_W	-676.65740284	61.97
78	hexagonal-f08_W	-676.65644582	62.57
79	158_closoTTP-A-m2_W	-676.65488623	63.55
80	108_closoTTP-A-e2_W	-676.65488596	63.55
81	180_closoTTP-B-c_W	-676.65378098	64.25
82	133_closoTTP-A-i2_W	-676.65377949	64.25
83	135_closoTTP-A-i4_W	-676.65253059	65.03

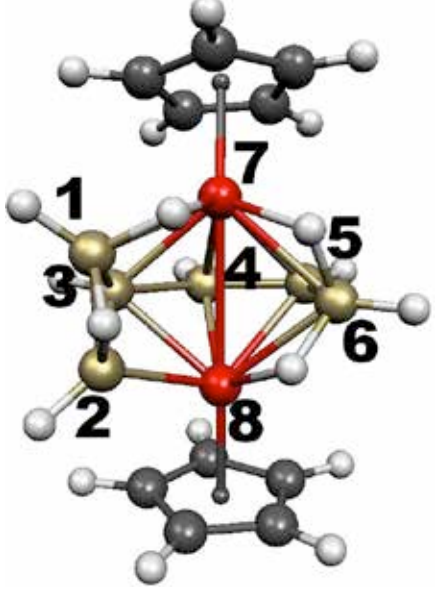
84	134_closoTTP-A-i3_W	-676.65252700	65.03
85	135_closoTTP-A-i4_W_r-30	-676.65252385	65.03
86	hexagonal-c06_W	-676.65229990	65.17
87	092_closoTTP-A-b1_W	-676.65059707	66.24
88	hexagonal-c13_W	-676.64954587	66.90
89	hexagonal-c11_W	-676.64954541	66.90
90	hexagonal-c08_W	-676.64950428	66.93
91	hexagonal-d15_W	-676.64694037	68.54
92	132_closoTTP-A-i1_W	-676.64467340	69.96
93	089_closoTTP-A-a1_W_r-60-62	-676.64312732	70.93
94	hexagonal-d03_W	-676.64308790	70.96
95	136_closoTTP-A-i5_W	-676.64282620	71.12
96	hexagonal-e04_W	-676.64253245	71.30
97	hexagonal-b4_W_r-98	-676.64191569	71.69
98	hexagonal-c07_W	-676.64185354	71.73
99	090_closoTTP-A-a2_W	-676.64183603	71.74
100	hexagonal-e15_W	-676.63982306	73.00
101	hexagonal-c09_W	-676.63798128	74.16
102	hexagonal-c12_W	-676.63780103	74.27
103	157_closoTTP-A-m1_W	-676.63779057	74.28
104	hexagonal-c04_W	-676.63677951	74.91
105	129_closoTTP-A-h3_W	-676.63675682	74.93
106	127_closoTTP-A-h1_W	-676.63675664	74.93
107	128_closoTTP-A-h2_W	-676.63675655	74.93
108	hexagonal-c03_W	-676.63611581	75.33
109	hexagonal-c02_W	-676.63611492	75.33
110	126_closoTTP-A-g5_W	-676.63603656	75.38
111	hexagonal-a1_W_r-182	-676.63545732	75.74
112	hexagonal-f09_W	-676.63519864	75.91
113	hexagonal-f12_W	-676.63519806	75.91
114	hexagonal-f03_W	-676.63519773	75.91
115	hexagonal-f01_W	-676.63519756	75.91
116	hexagonal-f02_W	-676.63519751	75.91
117	hexagonal-f14_W	-676.63519671	75.91
118	hexagonal-f04_W	-676.63519588	75.91
119	hexagonal-f15_W	-676.63503467	76.01
120	hexagonal-d14_W	-676.63479821	76.16
121	hexagonal-b2-_W	-676.63381242	76.78
122	hexagonal-b3-_W_ca	-676.63261339	77.53
123	hexagonal-b6_W	-676.63211982	77.84
124	hexagonal-f06_W	-676.63098905	78.55
125	hexagonal-f07_W	-676.63098891	78.55
126	130_closoTTP-A-h4_W	-676.63065369	78.76

127	131_closoTTP-A-h5_W	-676.63065308	78.76
128	111_closoTTP-A-e5_W	-676.63049144	78.86
129	hexagonal-f10_W	-676.63048885	78.86
130	110_closoTTP-A-e4_W	-676.63048873	78.86
131	hexagonal-e11_W	-676.63013793	79.08
132	174_closoTTP-A-o5_W	-676.62994763	79.20
133	138_closoTTP-A-j2_W	-676.62900508	79.79
134	hexagonal-a2_W	-676.62900436	79.79
135	178_closoTTP-B-a_W	-676.62900386	79.79
136	hexagonal-a6_W_r-75	-676.62898455	79.81
137	hexagonal-a3_W	-676.62898375	79.81
138	137_closoTTP-A-j1_W	-676.62863067	80.03
139	153_closoTTP-A-l4_W	-676.62838741	80.18
140	hexagonal-a4_W_caxqc	-676.62798889	80.43
141	hexagonal-a5_W	-676.62798816	80.43
142	097_closoTTP-A-c1_W	-676.62759780	80.68
143	101_closoTTP-A-c5_W	-676.62758860	80.68
144	hexagonal-d13_W	-676.62747713	80.75
145	hexagonal-d12_W	-676.62747522	80.75
146	hexagonal-d11_W	-676.62747420	80.75
147	hexagonal-f05_W	-676.62743661	80.78
148	hexagonal-b4- W_imag	-676.62414350	82.84
149	hexagonal-e07_W	-676.62332705	83.36
150	107_closoTTP-A-e1_W	-676.62044707	85.16
151	100_closoTTP-A-c4_W	-676.61920775	85.94
152	hexagonal-f13_W	-676.61725823	87.16
153	096_closoTTP-A-b5_W	-676.61700582	87.32
154	hexagonal-e14_W	-676.61628628	87.77
155	095_closoTTP-A-b4_W	-676.61550822	88.26
156	181_closoTTP-B-d_W	-676.61300537	89.83
157	141_closoTTP-A-j5-W	-676.61279159	89.97
158	139_closoTTP-A-j3_W	-676.61279155	89.97
159	hexagonal-f11_W	-676.61257665	90.10
160	146_closoTTP-A-k5_W	-676.61137432	90.86
161	hexagonal-c01_W	-676.61053862	91.38
162	hexagonal-c14_W	-676.60841524	92.71
163	hexagonal-d09_W	-676.60833124	92.77
164	hexagonal-d05_W	-676.60748703	93.29
165	hexagonal-d08_W	-676.60748698	93.29
166	106_closoTTP-A-d5_W	-676.60663668	93.83
167	hexagonal-a1_W_r-23	-676.60604192	94.20
168	hexagonal-a1_W_r-583	-676.60604136	94.20
169	182_closoTTP-B-e_W	-676.60496956	94.87

170	hexagonal-d04_W	-676.60474252	95.02
171	hexagonal-e12_W	-676.60395286	95.51
172	hexagonal-d06_W	-676.60283089	96.22
173	093_closoTTP-A-b2_W	-676.60072306	97.54
174	140_closoTTP-A-j4_W	-676.60013947	97.91
175	hexagonal-a1_W imag	-676.59876070	98.77
176	145_closoTTP-A-k4_W	-676.59778232	99.38
177	hexagonal-e13_W	-676.59750358	99.56
178	hexagonal-d01_W	-676.59667006	100.08
179	hexagonal-d02_W	-676.59666967	100.08
180	091_closoTTP-A-a3_W	-676.59647141	100.21
181	098_closoTTP-A-c2_W	-676.59552997	100.80
182	104_closoTTP-A-d3_W	-676.59512506	101.05
183	103_closoTTP-A-d2_W	-676.59512080	101.05
184	hexagonal-e03_W	-676.59322165	102.25
185	hexagonal-d07_W	-676.59142332	103.37
186	hexagonal-d10_W	-676.59142287	103.38
187	089_closoTTP-A-a1_W r-60-42	-676.58933038	104.69
188	089_closoTTP-A-a1_W	-676.58931270	104.70
189	089_closoTTP-A-a1_W-imag	-676.58758627	105.78
190	089_closoTTP-A-a1_W r-60	-676.58758627	105.78
191	094_closoTTP-A-b3_W	-676.58634963	106.56
192	hexagonal-e02_W	-676.58175224	109.44
193	hexagonal-a6_W i-75	-676.57974977	110.70
194	183_closoTTP-B-f_W	-676.57835081	111.58
195	hexagonal-c05_W	-676.57320884	114.80
196	105_closoTTP-A-d4_W	-676.56927460	117.27
197	hexagonal-b4_W	-676.56130378	122.27
198	102_closoTTP-A-d1_W	-676.54245668	134.10

Table 5A. Distance table for the lowest-lying $\text{Cp}_2\text{Re}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.815252</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.739077</td><td>3.192039</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.739096</td><td>3.192085</td><td>1.764457</td><td>0.000000</td><td></td></tr><tr><td>5 Re</td><td>2.275687</td><td>2.109637</td><td>3.182850</td><td>2.264670</td><td>0.000000</td></tr><tr><td>6 Re</td><td>2.275753</td><td>2.109575</td><td>2.264725</td><td>3.182815</td><td>2.834620</td></tr><tr><td>7 B</td><td>3.290423</td><td>2.066365</td><td>3.964337</td><td>3.964187</td><td>2.191805</td></tr><tr><td>8 B</td><td>3.444603</td><td>3.081505</td><td>3.427140</td><td>3.427094</td><td>2.242156</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.192066</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.241997</td><td>1.671745</td><td>0.000000</td><td></td><td></td></tr></table> Re6-H-B3 Re6-H 1.79 B3-H 1.35 Re5-H-B4 Re5-H 1.79 B4-H 1.35 B3-H-B4 B3-H 1.32 B4-H 1.32 B7-H-B8 B7-H 1.34 B8-H 1.31		1	2	3	4	5	1 B	0.000000					2 B	1.815252	0.000000				3 B	1.739077	3.192039	0.000000			4 B	1.739096	3.192085	1.764457	0.000000		5 Re	2.275687	2.109637	3.182850	2.264670	0.000000	6 Re	2.275753	2.109575	2.264725	3.182815	2.834620	7 B	3.290423	2.066365	3.964337	3.964187	2.191805	8 B	3.444603	3.081505	3.427140	3.427094	2.242156		6	7	8			6 Re	0.000000					7 B	2.192066	0.000000				8 B	2.241997	1.671745	0.000000		
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5 B	4.080925	3.996965	3.358923	1.736390	0.000000																																																																										
6 B	1.781719	1.748522	2.558999	3.492121	3.310573																																																																										
7 Re	2.263619	3.090048	2.249808	2.201456	2.353717																																																																										
8 Re	3.104629	2.208340	2.266766	2.141025	2.227315																																																																										
	6	7	8																																																																												
6 B	0.000000																																																																														
7 Re	2.348839	0.000000																																																																													
8 Re	2.308736	2.819020	0.000000																																																																												

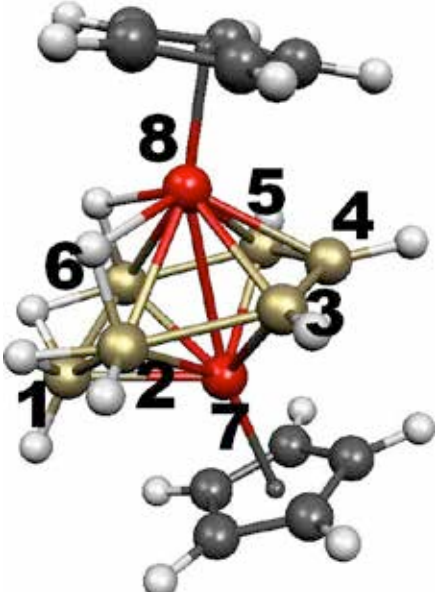


3. -698.842471 +12.4 C₁
WBI 0.47

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2 B	1.713806	0.000000			
3 B	1.746330	1.747373	0.000000		
4 B	3.347171	3.227471	1.914234	0.000000	
5 B	3.998181	3.909407	3.151745	1.745678	0.000000
6 B	3.699988	3.617289	3.537624	2.955096	1.645526
7 Re	2.325375	3.187520	2.254590	2.221323	2.249919
8 Re	3.148773	2.158077	2.250767	2.096381	2.242229

	6	7	8
6 B	0.000000		
7 Re	2.375425	0.000000	
8 Re	2.326223	2.928573	0.000000

Re7-H-B1 Re7-H 1.76 B1-H 1.36
Re7-H-B6 Re7-H 1.80 B6-H 1.36
Re8-H-B6 Re7-H 1.81 B6-H 1.36
B1-H-B2 B1-H 1.30 B2-H 1.34

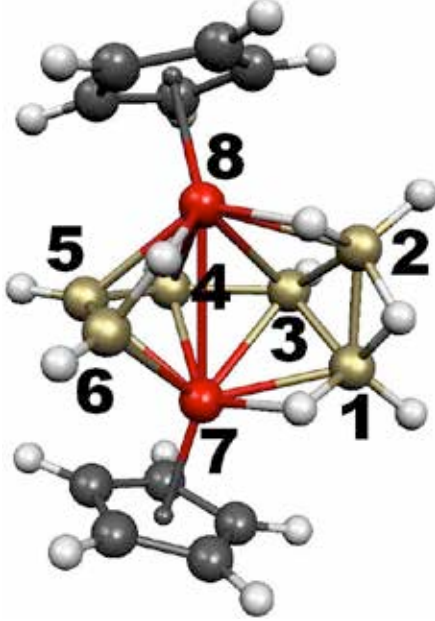


4. -698.842364 +12.5 C_s
WBI 0.47

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3 B	3.504513	2.113453	0.000000		
4 B	4.005226	3.241486	1.659707	0.000000	
5 B	3.504267	3.513614	2.878800	1.659613	0.000000
6 B	1.836593	2.737100	3.513498	3.241057	2.112897
7 Re	2.209951	2.194672	2.177139	2.232894	2.177394
8 Re	3.177986	2.404889	2.235677	2.229901	2.235867

	6	7	8
6 B	0.000000		
7 Re	2.194824	0.000000	
8 Re	2.404889	2.803613	0.000000

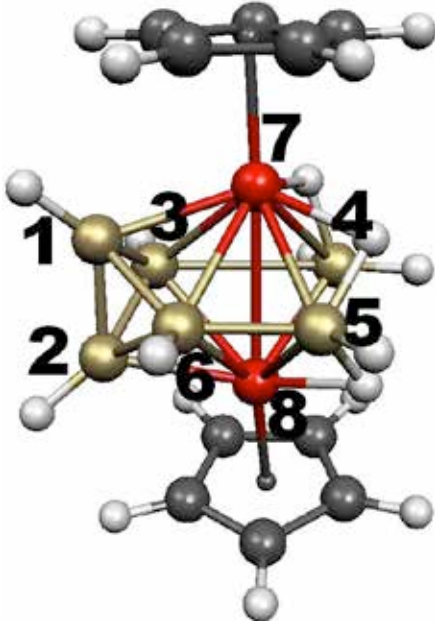
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Re8-H-B6 Re8-H 1.80 B6-H 1.34
B1-H-B2 B1-H 1.27 B2-H 1.43
B1-H-B6 B1-H 1.27 B6-H 1.43



5. -698.841258 +13.2 C₁
WBI 0.46

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2 B	1.745412	0.000000			
3 B	1.746541	1.735426	0.000000		
4 B	3.245822	3.290558	1.867933	0.000000	
5 B	4.002058	4.033490	3.152394	1.747586	0.000000
6 B	3.718708	3.823065	3.550874	2.923406	1.623709
7 Re	2.240841	3.190474	2.254398	2.122472	2.257500
8 Re	3.193847	2.305667	2.287900	2.223556	2.242879
	6	7	8		
6 B	0.000000				
7 Re	2.235806	0.000000			
8 Re	2.370792	2.879525	0.000000		

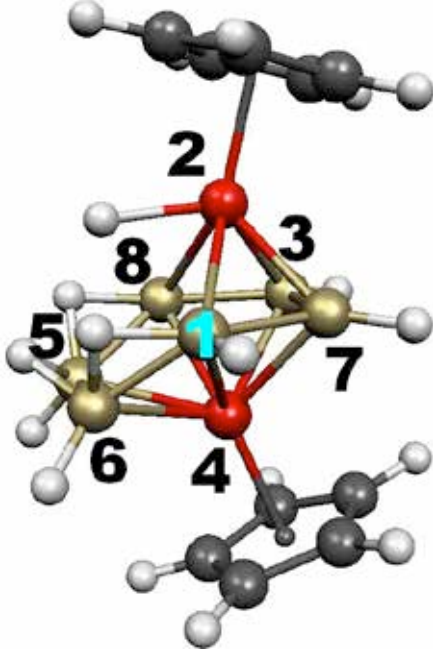
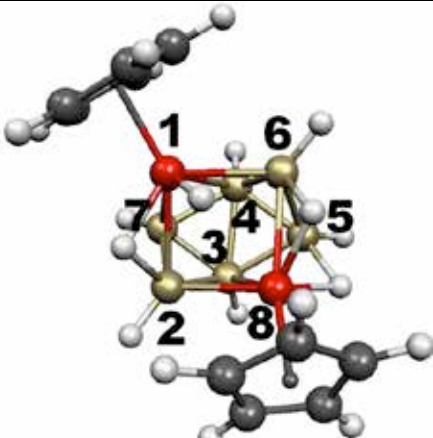
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Re8-H-B2 Re8-H 1.78 B2-H 1.35
Re8-H-B6 Re8-H 1.78 B6-H 1.37
B1-H-B2 B1-H 1.36 B2-H 1.30

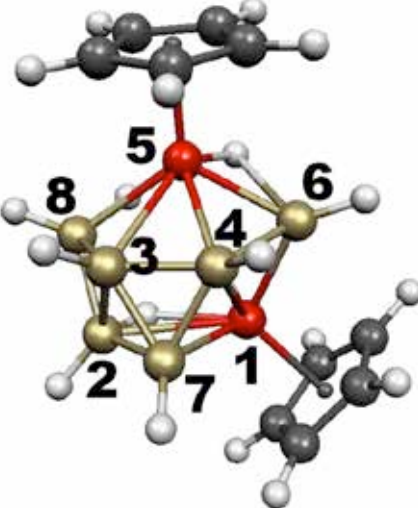
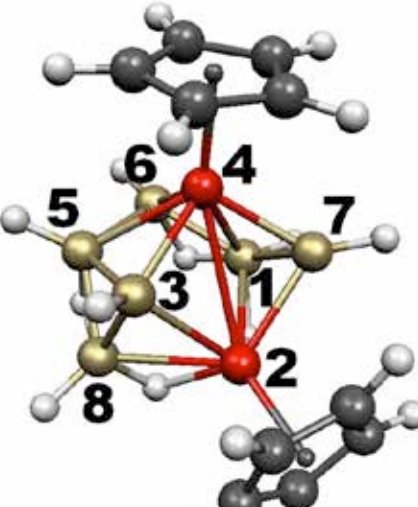


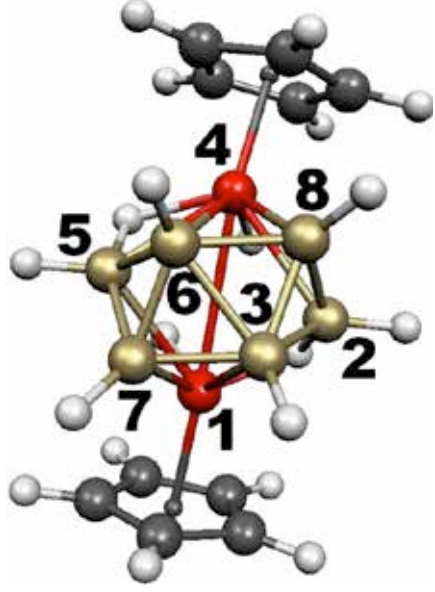
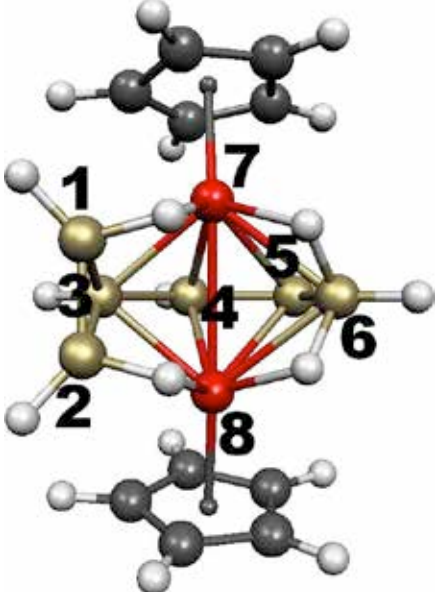
6. -698.838612 +14.9 C₁ (C_s)
WBI 0.52

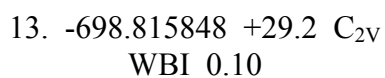
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3 B	1.729565	1.747200	0.000000		
4 B	3.877635	3.808497	2.670956	0.000000	
5 B	3.213578	3.199513	3.397578	3.054294	0.000000
6 B	1.773948	1.773773	2.554948	3.687191	1.776088
7 Re	2.210297	3.095944	2.257082	2.446084	2.256828
8 Re	3.053902	2.169602	2.235223	2.253042	2.229339
	6	7	8		
6 B	0.000000				
7 Re	2.300146	0.000000			
8 Re	2.276173	2.803829	0.000000		

Re7-H-B4 Re7-H 1.78 B4-H 1.32
Re7-H-B5 Re7-H 1.74 B5-H 1.38
Re8-H-B5 Re8-H 1.78 B5-H 1.31

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	1	2	3	4	5																																																																										
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4 Re	2.233479	2.918596	2.143506	0.000000																																																																											
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	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.239399</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.032073</td><td>1.777812</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.331194</td><td>2.741647</td><td>1.881924</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.323946</td><td>3.041293</td><td>1.791208</td><td>1.717353</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.193953</td><td>3.105097</td><td>2.788710</td><td>1.775582</td><td>1.791250</td></tr><tr><td>7 B</td><td>2.165777</td><td>1.736491</td><td>1.697424</td><td>1.757147</td><td>2.908118</td></tr><tr><td>8 Re</td><td>2.962746</td><td>2.223212</td><td>2.375545</td><td>3.037931</td><td>2.207425</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.018652</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Re</td><td>2.279312</td><td>3.313948</td><td>0.000000</td><td></td><td></td></tr></table> Re1-H-B2 Re1-H 1.68 B2-H 1.60 Re8-H-B6 Re8-H 1.68 B6-H 1.61 Re8-H-B5 Re8-H 1.68 B5-H 1.46 Re1-H 1.68		1	2	3	4	5	1 Re	0.000000					2 B	2.239399	0.000000				3 B	3.032073	1.777812	0.000000			4 B	2.331194	2.741647	1.881924	0.000000		5 B	3.323946	3.041293	1.791208	1.717353	0.000000	6 B	2.193953	3.105097	2.788710	1.775582	1.791250	7 B	2.165777	1.736491	1.697424	1.757147	2.908118	8 Re	2.962746	2.223212	2.375545	3.037931	2.207425		6	7	8			6 B	0.000000					7 B	3.018652	0.000000				8 Re	2.279312	3.313948	0.000000		
	1	2	3	4	5																																																																										
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5 B	3.323946	3.041293	1.791208	1.717353	0.000000																																																																										
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7 B	2.165777	1.736491	1.697424	1.757147	2.908118																																																																										
8 Re	2.962746	2.223212	2.375545	3.037931	2.207425																																																																										
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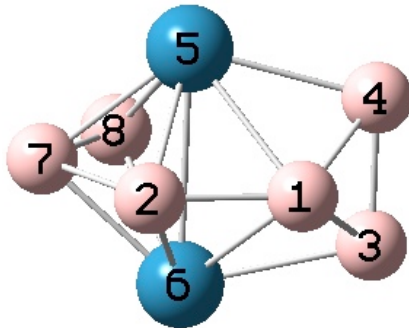
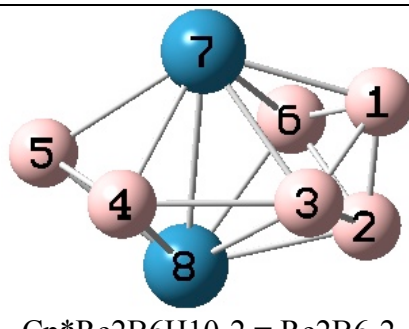
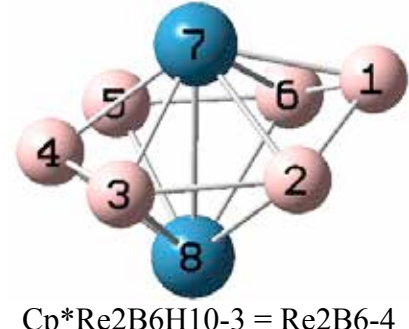
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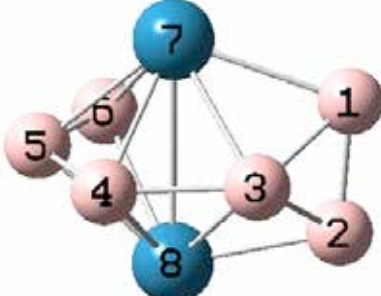
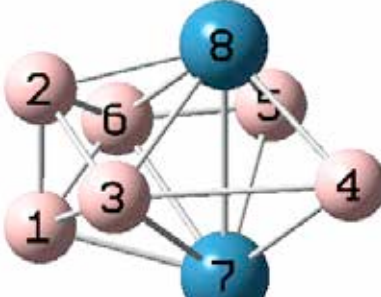
	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.244965</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.325506</td><td>1.779038</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Re</td><td>3.026887</td><td>2.351674</td><td>3.055378</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.355413</td><td>3.229049</td><td>2.823121</td><td>2.230733</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.050466</td><td>2.819648</td><td>1.921116</td><td>2.324695</td><td>1.772020</td></tr><tr><td>7 B</td><td>2.155049</td><td>3.038169</td><td>1.768454</td><td>3.275816</td><td>1.751192</td></tr><tr><td>8 B</td><td>3.276525</td><td>1.741253</td><td>1.696121</td><td>2.152668</td><td>3.030978</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.688798</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.770193</td><td>2.851928</td><td>0.000000</td><td></td><td></td></tr></table> Re1-H-B2 Re1-H 1.73 B2-H 1.37 Re4-H-B5 Re4-H 1.72 B5-H 1.40 Re1-H 1.66 Re4-H 1.66		1	2	3	4	5	1 Re	0.000000					2 B	2.244965	0.000000				3 B	2.325506	1.779038	0.000000			4 Re	3.026887	2.351674	3.055378	0.000000		5 B	2.355413	3.229049	2.823121	2.230733	0.000000	6 B	3.050466	2.819648	1.921116	2.324695	1.772020	7 B	2.155049	3.038169	1.768454	3.275816	1.751192	8 B	3.276525	1.741253	1.696121	2.152668	3.030978		6	7	8			6 B	0.000000					7 B	1.688798	0.000000				8 B	1.770193	2.851928	0.000000		
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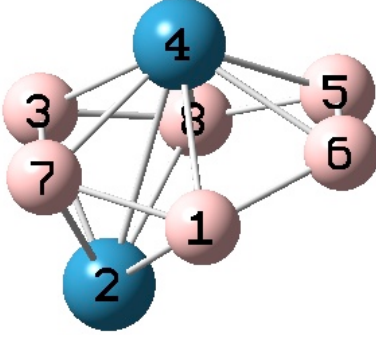
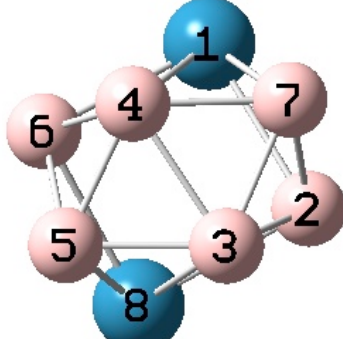
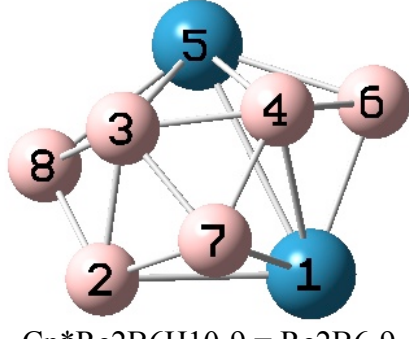


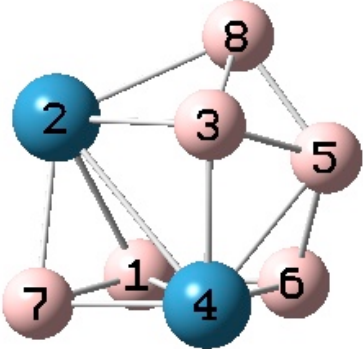
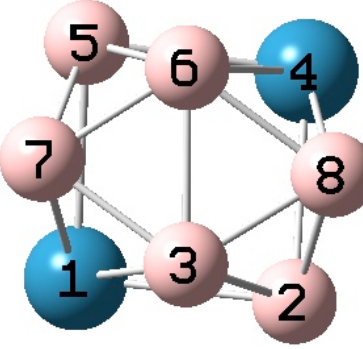
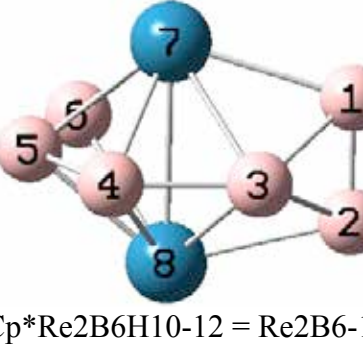
Re7-H-B4	Re7-H 1.78	B4-H 1.32
Re7-H-B5	Re7-H 1.78	B5-H 1.32
Re8-H-B4	Re7-H 1.78	B4-H 1.32
Re8-H-B5	Re7-H 1.78	B5-H 1.32

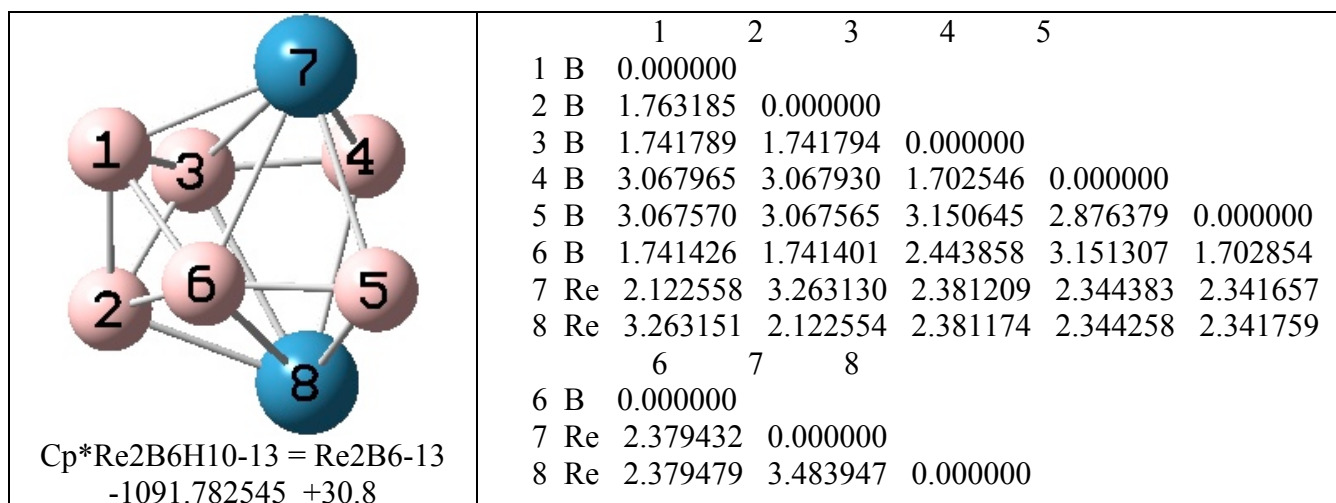
Table 5B. Distance table for the lowest-lying $\text{Cp}^*\text{Re}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Re2B6H10-1 = Re2B6-1 -1091.831570 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.814293</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.740396</td><td>3.189261</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.740259</td><td>3.189236</td><td>1.771899</td><td>0.000000</td><td></td></tr><tr><td>5 Re</td><td>2.283165</td><td>2.110009</td><td>3.188573</td><td>2.267930</td><td>0.000000</td></tr><tr><td>6 Re</td><td>2.283210</td><td>2.109992</td><td>2.267808</td><td>3.188216</td><td>2.834602</td></tr><tr><td>7 B</td><td>3.280729</td><td>2.041763</td><td>3.963714</td><td>3.963600</td><td>2.185677</td></tr><tr><td>8 B</td><td>3.462096</td><td>3.075112</td><td>3.454617</td><td>3.454402</td><td>2.243247</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.185668</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.243226</td><td>1.671238</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.814293	0.000000				3 B	1.740396	3.189261	0.000000			4 B	1.740259	3.189236	1.771899	0.000000		5 Re	2.283165	2.110009	3.188573	2.267930	0.000000	6 Re	2.283210	2.109992	2.267808	3.188216	2.834602	7 B	3.280729	2.041763	3.963714	3.963600	2.185677	8 B	3.462096	3.075112	3.454617	3.454402	2.243247		6	7	8			6 Re	0.000000					7 B	2.185668	0.000000				8 B	2.243226	1.671238	0.000000		
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 Cp*Re2B6H10-2 = Re2B6-2 -1091.827103 +2.8	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.628550</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.743446</td><td>1.737416</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.535172</td><td>3.478895</td><td>2.256936</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>4.069715</td><td>3.997594</td><td>3.395821</td><td>1.742695</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.788238</td><td>1.746464</td><td>2.566723</td><td>3.485608</td><td>3.268535</td></tr><tr><td>7 Re</td><td>2.252552</td><td>3.086604</td><td>2.246321</td><td>2.188066</td><td>2.354873</td></tr><tr><td>8 Re</td><td>3.101971</td><td>2.211575</td><td>2.267008</td><td>2.129294</td><td>2.236823</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Re</td><td>2.358631</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Re</td><td>2.306082</td><td>2.820638</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.628550	0.000000				3 B	1.743446	1.737416	0.000000			4 B	3.535172	3.478895	2.256936	0.000000		5 B	4.069715	3.997594	3.395821	1.742695	0.000000	6 B	1.788238	1.746464	2.566723	3.485608	3.268535	7 Re	2.252552	3.086604	2.246321	2.188066	2.354873	8 Re	3.101971	2.211575	2.267008	2.129294	2.236823		6	7	8			6 B	0.000000					7 Re	2.358631	0.000000				8 Re	2.306082	2.820638	0.000000		
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 Cp*Re2B6H10-10 = Re2B6-10 -1091.793768 +23.7	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Re</td><td>2.371825</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.224249</td><td>2.254250</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Re</td><td>2.251410</td><td>2.903275</td><td>2.137564</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.958739</td><td>3.159126</td><td>1.767282</td><td>2.257674</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.814975</td><td>3.447597</td><td>3.070318</td><td>2.039687</td><td>1.906337</td></tr><tr><td>7 B</td><td>1.893032</td><td>2.162865</td><td>3.078109</td><td>2.048474</td><td>3.724955</td></tr><tr><td>8 B</td><td>3.227772</td><td>2.299289</td><td>1.729704</td><td>3.230478</td><td>1.750694</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.168338</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.058659</td><td>3.856814</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 Re	2.371825	0.000000				3 B	3.224249	2.254250	0.000000			4 Re	2.251410	2.903275	2.137564	0.000000		5 B	2.958739	3.159126	1.767282	2.257674	0.000000	6 B	1.814975	3.447597	3.070318	2.039687	1.906337	7 B	1.893032	2.162865	3.078109	2.048474	3.724955	8 B	3.227772	2.299289	1.729704	3.230478	1.750694		6	7	8			6 B	0.000000					7 B	3.168338	0.000000				8 B	3.058659	3.856814	0.000000		
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8 B	3.058659	3.856814	0.000000																																																																												
 Cp*Re2B6H10-11 = Re2B6-12 -1091.791936 +24.9	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.251798</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.326546</td><td>1.781658</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Re</td><td>3.021213</td><td>2.354532</td><td>3.053423</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.356947</td><td>3.243834</td><td>2.827310</td><td>2.236610</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.048080</td><td>2.824103</td><td>1.918883</td><td>2.325934</td><td>1.774897</td></tr><tr><td>7 B</td><td>2.148547</td><td>3.040859</td><td>1.766585</td><td>3.273518</td><td>1.751230</td></tr><tr><td>8 B</td><td>3.274401</td><td>1.739084</td><td>1.698635</td><td>2.147130</td><td>3.035545</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.690545</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.771558</td><td>2.854017</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Re	0.000000					2 B	2.251798	0.000000				3 B	2.326546	1.781658	0.000000			4 Re	3.021213	2.354532	3.053423	0.000000		5 B	2.356947	3.243834	2.827310	2.236610	0.000000	6 B	3.048080	2.824103	1.918883	2.325934	1.774897	7 B	2.148547	3.040859	1.766585	3.273518	1.751230	8 B	3.274401	1.739084	1.698635	2.147130	3.035545		6	7	8			6 B	0.000000					7 B	1.690545	0.000000				8 B	1.771558	2.854017	0.000000		
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 Cp*Re2B6H10-12 = Re2B6-11 -1091.790731 +25.6	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.608723</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.807229</td><td>1.807272</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.355314</td><td>3.355397</td><td>1.863340</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>4.102870</td><td>4.102991</td><td>3.159964</td><td>1.750333</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.893434</td><td>3.893601</td><td>3.628192</td><td>2.972072</td><td>1.633014</td></tr><tr><td>7 Re</td><td>2.378238</td><td>3.205392</td><td>2.255421</td><td>2.147421</td><td>2.250139</td></tr><tr><td>8 Re</td><td>3.205203</td><td>2.378251</td><td>2.255358</td><td>2.147433</td><td>2.250196</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Re</td><td>2.373956</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Re</td><td>2.374073</td><td>2.870528</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.608723	0.000000				3 B	1.807229	1.807272	0.000000			4 B	3.355314	3.355397	1.863340	0.000000		5 B	4.102870	4.102991	3.159964	1.750333	0.000000	6 B	3.893434	3.893601	3.628192	2.972072	1.633014	7 Re	2.378238	3.205392	2.255421	2.147421	2.250139	8 Re	3.205203	2.378251	2.255358	2.147433	2.250196		6	7	8			6 B	0.000000					7 Re	2.373956	0.000000				8 Re	2.374073	2.870528	0.000000		
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$$\text{Cp}^*\text{Re}_2\text{B}_6\text{H}_{10-13} = \text{Re}_2\text{B}_6-13$$

$$-1091.782545 + 30.8$$

	1	2	3	4	5	
1 B	0.000000					
2 B	1.763185	0.000000				
3 B	1.741789	1.741794	0.000000			
4 B	3.067965	3.067930	1.702546	0.000000		
5 B	3.067570	3.067565	3.150645	2.876379	0.000000	
6 B	1.741426	1.741401	2.443858	3.151307	1.702854	
7 Re	2.122558	3.263130	2.381209	2.344383	2.341657	
8 Re	3.263151	2.122554	2.381174	2.344258	2.341759	
	6	7	8			
6 B	0.000000					
7 Re	2.379432	0.000000				
8 Re	2.379479	3.483947	0.000000			

Table 5C. Energy ranking for all of the $\text{Cp}_2\text{Re}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	hexagonal-b4_Re	-699.15118680	0.00
2	hexagonal-b4_Re	-699.15118621	0.00
3	B7Mo2-1F_c- Re	-699.14465020	4.10
4	hexagonal-b3_Re	-699.14361823	4.75
5	B7Mo2-1F_b1- Re	-699.12976414	13.44
6	B7Mo2-1F_a_Re_1imag	-699.12947276	13.63
7	B7Mo2-1F_b3- Re	-699.12785851	14.64
8	B7Mo2-1F_b3_Re	-699.12785847	14.64
9	B7Mo2-1F_d- 1 Re	-699.12688569	15.25
10	156_closoTTP-A-l-5_Re_r-23	-699.12453014	16.73
11	hexagonal-e01_Re_r-22	-699.12453003	16.73
12	hexagonal-e01_Re	-699.12451505	16.74
13	156_closoTTP-A-l-5_Re	-699.12451493	16.74
14	160_closoTTP-A-n1_Re	-699.11487741	22.78
15	115_closoTTP-A-f-2_Re	-699.11428349	23.16
16	118_closoTTP-A-f4_Re	-699.11426185	23.17
17	114_closoTTP-A-f2_Re	-699.11425515	23.17
18	119_closoTTP-A-f-4_Re	-699.11425470	23.17
19	151_closoTTP-A-l3_Re	-699.11404260	23.31
20	hexagonal-e04_Re	-699.11327283	23.79
21	150_closoTTP-A-l-2_Re	-699.11325936	23.80
22	hexagonal-d13_Re_ca	-699.11266338	24.17
23	152_closoTTP-A-l-3_Re	-699.11249738	24.28
24	154_closoTTP-A-l-4_Re	-699.11246556	24.30
25	164_closoTTP-A-n3_Re	-699.10862630	26.71
26	186_closoTTP-B-i_Re	-699.10850021	26.79
27	162_closoTTP-A-n2_Re	-699.10795466	27.13
28	163_closoTTP-A-n-2_Re	-699.10795430	27.13
29	106_closoTTP-A-d5_Re_r-33	-699.10547898	28.68
30	106_closoTTP-A-d5_Re	-699.10529779	28.80
31	148_closoTTP-A-l-1_Re	-699.10462369	29.22
32	B7Mo2-1F_b2- Re	-699.10404947	29.58
33	177_closoTTP-A-p3_Re	-699.10267601	30.44
34	B7Mo2-1F_d_Re	-699.10262688	30.47
35	165_closoTTP-A-n-3_Re	-699.10178526	31.00
36	hexagonal-b3_Re_caxqc--freq	-699.10143637	31.22
37	hexagonal-e15_Re	-699.10132115	31.29
38	hexagonal-e15_Re--freq	-699.10131537	31.29

39	171_closoTTP-A-o2_Re	-699.10131006	31.30
40	hexagonal-b4_Re_irqc	-699.10088409	31.56
41	159_closoTTP-A-m3_Re	-699.10080764	31.61
42	187_closoTTP-B-j_Re_r-333	-699.10079079	31.62
43	187_closoTTP-B-j_Re_i-333	-699.10050165	31.80
44	149_closoTTP-A-l2_Re	-699.09997636	32.13
45	116_closoTTP-A-f3_Re	-699.09937952	32.51
46	121_closoTTP-A-f-5_Re	-699.09815497	33.28
47	184_closoTTP-B-g_Re	-699.09765874	33.59
48	112_closoTTP-A-fl_Re	-699.09765869	33.59
49	181_closoTTP-B-d_Re	-699.09548603	34.95
50	153_closoTTP-A-l4_Re	-699.09548405	34.95
51	158_closoTTP-A-m2_Re	-699.09453624	35.55
52	134_closoTTP-A-i3_Re	-699.09298875	36.52
53	135_closoTTP-A-i4_Re	-699.09298746	36.52
54	168_closoTTP-A-n5_Re	-699.09286141	36.60
55	175_closoTTP-A-pl_Re_r-377	-699.09270224	36.70
56	hexagonal-b1_Re	-699.09158769	37.40
57	B7Mo2-1F_c_Re	-699.09101544	37.76
58	hexagonal-b1-_Re_r-71	-699.09078742	37.90
59	117_closoTTP-A-f-3_Re	-699.08966030	38.61
60	hexagonal-b4-_Re_r-130	-699.08909717	38.96
61	hexagonal-b3-_Re_r-116	-699.08899325	39.03
62	143_closoTTP-A-k2_Re	-699.08880016	39.15
63	142_closoTTP-A-k1_Re	-699.08880001	39.15
64	hexagonal-b1-_Re_i-71	-699.08865631	39.24
65	113_closoTTP-A-f-1_Re	-699.08844949	39.37
66	166_closoTTP-A-n4_Re	-699.08746923	39.98
67	167_closoTTP-A-n-4_Re	-699.08744114	40.00
68	169_closoTTP-A-n-5_Re	-699.08733821	40.06
69	hexagonal-c02_Re_ca--freq	-699.08710148	40.21
70	hexagonal-c03_Re	-699.08709902	40.22
71	hexagonal-c04_Re_r-37	-699.08709864	40.22
72	hexagonal-c04_Re_i-37	-699.08629305	40.72
73	hexagonal-e05_Re	-699.08551618	41.21
74	hexagonal-c14_Re	-699.08525696	41.37
75	122_closoTTP-A-gl_Re	-699.08518277	41.42
76	hexagonal-c12_Re	-699.08507500	41.49
77	hexagonal-e08_Re-cont	-699.08505555	41.50
78	144_closoTTP-A-k3_Re	-699.08505450	41.50
79	hexagonal-e09_Re	-699.08505394	41.50

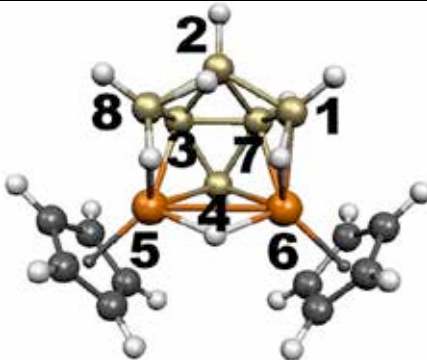
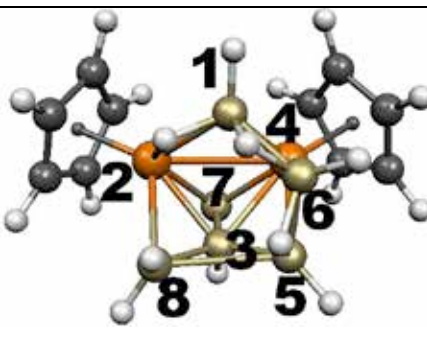
80	hexagonal-e14 Re	-699.08505334	41.50
81	147_closoTTP-A-l1 Re	-699.08359619	42.41
82	157_closoTTP-A-m1 Re r-408	-699.08299327	42.79
83	099_closoTTP-A-c3 Re	-699.08108460	43.99
84	100_closoTTP-A-c4 Re	-699.08099971	44.04
85	hexagonal-b2- Re	-699.08097104	44.06
86	hexagonal-f02 Re	-699.08093864	44.08
87	hexagonal-f04 Re	-699.08092697	44.09
88	hexagonal-f03 Re	-699.08091973	44.09
89	hexagonal-f01 Re	-699.08053270	44.34
90	157_closoTTP-A-m1 Re i-408	-699.07904656	45.27
91	132_closoTTP-A-i1 Re	-699.07756198	46.20
92	hexagonal-d15 Re	-699.07736950	46.32
93	hexagonal-a1 Re ca	-699.07711502	46.48
94	141_closoTTP-A-j5-Re	-699.07709500	46.49
95	140_closoTTP-A-j4 Re	-699.07709480	46.49
96	092_closoTTP-A-b1 Re	-699.07709425	46.49
97	139_closoTTP-A-j3 Re	-699.07709367	46.49
98	173_closoTTP-A-o4 Re	-699.07708577	46.50
99	174_closoTTP-A-o5 Re	-699.07708559	46.50
100	172_closoTTP-A-o3 Re	-699.07708543	46.50
101	108_closoTTP-A-e2 Re	-699.07708498	46.50
102	107_closoTTP-A-e1 Re	-699.07708473	46.50
103	hexagonal-d14 Re	-699.07678257	46.69
104	124_closoTTP-A-g3 Re	-699.07552035	47.48
105	125_closoTTP-A-g4 Re	-699.07552002	47.48
106	hexagonal-f09 Re	-699.07418773	48.32
107	hexagonal-f12 Re	-699.07415217	48.34
108	090_closoTTP-A-a2 Re	-699.07396071	48.46
109	hexagonal-b2- Re	-699.07373958	48.60
110	hexagonal-b6 Re	-699.07373948	48.60
111	110_closoTTP-A-e4 Re	-699.07372846	48.61
112	hexagonal-f10 Re	-699.07372810	48.61
113	hexagonal-f08 Re	-699.07353472	48.73
114	hexagonal-f13 Re	-699.07349460	48.75
115	hexagonal-f11 Re	-699.07349382	48.75
116	089_closoTTP-A-a1 Re r-40-34	-699.07214186	49.60
117	hexagonal-f14 Re	-699.07197859	49.70
118	hexagonal-f15 Re	-699.07197844	49.70
119	hexagonal-a4 Re r-399	-699.07156623	49.96
120	hexagonal-a3 Re r-124	-699.07138300	50.08

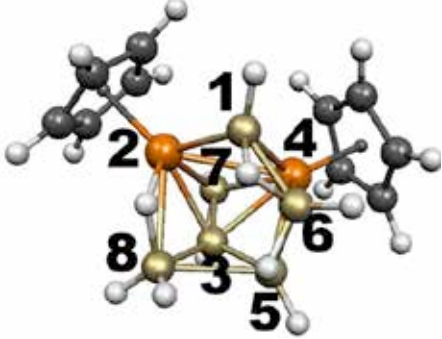
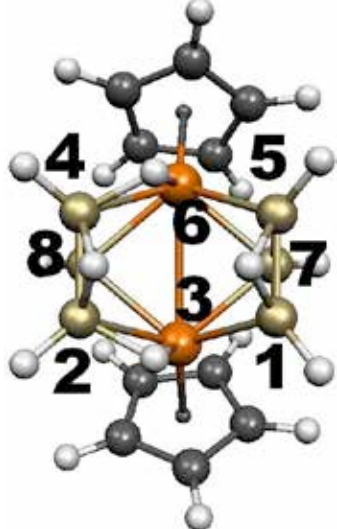
121	hexagonal-a2_Re	-699.07116375	50.21
122	hexagonal-a4_Re r-44	-699.07115929	50.22
123	120_closoTTP-A-f5_Re	-699.07092297	50.37
124	hexagonal-b5-_Re	-699.07048722	50.64
125	089_closoTTP-A-a1_Re r-40	-699.07038783	50.70
126	089_closoTTP-A-a1_Re	-699.07035366	50.72
127	hexagonal-e07_Re	-699.07013399	50.86
128	hexagonal-e03_Re-cont	-699.06985873	51.03
129	176_closoTTP-A-p2_Re	-699.06851519	51.88
130	B7Mo2-1F_b2_Re	-699.06786487	52.28
131	hexagonal-a5_Re	-699.06738381	52.59
132	hexagonal-c09_Re	-699.06730664	52.63
133	145_closoTTP-A-k4_Re	-699.06702457	52.81
134	155_closoTTP-A-l5_Re	-699.06691130	52.88
135	091_closoTTP-A-a3_Re	-699.06689266	52.89
136	hexagonal-d05_Re	-699.06624710	53.30
137	133_closoTTP-A-i2_Re	-699.06617881	53.34
138	104_closoTTP-A-d3_Re	-699.06591328	53.51
139	111_closoTTP-A-e5_Re	-699.06546552	53.79
140	170_closoTTP-A-o1_Re	-699.06546260	53.79
141	hexagonal-c09_Re	-699.06531853	53.88
142	hexagonal-d01_Re	-699.06448525	54.41
143	hexagonal-d09_Re	-699.06433493	54.50
144	161_closoTTP-A-n-1_Re	-699.06354528	55.00
145	136_closoTTP-A-i5_Re	-699.06347600	55.04
146	hexagonal-f07_Re	-699.06347436	55.04
147	hexagonal-f06_Re	-699.06347401	55.04
148	185_closoTTP-B-h_Re	-699.06236643	55.73
149	hexagonal-c13_Re	-699.06209428	55.91
150	hexagonal-c11_Re	-699.06209345	55.91
151	hexagonal-b2_Re	-699.06097061	56.61
152	hexagonal-c10_Re	-699.06095280	56.62
153	183_closoTTP-B-f_Re	-699.06084748	56.69
154	hexagonal-d11_Re	-699.06070770	56.78
155	137_closoTTP-A-j1_Re	-699.06037567	56.98
156	138_closoTTP-A-j2_Re	-699.06037541	56.98
157	123_closoTTP-A-g2_Re	-699.06021144	57.09
158	hexagonal-c08_Re	-699.05954035	57.51
159	hexagonal-c01_Re	-699.05946683	57.55
160	hexagonal-b5_Re	-699.05932664	57.64
161	hexagonal-d08_Re	-699.05919544	57.72

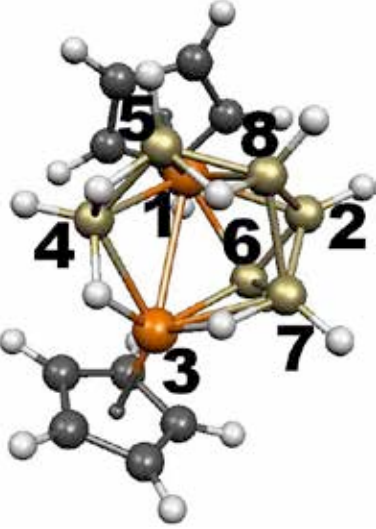
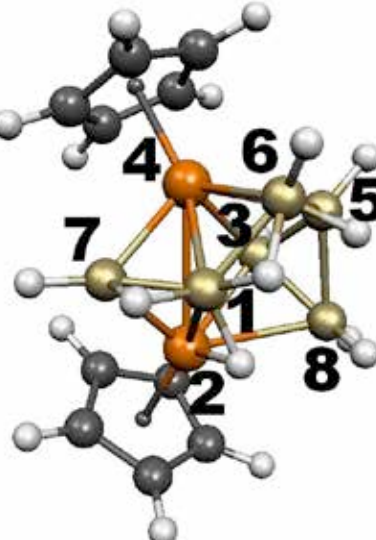
162	hexagonal-c07_Re	-699.05845242	58.19
163	hexagonal-c05_Re	-699.05588012	59.80
164	109_closoTTP-A-e3_Re	-699.05574850	59.89
165	129_closoTTP-A-h3_Re	-699.05538624	60.11
166	094_closoTTP-A-b3_Re	-699.05538366	60.12
167	B7Mo2-1F_b1_Re.log	-699.05527040	60.19
168	hexagonal-d12_Re	-699.05498439	60.37
169	hexagonal-c06_Re	-699.05495675	60.38
170	hexagonal-a3_Re i-124	-699.05427825	60.81
171	130_closoTTP-A-h4_Re	-699.05414824	60.89
172	hexagonal-d06_Re	-699.05411306	60.91
173	hexagonal-d02_Re-ca	-699.05174502	62.40
174	hexagonal-d04_Re	-699.05083566	62.97
175	hexagonal-a4_Re imag	-699.04900190	64.12
176	146_closoTTP-A-k5_Re	-699.04729374	65.19
177	hexagonal-d07_Re	-699.04576078	66.15
178	hexagonal-d10_Re	-699.04572709	66.18
179	126_closoTTP-A-g5_Re	-699.04169497	68.71
180	128_closoTTP-A-h2_Re	-699.04134919	68.92
181	hexagonal-e13_Re	-699.04033898	69.56
182	hexagonal-e12_Re	-699.03943064	70.13
183	098_closoTTP-A-c2_Re	-699.03809623	70.96
184	180_closoTTP-B-c_Re	-699.03768031	71.23
185	179_closoTTP-B-b_Re	-699.03340176	73.91
186	131_closoTTP-A-h5_Re	-699.03125683	75.26
187	093_closoTTP-A-b2_Re	-699.02931870	76.47
188	102_closoTTP-A-d1_Re	-699.02905791	76.64
189	hexagonal-f05_Re	-699.02820173	77.17
190	095_closoTTP-A-b4_Re	-699.02775647	77.45
191	097_closoTTP-A-c1_Re	-699.02736875	77.70
192	096_closoTTP-A-b5_Re	-699.02706370	77.89
193	105_closoTTP-A-d4_Re	-699.02512447	79.10
194	hexagonal-a6_Re_caxqc	-699.02506830	79.14
195	hexagonal-a6_Re_caxqc	-699.02506830	79.14
196	101_closoTTP-A-c5_Re	-699.02473838	79.35
197	178_closoTTP-B-a_Re_r-86	-699.02348282	80.13
198	182_closoTTP-B-e_Re	-699.02321016	80.31
199	hexagonal-e11_Re	-699.02291811	80.49
200	127_closoTTP-A-h1_Re	-699.02248644	80.76
201	hexagonal-e10_Re	-699.02220319	80.94
202	hexagonal-b4-_Re	-699.01969890	82.51

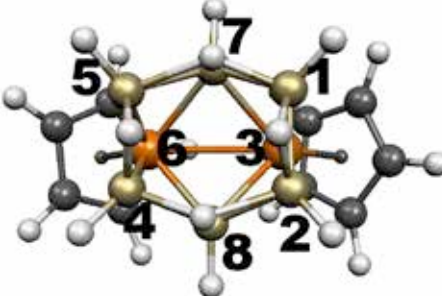
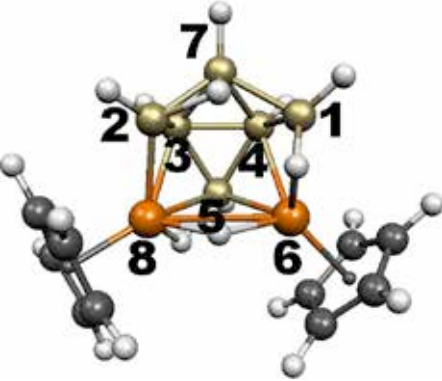
203	hexagonal-e02_Re	-699.01937341	82.71
204	hexagonal-e06_Re	-699.01932742	82.74
205	103_closoTTP-A-d2_Re	-699.01163441	87.57
206	175_closoTTP-A-p1_Re i-377	-699.00913453	89.14
207	hexagonal-b6-_Re	-699.00868364	89.42
208	hexagonal-b3-_Re	-699.00592719	91.15
209	hexagonal-d03_Re	-699.00270308	93.17
210	178_closoTTP-B-a_Re i-86	-698.98877562	101.91

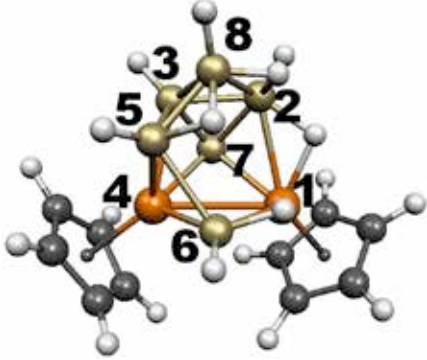
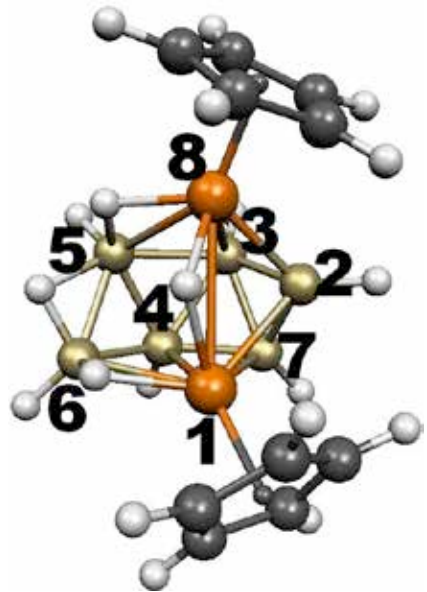
Table 6A. Distance table for the lowest-lying $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 1. -732.059181 0.0 C₁(C_s) WBI 0.30	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.878122</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.920416</td><td>1.754423</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.990508</td><td>2.925232</td><td>1.762375</td><td>0.000000</td><td></td></tr><tr><td>5 Ru</td><td>3.657106</td><td>3.297785</td><td>2.256927</td><td>2.108907</td><td>0.000000</td></tr><tr><td>6 Ru</td><td>2.104612</td><td>3.299788</td><td>3.210588</td><td>2.129996</td><td>2.878859</td></tr><tr><td>7 B</td><td>1.716428</td><td>1.743955</td><td>1.778322</td><td>1.755989</td><td>3.182620</td></tr><tr><td>8 B</td><td>3.004220</td><td>1.787314</td><td>1.742497</td><td>3.000225</td><td>2.167546</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Ru</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.259252</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.611493</td><td>2.852062</td><td>0.000000</td><td></td><td></td></tr></table> Ru5-H-Ru6 Ru5-H 1.75 Ru6-H 1.77 Ru5-H-B8 Ru5-H 1.72 B8-H 1.34 Ru6-H-B1 Ru6-H 1.73 B1-H 1.33 B1-H-B8 B1-H 1.97 B8-H 1.48		1	2	3	4	5	1 B	0.000000					2 B	1.878122	0.000000				3 B	2.920416	1.754423	0.000000			4 B	2.990508	2.925232	1.762375	0.000000		5 Ru	3.657106	3.297785	2.256927	2.108907	0.000000	6 Ru	2.104612	3.299788	3.210588	2.129996	2.878859	7 B	1.716428	1.743955	1.778322	1.755989	3.182620	8 B	3.004220	1.787314	1.742497	3.000225	2.167546		6	7	8			6 Ru	0.000000					7 B	2.259252	0.000000				8 B	3.611493	2.852062	0.000000		
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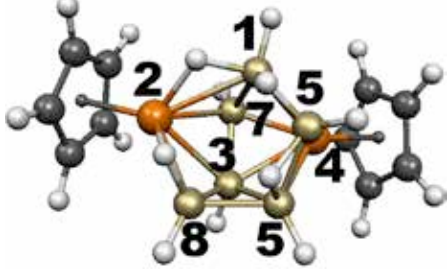
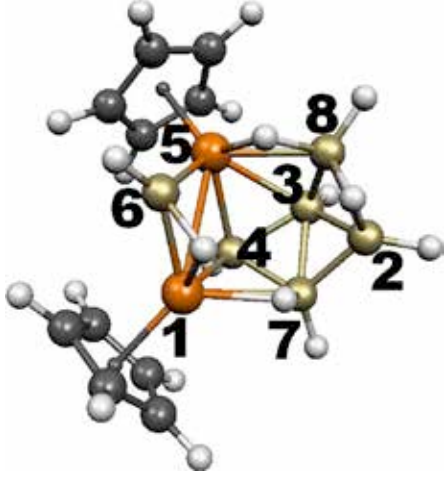
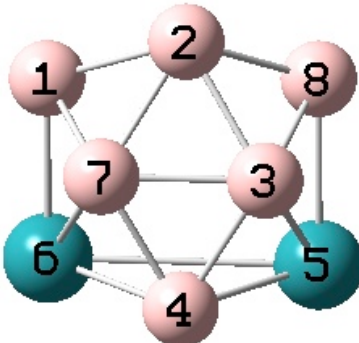
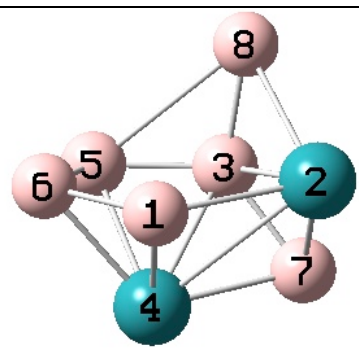
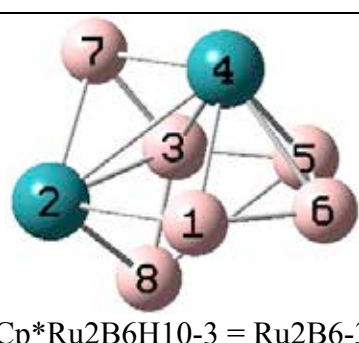
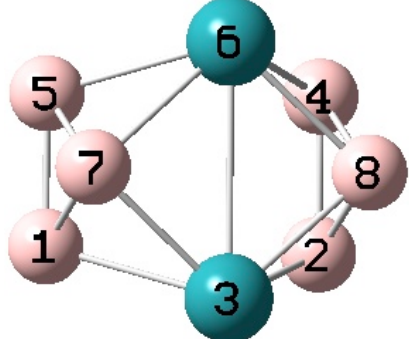
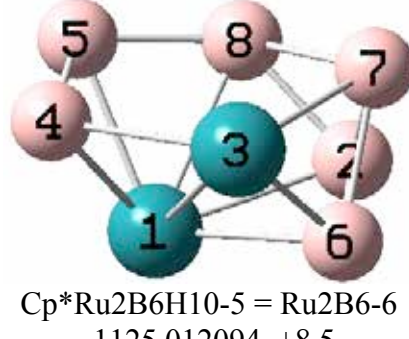
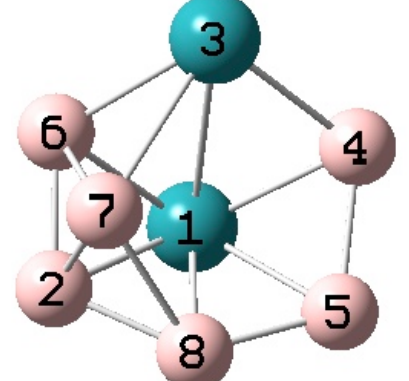
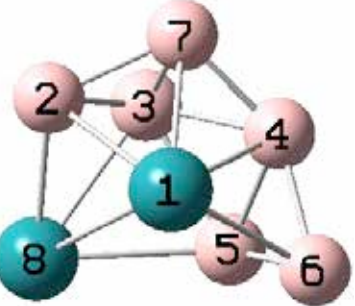
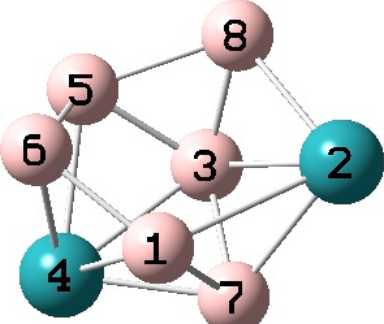
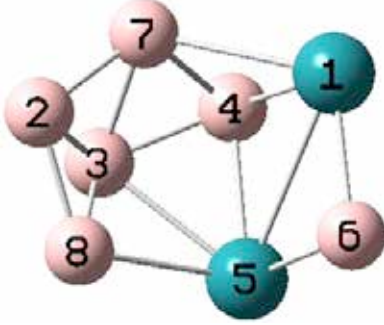
 11. -732.038011 +13.3 C₁ WBI 0.14	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ru</td><td>2.451317</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.741491</td><td>2.304988</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ru</td><td>2.200701</td><td>3.617195</td><td>2.175109</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.839840</td><td>3.304386</td><td>1.742557</td><td>2.146432</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.833258</td><td>3.510651</td><td>2.869566</td><td>2.075619</td><td>1.815123</td></tr><tr><td>7 B</td><td>1.926994</td><td>2.146884</td><td>1.792475</td><td>2.008019</td><td>2.981698</td></tr><tr><td>8 B</td><td>3.157003</td><td>2.128736</td><td>1.694799</td><td>3.404408</td><td>1.883789</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td></tr><tr><td>7 B</td><td>3.076439</td><td>0.000000</td><td></td></tr><tr><td>8 B</td><td>2.978767</td><td>3.020373</td><td>0.000000</td></tr></table> Ru2-H-B1 Ru2-H 1.70 B1-H 1.37 Ru2-H-B8 Ru2-H 1.71 B8-H 1.35 B1-H-B6 B1-H 1.36 B6-H 1.29 B5-H-B6 B5-H 1.32 B6-H 1.37		1	2	3	4	5	1 B	0.000000					2 Ru	2.451317	0.000000				3 B	2.741491	2.304988	0.000000			4 Ru	2.200701	3.617195	2.175109	0.000000		5 B	2.839840	3.304386	1.742557	2.146432	0.000000	6 B	1.833258	3.510651	2.869566	2.075619	1.815123	7 B	1.926994	2.146884	1.792475	2.008019	2.981698	8 B	3.157003	2.128736	1.694799	3.404408	1.883789		6	7	8	6 B	0.000000			7 B	3.076439	0.000000		8 B	2.978767	3.020373	0.000000
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Table 6B. Distance table for the lowest-lying $\text{Cp}^*\text{Ru}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Ru2B6H10-1 = Ru2B6-1 -1125.025691 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.862723</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.896621</td><td>1.751270</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.978794</td><td>2.927211</td><td>1.763515</td><td>0.000000</td><td></td></tr><tr><td>5 Ru</td><td>3.651582</td><td>3.316571</td><td>2.253355</td><td>2.118948</td><td>0.000000</td></tr><tr><td>6 Ru</td><td>2.106145</td><td>3.321998</td><td>3.226283</td><td>2.137676</td><td>2.938953</td></tr><tr><td>7 B</td><td>1.721402</td><td>1.744169</td><td>1.779247</td><td>1.757717</td><td>3.202751</td></tr><tr><td>8 B</td><td>2.946065</td><td>1.787764</td><td>1.742053</td><td>2.991306</td><td>2.160642</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Ru</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.265112</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.616747</td><td>2.844002</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.862723	0.000000				3 B	2.896621	1.751270	0.000000			4 B	2.978794	2.927211	1.763515	0.000000		5 Ru	3.651582	3.316571	2.253355	2.118948	0.000000	6 Ru	2.106145	3.321998	3.226283	2.137676	2.938953	7 B	1.721402	1.744169	1.779247	1.757717	3.202751	8 B	2.946065	1.787764	1.742053	2.991306	2.160642		6	7	8			6 Ru	0.000000					7 B	2.265112	0.000000				8 B	3.616747	2.844002	0.000000		
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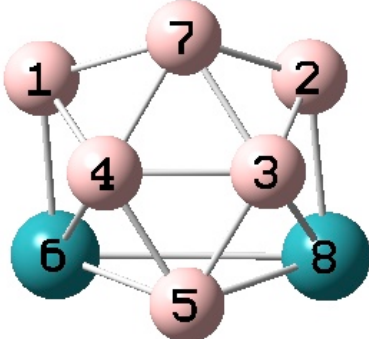
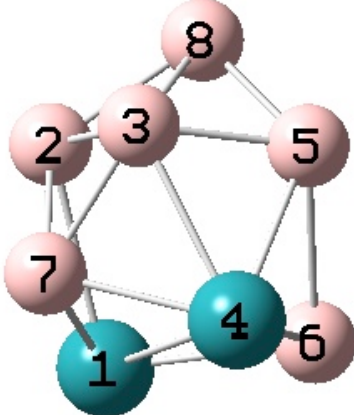
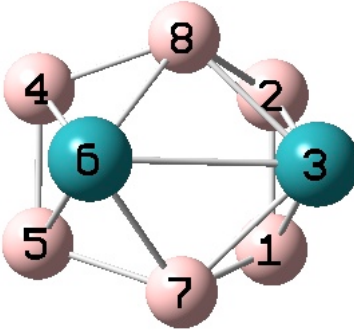
 Cp*Ru2B6H10-10 = Ru2B6-8 -1125.005227 +12.8	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.940337</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.950595</td><td>1.726876</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.714529</td><td>2.786691</td><td>1.796326</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.046238</td><td>2.960262</td><td>1.771257</td><td>1.756481</td><td>0.000000</td></tr><tr><td>6 Ru</td><td>2.109952</td><td>3.481961</td><td>3.232484</td><td>2.260415</td><td>2.209540</td></tr><tr><td>7 B</td><td>1.864609</td><td>1.760274</td><td>1.764989</td><td>1.741885</td><td>2.936936</td></tr><tr><td>8 Ru</td><td>3.759746</td><td>2.084567</td><td>2.256365</td><td>3.230792</td><td>2.202171</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 Ru</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.272514</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Ru</td><td>2.974917</td><td>3.312404</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	2.940337	0.000000				3 B	2.950595	1.726876	0.000000			4 B	1.714529	2.786691	1.796326	0.000000		5 B	3.046238	2.960262	1.771257	1.756481	0.000000	6 Ru	2.109952	3.481961	3.232484	2.260415	2.209540	7 B	1.864609	1.760274	1.764989	1.741885	2.936936	8 Ru	3.759746	2.084567	2.256365	3.230792	2.202171		6	7	8			6 Ru	0.000000					7 B	3.272514	0.000000				8 Ru	2.974917	3.312404	0.000000		
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 Cp*Ru2B6H10-11 = Ru2B6-9 -1124.995742 +18.8	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ru</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.353599</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.203651</td><td>1.812738</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ru</td><td>2.827384</td><td>3.223421</td><td>2.210953</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.414916</td><td>2.807292</td><td>1.764762</td><td>2.060540</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.201996</td><td>3.300933</td><td>3.142040</td><td>2.003994</td><td>2.199893</td></tr><tr><td>7 B</td><td>2.151259</td><td>1.862178</td><td>1.761364</td><td>2.063234</td><td>2.926866</td></tr><tr><td>8 B</td><td>3.487955</td><td>1.849965</td><td>1.739312</td><td>3.324531</td><td>1.756852</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.032394</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.222028</td><td>3.033195</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Ru	0.000000					2 B	2.353599	0.000000				3 B	3.203651	1.812738	0.000000			4 Ru	2.827384	3.223421	2.210953	0.000000		5 B	3.414916	2.807292	1.764762	2.060540	0.000000	6 B	2.201996	3.300933	3.142040	2.003994	2.199893	7 B	2.151259	1.862178	1.761364	2.063234	2.926866	8 B	3.487955	1.849965	1.739312	3.324531	1.756852		6	7	8			6 B	0.000000					7 B	3.032394	0.000000				8 B	3.222028	3.033195	0.000000		
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 Cp*Ru2B6H10-12 = Ru2B6-7 -1124.988419 +23.4	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.779715</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Ru</td><td>2.035374</td><td>2.038306</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.343242</td><td>2.824989</td><td>3.448112</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.824710</td><td>3.334609</td><td>3.450546</td><td>1.780505</td><td>0.000000</td></tr><tr><td>6 Ru</td><td>3.452202</td><td>3.455119</td><td>2.747476</td><td>2.037057</td><td>2.039548</td></tr><tr><td>7 B</td><td>1.849938</td><td>2.939727</td><td>2.159250</td><td>2.938878</td><td>1.849176</td></tr><tr><td>8 B</td><td>2.940656</td><td>1.852184</td><td>2.155441</td><td>1.846128</td><td>2.937996</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 Ru</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.154859</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.161178</td><td>2.932125</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.779715	0.000000				3 Ru	2.035374	2.038306	0.000000			4 B	3.343242	2.824989	3.448112	0.000000		5 B	2.824710	3.334609	3.450546	1.780505	0.000000	6 Ru	3.452202	3.455119	2.747476	2.037057	2.039548	7 B	1.849938	2.939727	2.159250	2.938878	1.849176	8 B	2.940656	1.852184	2.155441	1.846128	2.937996		6	7	8			6 Ru	0.000000					7 B	2.154859	0.000000				8 B	2.161178	2.932125	0.000000		
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Table 6C. Energy ranking for all of the $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_{10}$ optimized structures:

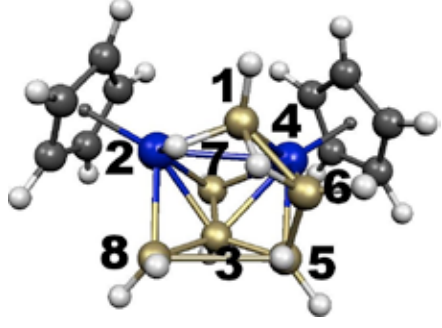
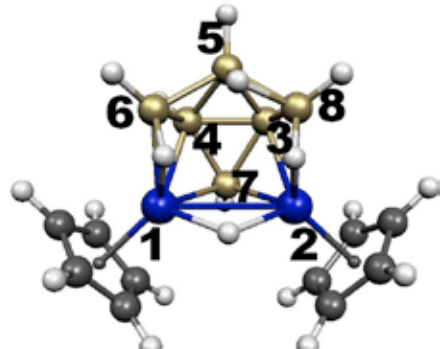
Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	109_closoTTP-A-e3_Ru	-732.1513258	0.00
2	110_closoTTP-A-e4_Ru	-732.1513238	0.00
3	083_hexagonal-f10_Ru	-732.1513224	0.00
4	159_closoTTP-A-m3_Ru	-732.1513216	0.00
5	177_closoTTP-A-p3_Ru	-732.1513201	0.00
6	178_closoTTP-B-a_Ru	-732.1398734	7.19
7	025_hexagonal-b4- Ru	-732.1398699	7.19
8	148_closoTTP-A-l-1_Ru	-732.1377875	8.50
9	057_hexagonal-d14_Ru	-732.1333031	11.31
10	135_closoTTP-A-i4_Ru	-732.1317649	12.27
11	134_closoTTP-A-i3_Ru	-732.1317643	12.28
12	128_closoTTP-A-h2_Ru	-732.1317637	12.28
13	127_closoTTP-A-h1_Ru	-732.1317637	12.28
14	052_hexagonal-d09_Ru	-732.1317636	12.28
15	180_closoTTP-B-c_Ru	-732.1317634	12.28
16	113_closoTTP-A-f-1_Ru	-732.1314235	12.49
17	051_hexagonal-d08_Ru	-732.1310568	12.72
18	156_closoTTP-A-l-5_Ru	-732.1272045	15.14
19	154_closoTTP-A-l-4_Ru	-732.1272043	15.14
20	142_closoTTP-A-k1_Ru	-732.1269296	15.31
21	184_closoTTP-B-g_Ru	-732.1269296	15.31
22	153_closoTTP-A-l4_Ru	-732.1269296	15.31
23	143_closoTTP-A-k2_Ru	-732.1269286	15.31
24	145_closoTTP-A-k4_Ru	-732.1269278	15.31
25	181_closoTTP-B-d_Ru	-732.1269179	15.32
26	149_closoTTP-A-l2_Ru	-732.1243823	16.91
27	151_closoTTP-A-l3_Ru	-732.1243823	16.91
28	089_closoTTP-A-a1_Ru-i67	-732.1243823	16.91
29	061_hexagonal-e03_Ru	-732.1243822	16.91
30	152_closoTTP-A-l-3_Ru	-732.1243822	16.91
31	014_hexagonal-a3_Ru	-732.124372	16.91
32	137_closoTTP-A-j1_Ru	-732.1243602	16.92
33	138_closoTTP-A-j2_Ru	-732.1243593	16.92
34	015_hexagonal-a4_Ru-i40	-732.1221739	18.29
35	066_hexagonal-e08_Ru	-732.1211886	18.91
36	064_hexagonal-e06_Ru	-732.1211884	18.91
37	065_hexagonal-e07_Ru	-732.1211883	18.91
38	062_hexagonal-e04_Ru	-732.1211882	18.91
39	144_closoTTP-A-k3_Ru-i3	-732.121188	18.91
40	028_hexagonal-b6_Ru	-732.1203753	19.42
41	020_hexagonal-b2_Ru	-732.1203751	19.42
42	121_closoTTP-A-f-5_Ru	-732.1174841	21.24
43	116_closoTTP-A-f3_Ru	-732.1174841	21.24
44	017_hexagonal-a6_Ru-i84	-732.1174189	21.28
45	117_closoTTP-A-f-3_Ru	-732.1172674	21.37

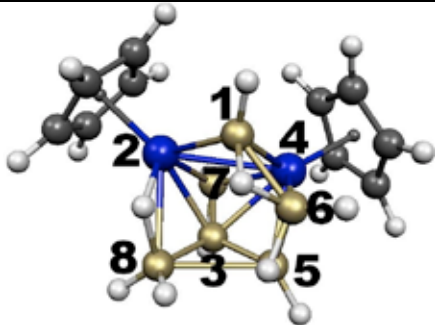
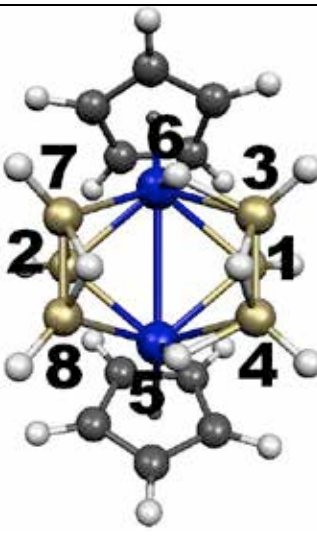
46	112_closoTTP-A-f1_Ru	-732.1171652	21.44
47	027_hexagonal-b5- Ru	-732.116458	21.88
48	026_hexagonal-b5 Ru	-732.1164579	21.88
49	115_closoTTP-A-f-2_Ru	-732.1159772	22.18
50	120_closoTTP-A-f5_Ru	-732.1159771	22.18
51	150_closoTTP-A-l-2_Ru	-732.115813	22.28
52	146_closoTTP-A-k5_Ru	-732.1155959	22.42
53	166_closoTTP-A-n4_Ru	-732.1153366	22.58
54	169_closoTTP-A-n-5_Ru	-732.1153363	22.58
55	187_closoTTP-B-j Ru-i329	-732.115336	22.58
56	168_closoTTP-A-n5_Ru	-732.1150649	22.75
57	186_closoTTP-B-i Ru	-732.1138559	23.51
58	160_closoTTP-A-n1_Ru	-732.1138227	23.53
59	118_closoTTP-A-f4_Ru	-732.1138194	23.54
60	023_hexagonal-b3- Ru-i250	-732.1129561	24.08
61	022_hexagonal-b3_Ru	-732.1129557	24.08
62	039_hexagonal-c10_Ru	-732.1127718	24.19
63	125_closoTTP-A-g4_Ru	-732.1127717	24.19
64	123_closoTTP-A-g2_Ru	-732.1127716	24.19
65	124_closoTTP-A-g3_Ru	-732.1127714	24.19
66	089_closoTTP-A-a1_Ru-i303	-732.1105304	25.60
67	136_closoTTP-A-i5_Ru	-732.1092912	26.38
68	163_closoTTP-A-n-2_Ru	-732.109207	26.43
69	001_B7Mo2-1F a Ru	-732.1091968	26.44
70	164_closoTTP-A-n3_Ru	-732.1088973	26.62
71	165_closoTTP-A-n-3_Ru	-732.1088973	26.62
72	162_closoTTP-A-n2_Ru	-732.1088972	26.62
73	073_hexagonal-e15_Ru	-732.1085994	26.81
74	072_hexagonal-e14_Ru	-732.1085988	26.81
75	114_closoTTP-A-f2_Ru	-732.1075742	27.45
76	011_B7Mo2-1F d- Ru	-732.106544	28.10
77	019_hexagonal-b1- Ru-i15	-732.1061835	28.33
78	018_hexagonal-b1_Ru	-732.1061833	28.33
79	021_hexagonal-b2- Ru	-732.1061825	28.33
80	043_hexagonal-c14_Ru	-732.1060239	28.43
81	091_closoTTP-A-a3_Ru	-732.1050664	29.03
82	161_closoTTP-A-n-1_Ru	-732.1049452	29.10
83	006_B7Mo2-1F b3_Ru	-732.1044089	29.44
84	003_B7Mo2-1F b1_Ru	-732.1044089	29.44
85	002_B7Mo2-1F b1- Ru	-732.1044085	29.44
86	063_hexagonal-e05_Ru	-732.1037759	29.84
87	067_hexagonal-e09_Ru-i24	-732.1037758	29.84
88	175_closoTTP-A-p1_Ru-i122	-732.1027152	30.50
89	041_hexagonal-c12_Ru	-732.1024707	30.66
90	122_closoTTP-A-g1_Ru	-732.1024706	30.66
91	185_closoTTP-B-h_Ru	-732.1017644	31.10
92	031_hexagonal-c02_Ru	-732.1005897	31.84
93	126_closoTTP-A-g5_Ru	-732.100589	31.84

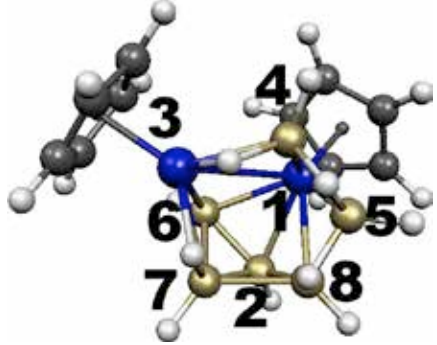
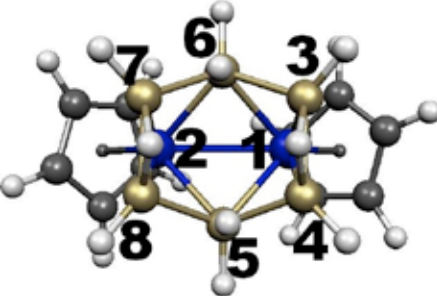
94	170_closoTTP-A-o1_Ru	-732.0999379	32.25
95	111_closoTTP-A-e5_Ru	-732.0999377	32.25
96	037_hexagonal-c08_Ru	-732.0994654	32.54
97	035_hexagonal-c06_Ru	-732.0994647	32.54
98	036_hexagonal-c07_Ru	-732.0994646	32.54
99	032_hexagonal-c03_Ru	-732.0985359	33.13
100	033_hexagonal-c04_Ru	-732.0985359	33.13
101	106_closoTTP-A-d5_Ru	-732.0983599	33.24
102	147_closoTTP-A-l1_Ru	-732.0982162	33.33
103	059_hexagonal-e01_Ru	-732.0982156	33.33
104	008_B7Mo2-1F_c_Ru	-732.0981151	33.39
105	009_B7Mo2-1F_c-_Ru	-732.098115	33.39
106	157_closoTTP-A-m1_Ru-i106	-732.0975111	33.77
107	157_closoTTP-A-m1_Ru-i33	-732.097511	33.77
108	158_closoTTP-A-m2_Ru	-732.0975109	33.77
109	107_closoTTP-A-e1_Ru	-732.0975101	33.77
110	086_hexagonal-f13_Ru	-732.0970595	34.05
111	119_closoTTP-A-f-4_Ru	-732.0970245	34.07
112	076_hexagonal-f03_Ru	-732.0963431	34.50
113	099_closoTTP-A-c3_Ru	-732.0963428	34.50
114	087_hexagonal-f14_Ru	-732.0963428	34.50
115	040_hexagonal-c11_Ru	-732.096204	34.59
116	074_hexagonal-f01_Ru	-732.0958109	34.84
117	085_hexagonal-f12_Ru	-732.0958106	34.84
118	082_hexagonal-f09_Ru	-732.0958104	34.84
119	075_hexagonal-f02_Ru	-732.0958103	34.84
120	042_hexagonal-c13_Ru	-732.0955116	35.02
121	100_closoTTP-A-c4_Ru	-732.0954721	35.05
122	101_closoTTP-A-c5_Ru	-732.0954717	35.05
123	081_hexagonal-f08_Ru	-732.0952177	35.21
124	084_hexagonal-f11_Ru	-732.0952162	35.21
125	095_closoTTP-A-b4	-732.095066	35.30
126	155_closoTTP-A-l5_Ru	-732.0923619	37.00
127	024_hexagonal-b4_Ru	-732.091744	37.39
128	171_closoTTP-A-o2_Ru	-732.0915002	37.54
129	090_closoTTP-A-a2_Ru	-732.0910592	37.82
130	131_closoTTP-A-h5_Ru	-732.0906426	38.08
131	130_closoTTP-A-h4_Ru	-732.090583	38.12
132	049_hexagonal-d06_Ru	-732.090554	38.13
133	069_hexagonal-e11_Ru	-732.0904277	38.21
134	068_hexagonal-e10_Ru	-732.0904258	38.22
135	044_hexagonal-d01_Ru	-732.0886775	39.31
136	012_hexagonal-a1_Ru	-732.0886327	39.34
137	141_closoTTP-A-j5-Ru	-732.0886327	39.34
138	140_closoTTP-A-j4_Ru	-732.0886325	39.34
139	139_closoTTP-A-j3_Ru	-732.0886315	39.34
140	045_hexagonal-d02_Ru	-732.0868817	40.44
141	046_hexagonal-d03_Ru	-732.0868815	40.44

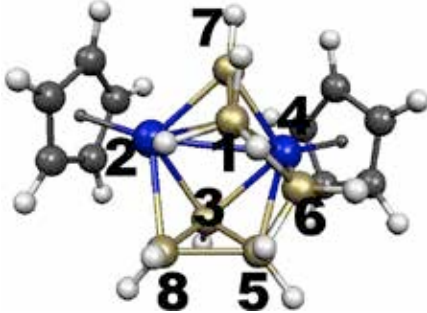
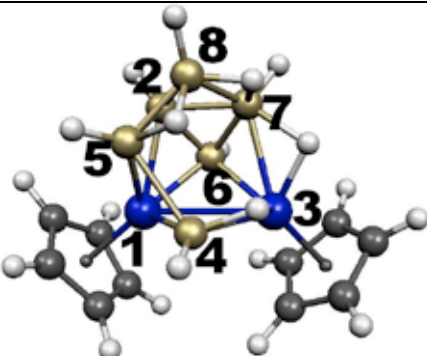
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143	038_hexagonal-c09_Ru	-732.0857802	41.13
144	050_hexagonal-d07_Ru	-732.0855109	41.30
145	053_hexagonal-d10_Ru	-732.0855109	41.30
146	129_closoTTP-A-h3_Ru	-732.0855107	41.30
147	048_hexagonal-d05_Ru	-732.0840755	42.20
148	030_hexagonal-c01_Ru	-732.0838117	42.37
149	094_closoTTP-A-b3_Ru	-732.082153	43.41
150	034_hexagonal-c05_Ru	-732.0821529	43.41
151	079_hexagonal-f06_Ru	-732.0809017	44.19
152	080_hexagonal-f07_Ru	-732.0809017	44.19
153	104_closoTTP-A-d3_Ru	-732.0800089	44.75
154	103_closoTTP-A-d2_Ru	-732.0800064	44.75
155	173_closoTTP-A-o4_Ru	-732.0797131	44.94
156	108_closoTTP-A-e2_Ru	-732.0797129	44.94
157	132_closoTTP-A-i1_Ru	-732.0761062	47.20
158	058_hexagonal-d15_Ru	-732.0761062	47.20
159	055_hexagonal-d12_Ru	-732.0752864	47.72
160	102_closoTTP-A-d1_Ru	-732.0746469	48.12
161	105_closoTTP-A-d4_Ru	-732.0724372	49.50
162	088_hexagonal-f15_Ru	-732.0717169	49.96
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164	133_closoTTP-A-i2_Ru	-732.0701578	50.93
165	174_closoTTP-A-o5_Ru	-732.0651864	54.05
166	054_hexagonal-d11_Ru	-732.0646613	54.38
167	056_hexagonal-d13_Ru	-732.0643285	54.59
168	060_hexagonal-e02_Ru	-732.0626744	55.63
169	172_closoTTP-A-o3_Ru	-732.0625751	55.69
170	016_hexagonal-a5_Ru	-732.0603152	57.11
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172	047_hexagonal-d04_Ru	-732.0592971	57.75
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175	096_closoTTP-A-b5_Ru	-732.0588598	58.02
176	092_closoTTP-A-b1_Ru	-732.0588585	58.02
177	078_hexagonal-f05_Ru	-732.0551933	60.32
178	098_closoTTP-A-c2_Ru	-732.0507802	63.09
179	097_closoTTP-A-c1_Ru	-732.0495968	63.84
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182	176_closoTTP-A-p2_Ru	-732.0462134	65.96
183	029_hexagonal-b6- Ru-i43	-732.036137	72.28
184	182_closoTTP-B-e_Ru	-732.0336608	73.84
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186	005_B7Mo2-1F_b2- Ru	-732.0051119	91.75

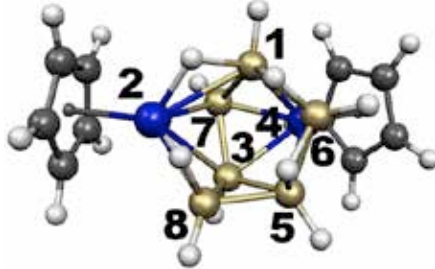
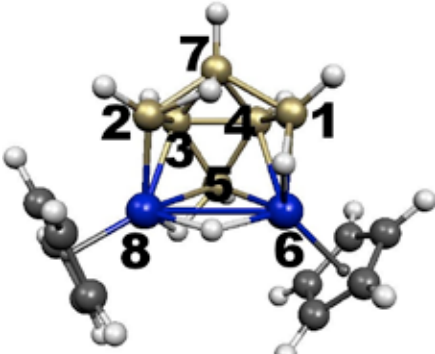
Table 7A. Distance table for the lowest-lying $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

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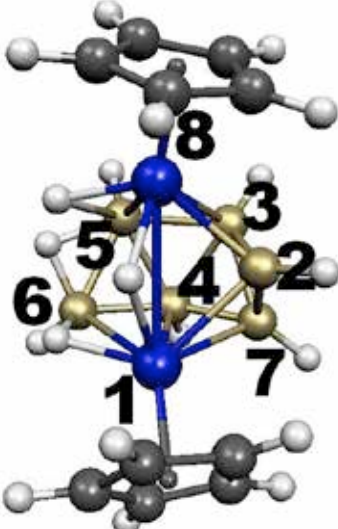
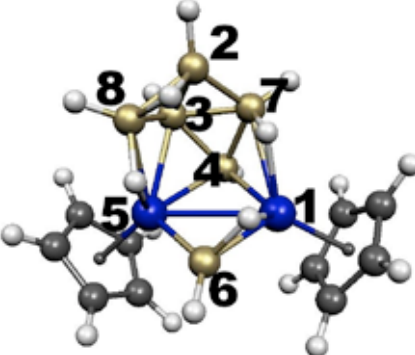
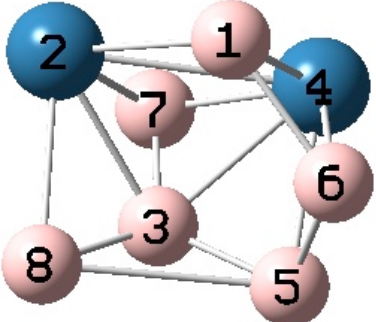
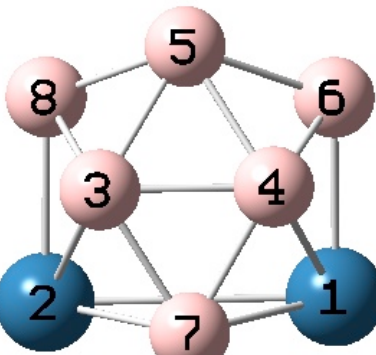
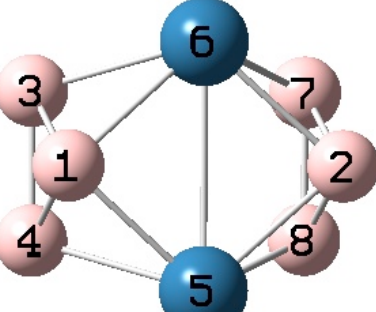
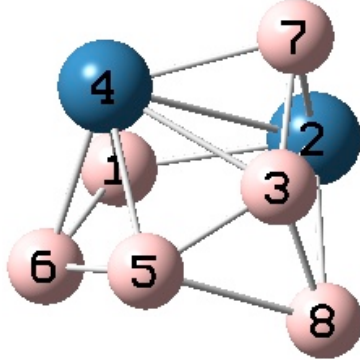
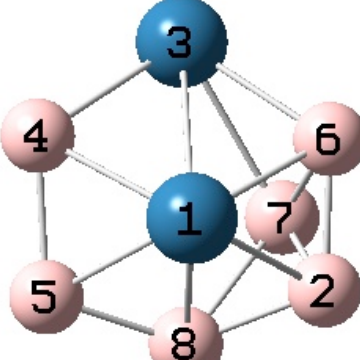
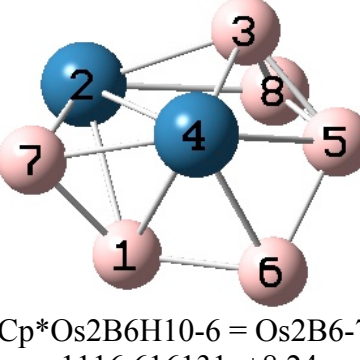
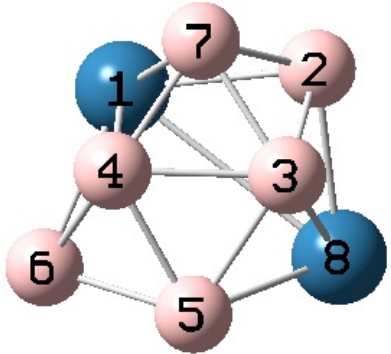
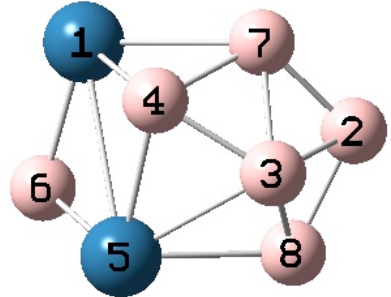
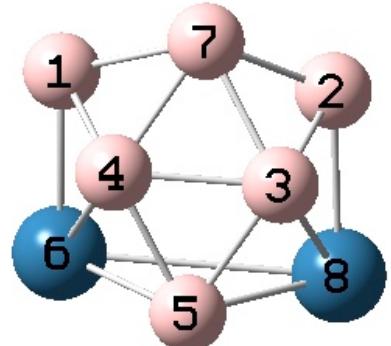
	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.258288</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.939495</td><td>1.755394</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.297124</td><td>2.731782</td><td>1.855972</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.016625</td><td>3.030906</td><td>1.851826</td><td>1.813219</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.330038</td><td>3.612330</td><td>3.004386</td><td>1.682381</td><td>1.790427</td></tr><tr><td>7 B</td><td>2.217266</td><td>1.693913</td><td>1.715399</td><td>1.675130</td><td>2.932096</td></tr><tr><td>8 Os</td><td>2.930923</td><td>2.133823</td><td>2.240082</td><td>3.231369</td><td>2.232539</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td></tr><tr><td>7 B</td><td>3.100671</td><td>0.000000</td><td></td></tr><tr><td>8 Os</td><td>3.271954</td><td>3.280153</td><td>0.000000</td></tr></table> Os1-H- Os8 Os1-H 1.89 Os8-H 1.74 Os1-H-B6 Os1-H 1.74 B6-H 1.36 Os8-H-B5 Os8-H 1.62 B5-H 2.1 B5-H-B6 B5-H 1.38 B6-H 1.26		1	2	3	4	5	1 Os	0.000000					2 B	2.258288	0.000000				3 B	2.939495	1.755394	0.000000			4 B	2.297124	2.731782	1.855972	0.000000		5 B	3.016625	3.030906	1.851826	1.813219	0.000000	6 B	2.330038	3.612330	3.004386	1.682381	1.790427	7 B	2.217266	1.693913	1.715399	1.675130	2.932096	8 Os	2.930923	2.133823	2.240082	3.231369	2.232539		6	7	8	6 B	0.000000			7 B	3.100671	0.000000		8 Os	3.271954	3.280153	0.000000
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Table 7B. Distance table for the lowest-lying Cp*₂Os₂B₆H₁₀ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Os2B6H10-1 = Os2B6-1 -1116.629257 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Os</td><td>2.282165</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.902032</td><td>2.198529</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Os</td><td>2.152915</td><td>2.816634</td><td>2.225773</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.926387</td><td>3.436652</td><td>1.671555</td><td>2.180296</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.824007</td><td>3.489806</td><td>2.799645</td><td>2.177457</td><td>1.777036</td></tr><tr><td>7 B</td><td>3.332797</td><td>2.142407</td><td>1.654949</td><td>2.154077</td><td>2.969400</td></tr><tr><td>8 B</td><td>3.166555</td><td>2.267520</td><td>1.713770</td><td>3.570765</td><td>2.606317</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.781683</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.271993</td><td>3.026009</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 Os	2.282165	0.000000				3 B	2.902032	2.198529	0.000000			4 Os	2.152915	2.816634	2.225773	0.000000		5 B	2.926387	3.436652	1.671555	2.180296	0.000000	6 B	1.824007	3.489806	2.799645	2.177457	1.777036	7 B	3.332797	2.142407	1.654949	2.154077	2.969400	8 B	3.166555	2.267520	1.713770	3.570765	2.606317		6	7	8			6 B	0.000000					7 B	3.781683	0.000000				8 B	3.271993	3.026009	0.000000		
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 Cp*Os2B6H10-2 = Os2B6-2 -1116.626691 +1.6	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Os</td><td>2.973644</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.247480</td><td>2.272478</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.278846</td><td>3.227186</td><td>1.782928</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.334897</td><td>3.333115</td><td>1.754251</td><td>1.745793</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.115275</td><td>3.670452</td><td>2.898971</td><td>1.723648</td><td>1.858158</td></tr><tr><td>7 B</td><td>2.155643</td><td>2.142116</td><td>1.767710</td><td>1.761264</td><td>2.931095</td></tr><tr><td>8 B</td><td>3.639886</td><td>2.168800</td><td>1.739760</td><td>2.848244</td><td>1.789385</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.983970</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.950500</td><td>2.995267</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Os	0.000000					2 Os	2.973644	0.000000				3 B	3.247480	2.272478	0.000000			4 B	2.278846	3.227186	1.782928	0.000000		5 B	3.334897	3.333115	1.754251	1.745793	0.000000	6 B	2.115275	3.670452	2.898971	1.723648	1.858158	7 B	2.155643	2.142116	1.767710	1.761264	2.931095	8 B	3.639886	2.168800	1.739760	2.848244	1.789385		6	7	8			6 B	0.000000					7 B	2.983970	0.000000				8 B	2.950500	2.995267	0.000000		
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 Cp*Os2B6H10-11 = Os2B6-8 -1116.601731 +17.3	<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.236630</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Os</td><td>2.871889</td><td>3.241281</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.019997</td><td>3.172234</td><td>2.208094</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.078404</td><td>1.768649</td><td>3.469045</td><td>2.255248</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.088883</td><td>1.764805</td><td>2.176916</td><td>3.041157</td><td>2.939854</td></tr><tr><td>7 B</td><td>3.222288</td><td>1.819991</td><td>2.332810</td><td>3.283782</td><td>2.817827</td></tr><tr><td>8 B</td><td>3.330464</td><td>1.741887</td><td>3.482798</td><td>3.222445</td><td>1.758013</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.831276</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.016086</td><td>1.849420</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Os	0.000000					2 B	2.236630	0.000000				3 Os	2.871889	3.241281	0.000000			4 B	2.019997	3.172234	2.208094	0.000000		5 B	2.078404	1.768649	3.469045	2.255248	0.000000	6 B	2.088883	1.764805	2.176916	3.041157	2.939854	7 B	3.222288	1.819991	2.332810	3.283782	2.817827	8 B	3.330464	1.741887	3.482798	3.222445	1.758013		6	7	8			6 B	0.000000					7 B	1.831276	0.000000				8 B	3.016086	1.849420	0.000000		
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 Cp*Os2B6H10-12 = Os2B6-6 -1116.597476 +19.9	<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Os</td><td>2.767851</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.056141</td><td>3.481087</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.065183</td><td>3.482806</td><td>1.784829</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.176971</td><td>2.187023</td><td>2.955228</td><td>1.858689</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.186471</td><td>2.179926</td><td>1.857911</td><td>2.954427</td><td>2.957209</td></tr><tr><td>7 B</td><td>3.480558</td><td>2.062424</td><td>2.845419</td><td>3.346529</td><td>2.952817</td></tr><tr><td>8 B</td><td>3.479916</td><td>2.053957</td><td>3.370304</td><td>2.846349</td><td>1.859810</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.859117</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.955503</td><td>1.782023</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Os	0.000000					2 Os	2.767851	0.000000				3 B	2.056141	3.481087	0.000000			4 B	2.065183	3.482806	1.784829	0.000000		5 B	2.176971	2.187023	2.955228	1.858689	0.000000	6 B	2.186471	2.179926	1.857911	2.954427	2.957209	7 B	3.480558	2.062424	2.845419	3.346529	2.952817	8 B	3.479916	2.053957	3.370304	2.846349	1.859810		6	7	8			6 B	0.000000					7 B	1.859117	0.000000				8 B	2.955503	1.782023	0.000000		
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8 B	2.955503	1.782023	0.000000																																																																												

Table 7C. Energy ranking for all of the $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	159_closoTTP-A-m3_Os	-723.74232620	0.00
2	025_hexagonal-b4-_Os	-723.73879000	2.22
3	178_closoTTP-B-a_Os-i34	-723.73878669	2.22
4	148_closoTTP-A-l-1_Os	-723.73836408	2.49
5	027_hexagonal-b5-_Os	-723.73745969	3.05
6	023_hexagonal-b3-_Os	-723.73738501	3.10
7	134_closoTTP-A-i3_Os	-723.73065561	7.32
8	180_closoTTP-B-c_Os	-723.73065512	7.32
9	135_closoTTP-A-i4_Os	-723.73065479	7.32
10	136_closoTTP-A-i5_Os	-723.73029685	7.55
11	051_hexagonal-d08_Os	-723.72924739	8.21
12	014_hexagonal-a3_Os	-723.72916144	8.26
13	138_closoTTP-A-j2_Os	-723.72915677	8.26
14	137_closoTTP-A-j1_Os	-723.72915676	8.26
15	156_closoTTP-A-l-5_Os	-723.72714814	9.52
16	015_hexagonal-a4_Os-i39	-723.72713071	9.54
17	152_closoTTP-A-l-3_Os	-723.72706570	9.58
18	113_closoTTP-A-f-1_Os	-723.72652726	9.91
19	149_closoTTP-A-l2_Os	-723.72179211	12.89
20	151_closoTTP-A-l3_Os	-723.72179210	12.89
21	177_closoTTP-A-p3_Os	-723.72134089	13.17
22	184_closoTTP-B-g_Os	-723.72112123	13.31
23	145_closoTTP-A-k4_Os	-723.72112109	13.31
24	142_closoTTP-A-k1_Os	-723.72112086	13.31
25	143_closoTTP-A-k2_Os	-723.72112071	13.31
26	153_closoTTP-A-l4_Os	-723.72112070	13.31
27	061_hexagonal-e03_Os	-723.72112006	13.31
28	181_closoTTP-B-d_Os	-723.72110032	13.32
29	090_closoTTP-A-a2_Os	-723.72109766	13.32
30	154_closoTTP-A-l-4_Os	-723.72073829	13.55
31	150_closoTTP-A-l-2_Os	-723.72039147	13.76
32	146_closoTTP-A-k5_Os	-723.71903904	14.61
33	066_hexagonal-e08_Os	-723.71764035	15.49
34	144_closoTTP-A-k3_Os	-723.71764027	15.49
35	062_hexagonal-e04_Os	-723.71764018	15.49
36	065_hexagonal-e07_Os	-723.71764016	15.49
37	064_hexagonal-e06_Os	-723.71763988	15.49
38	089_closoTTP-A-a1_Os-i147	-723.71534160	16.93
39	089_closoTTP-A-a1_Os-i198	-723.71534049	16.93
40	026_hexagonal-b5_Os	-723.71522243	17.01
41	035_hexagonal-c06_Os	-723.71376357	17.92

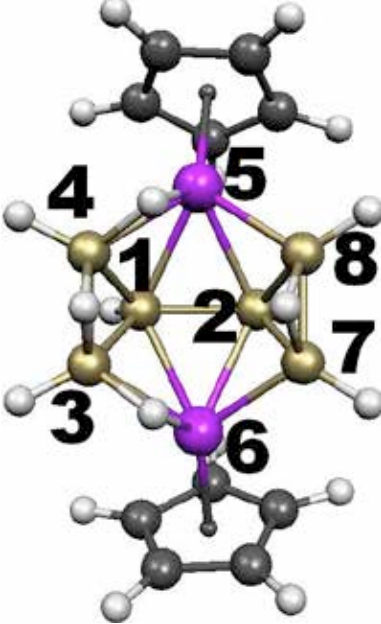
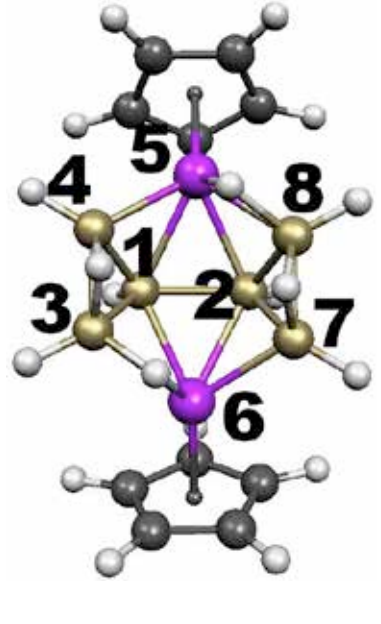
42	028_hexagonal-b6_Os	-723.71359531	18.03
43	020_hexagonal-b2_Os	-723.71359458	18.03
44	160_closoTTP-A-n1_Os	-723.71094897	19.69
45	118_closoTTP-A-f4_Os	-723.71094824	19.69
46	116_closoTTP-A-f3_Os	-723.71086067	19.74
47	112_closoTTP-A-f1_Os	-723.70961951	20.52
48	091_closoTTP-A-a3_Os	-723.70920489	20.78
49	123_closoTTP-A-g2_Os	-723.70917970	20.80
50	124_closoTTP-A-g3_Os	-723.70917927	20.80
51	125_closoTTP-A-g4_Os	-723.70917915	20.80
52	039_hexagonal-c10_Os	-723.70917883	20.80
53	166_closoTTP-A-n4_Os	-723.70890159	20.97
54	167_closoTTP-A-n-4_Os	-723.70890125	20.97
55	114_closoTTP-A-f2_Os	-723.70873459	21.08
56	187_closoTTP-B-j_Os-i326	-723.70799787	21.54
57	169_closoTTP-A-n-5_Os	-723.70799663	21.54
58	187_closoTTP-B-j_Os-i20	-723.70799643	21.54
59	168_closoTTP-A-n5_Os	-723.70764872	21.76
60	120_closoTTP-A-f5_Os	-723.70656039	22.44
61	186_closoTTP-B-i_Os	-723.70640002	22.54
62	022_hexagonal-b3_Os	-723.70606920	22.75
63	073_hexagonal-e15_Os	-723.70558939	23.05
64	043_hexagonal-c14_Os	-723.70547829	23.12
65	033_hexagonal-c04_Os	-723.70547828	23.12
66	032_hexagonal-c03_Os	-723.70547718	23.12
67	122_closoTTP-A-g1_Os	-723.70352169	24.35
68	126_closoTTP-A-g5_Os	-723.70352114	24.35
69	031_hexagonal-c02_Os	-723.70352105	24.35
70	041_hexagonal-c12_Os	-723.70352066	24.35
71	063_hexagonal-e05_Os	-723.70258172	24.94
72	176_closoTTP-A-p2_Os	-723.70177779	25.44
73	164_closoTTP-A-n3_Os	-723.69972312	26.73
74	162_closoTTP-A-n2_Os	-723.69972116	26.74
75	155_closoTTP-A-l5_Os	-723.69858944	27.45
76	006_B7Mo2-1F_b3_Os	-723.69814021	27.73
77	003_B7Mo2-1F_b1_Os	-723.69814019	27.73
78	106_closoTTP-A-d5_Os	-723.69785092	27.91
79	009_B7Mo2-1F_c-_Os	-723.69656742	28.71
80	185_closoTTP-B-h_Os	-723.69650928	28.75
81	037_hexagonal-c08_Os	-723.69568333	29.27
82	059_hexagonal-e01_Os	-723.69528457	29.52
83	147_closoTTP-A-l1_Os	-723.69528454	29.52
84	161_closoTTP-A-n-1_Os	-723.69371788	30.50

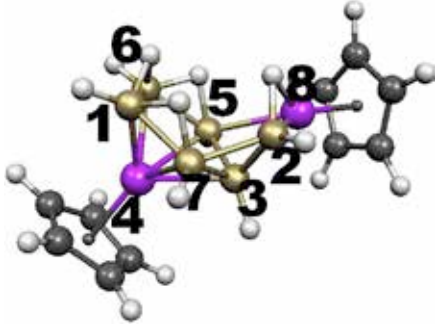
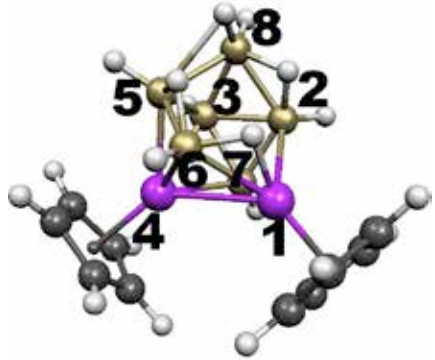
85	163_closoTTP-A-n-2_Os	-723.69371773	30.50
86	165_closoTTP-A-n-3_Os	-723.69371767	30.50
87	158_closoTTP-A-m2_Os	-723.69367325	30.53
88	157_closoTTP-A-m1_Os-i149	-723.69367324	30.53
89	157_closoTTP-A-m1_Os-i37	-723.69367293	30.53
90	040_hexagonal-c11_Os	-723.69302770	30.94
91	018_hexagonal-b1_Os	-723.69291182	31.01
92	019_hexagonal-b1-_Os-23	-723.69291180	31.01
93	021_hexagonal-b2-_Os	-723.69291148	31.01
94	072_hexagonal-e14_Os	-723.69272986	31.12
95	082_hexagonal-f09_Os	-723.69271532	31.13
96	085_hexagonal-f12_Os	-723.69271525	31.13
97	075_hexagonal-f02_Os	-723.69271516	31.13
98	074_hexagonal-f01_Os	-723.69271488	31.13
99	115_closoTTP-A-f-2_Os	-723.69256935	31.22
100	076_hexagonal-f03_Os	-723.69209803	31.52
101	099_closoTTP-A-c3_Os	-723.69209783	31.52
102	087_hexagonal-f14_Os	-723.69209773	31.52
103	048_hexagonal-d05_Os	-723.69203836	31.56
104	047_hexagonal-d04_Os	-723.69203819	31.56
105	069_hexagonal-e11_Os	-723.69163842	31.81
106	068_hexagonal-e10_Os	-723.69163831	31.81
107	044_hexagonal-d01_Os	-723.69097568	32.22
108	045_hexagonal-d02_Os	-723.69096151	32.23
109	111_closoTTP-A-e5_Os	-723.69052909	32.50
110	058_hexagonal-d15_Os	-723.69048967	32.53
111	034_hexagonal-c05_Os	-723.69033461	32.63
112	030_hexagonal-c01_Os	-723.69017196	32.73
113	038_hexagonal-c09_Os	-723.69017186	32.73
114	008_B7Mo2-1F c_Os	-723.69002532	32.82
115	104_closoTTP-A-d3_Os	-723.68989300	32.90
116	119_closoTTP-A-f-4_Os	-723.68980526	32.96
117	042_hexagonal-c13_Os	-723.68880924	33.58
118	052_hexagonal-d09_Os	-723.68791922	34.14
119	002_B7Mo2-1F b1-_Os	-723.68770499	34.28
120	071_hexagonal-e13_Os	-723.68743757	34.44
121	140_closoTTP-A-j4_Os	-723.68710795	34.65
122	012_hexagonal-a1_Os	-723.68710790	34.65
123	141_closoTTP-A-j5-Os	-723.68710733	34.65
124	139_closoTTP-A-j3_Os	-723.68710703	34.65
125	109_closoTTP-A-e3_Os	-723.68624737	35.19
126	086_hexagonal-f13_Os	-723.68623046	35.20
127	081_hexagonal-f08_Os	-723.68589463	35.41

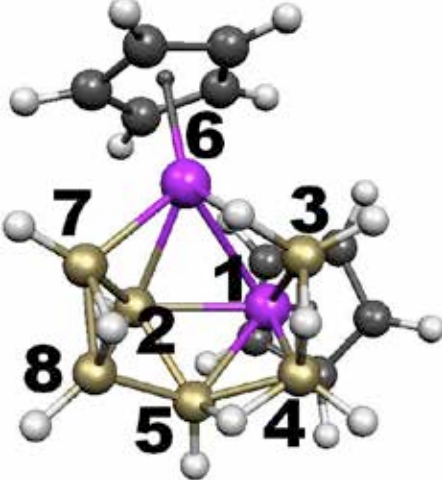
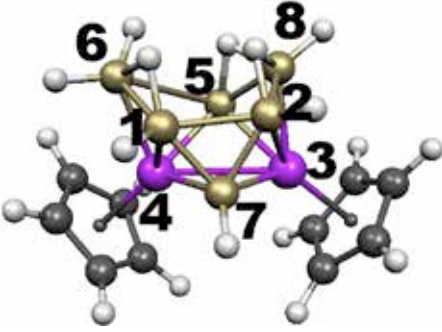
128	084_hexagonal-f11_Os	-723.68589404	35.41
129	121_closoTTP-A-f-5_Os	-723.68460247	36.22
130	011_B7Mo2-1F_d_Os	-723.68417783	36.49
131	183_closoTTP-B-f_Os	-723.68415679	36.50
132	024_hexagonal-b4_Os	-723.68353048	36.89
133	129_closoTTP-A-h3_Os	-723.68352750	36.90
134	050_hexagonal-d07_Os	-723.68335068	37.01
135	053_hexagonal-d10_Os	-723.68334590	37.01
136	108_closoTTP-A-e2_Os	-723.68265887	37.44
137	107_closoTTP-A-e1_Os	-723.68265753	37.44
138	173_closoTTP-A-o4_Os	-723.68265718	37.44
139	088_hexagonal-f15_Os	-723.68255830	37.50
140	170_closoTTP-A-o1_Os	-723.68230292	37.67
141	174_closoTTP-A-o5_Os	-723.68230139	37.67
142	171_closoTTP-A-o2_Os	-723.68118087	38.37
143	131_closoTTP-A-h5_Os	-723.67986201	39.20
144	101_closoTTP-A-c5_Os	-723.67836663	40.14
145	100_closoTTP-A-c4_Os	-723.67836646	40.14
146	055_hexagonal-d12_Os	-723.67817487	40.26
147	132_closoTTP-A-i1_Os	-723.67683575	41.10
148	078_hexagonal-f05_Os	-723.67584531	41.72
149	077_hexagonal-f04_Os	-723.67584169	41.72
150	049_hexagonal-d06_Os	-723.67559702	41.87
151	079_hexagonal-f06_Os	-723.67461797	42.49
152	080_hexagonal-f07_Os	-723.67461783	42.49
153	103_closoTTP-A-d2_Os	-723.67320788	43.37
154	117_closoTTP-A-f-3_Os	-723.67283498	43.61
155	130_closoTTP-A-h4_Os	-723.66967491	45.59
156	067_hexagonal-e09_Os	-723.66964387	45.61
157	105_closoTTP-A-d4_Os	-723.66910731	45.95
158	083_hexagonal-f10_Os	-723.66863825	46.24
159	110_closoTTP-A-e4_Os	-723.66863808	46.24
160	095_closoTTP-A-b4_Os	-723.66819930	46.52
161	133_closoTTP-A-i2_Os	-723.66724553	47.11
162	010_B7Mo2-1F_d_Os -i147-i279	-723.69656708	28.71
163	013_hexagonal-a2_Os	-723.66407121	49.11
164	016_hexagonal-a5_Os	-723.66407107	49.11
165	060_hexagonal-e02_Os	-723.66310097	49.71
166	175_closoTTP-A-p1_Os	-723.66140010	50.78
167	001_B7Mo2-1F_a_Os	-723.66062011	51.27
168	092_closoTTP-A-b1_Os	-723.66004026	51.64
169	172_closoTTP-A-o3_Os	-723.66002451	51.65
170	179_closoTTP-B-b_Os	-723.65997151	51.68

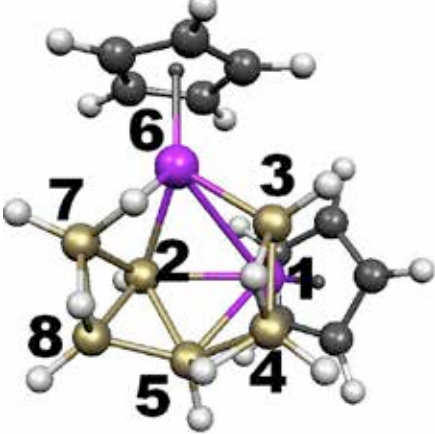
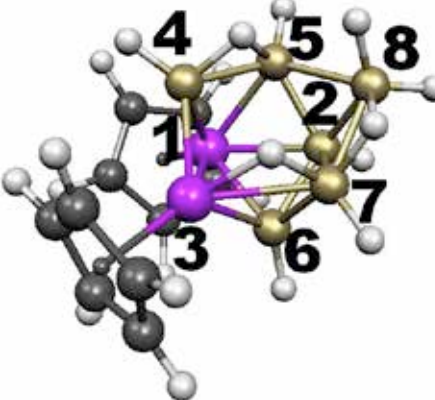
171	096_closoTTP-A-b5_Os	-723.65997144	51.68
172	017_hexagonal-a6_Os-i84-i42	-723.65990484	51.72
173	017_hexagonal-a6_Os-i84-i55	-723.65990468	51.72
174	054_hexagonal-d11_Os	-723.65929442	52.10
175	056_hexagonal-d13_Os	-723.65929438	52.10
176	093_closoTTP-A-b2_Os	-723.65916635	52.18
177	128_closoTTP-A-h2_Os	-723.65871416	52.47
178	127_closoTTP-A-h1_Os	-723.65871037	52.47
179	070_hexagonal-e12_Os	-723.65743149	53.27
180	046_hexagonal-d03_Os	-723.65093415	57.35
181	057_hexagonal-d14_Os	-723.65093410	57.35
182	098_closoTTP-A-c2_Os	-723.64792503	59.24
183	007_B7Mo2-1F_b3-_Os	-723.64680994	59.94
184	097_closoTTP-A-c1_Os	-723.64130169	63.39
185	102_closoTTP-A-d1_Os	-723.63748289	65.79
186	029_hexagonal-b6-_Os-i31	-723.63421155	67.84
187	182_closoTTP-B-e_Os	-723.63142149	69.59
188	004_B7Mo2-1F_b2_Os	-723.61592394	79.32
189	017_hexagonal-a6_Os-i84	-723.60938141	83.42
190	005_B7Mo2-1F_b2-_Os	-723.60296928	87.45

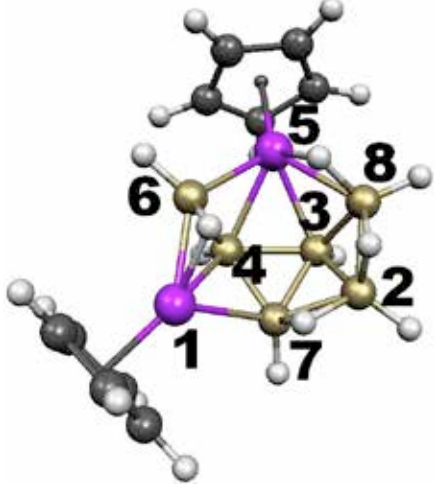
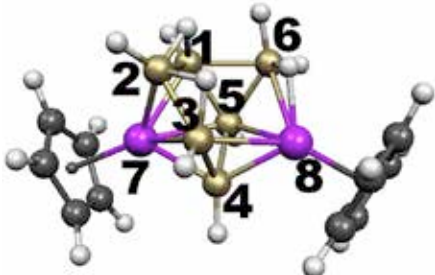
Table 8A. Distance table for the lowest-lying $\text{Cp}_2\text{Rh}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.868940</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.767888</td><td>3.059452</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.767888</td><td>3.059452</td><td>1.708480</td><td>0.000000</td><td></td></tr><tr><td>5 Rh</td><td>2.206133</td><td>2.204622</td><td>3.353910</td><td>2.157973</td><td>0.000000</td></tr><tr><td>6 Rh</td><td>2.206133</td><td>2.204622</td><td>2.157973</td><td>3.353910</td><td>3.858324</td></tr><tr><td>7 B</td><td>2.996899</td><td>1.736002</td><td>3.264660</td><td>3.673584</td><td>3.299821</td></tr><tr><td>8 B</td><td>2.996899</td><td>1.736002</td><td>3.673584</td><td>3.264660</td><td>2.116942</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.116942</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.299821</td><td>1.660664</td><td>0.000000</td><td></td><td></td></tr></table> Rh5-H-B4 Rh5-H 1.68 B4-H 1.39 Rh6-H-B3 Rh6-H 1.68 B3-H 1.39 B3-H-B4 B3-H 1.33 B4-H 1.33 B7-H-B8 B7-H 1.34 B8-H 1.34		1	2	3	4	5	1 B	0.000000					2 B	1.868940	0.000000				3 B	1.767888	3.059452	0.000000			4 B	1.767888	3.059452	1.708480	0.000000		5 Rh	2.206133	2.204622	3.353910	2.157973	0.000000	6 Rh	2.206133	2.204622	2.157973	3.353910	3.858324	7 B	2.996899	1.736002	3.264660	3.673584	3.299821	8 B	2.996899	1.736002	3.673584	3.264660	2.116942		6	7	8			6 Rh	0.000000					7 B	2.116942	0.000000				8 B	3.299821	1.660664	0.000000		
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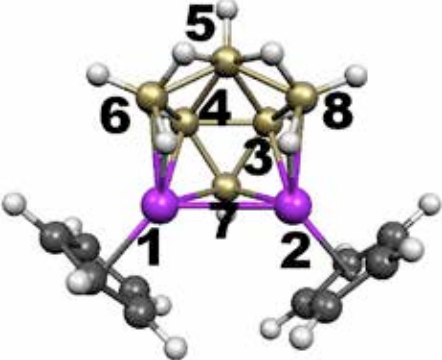
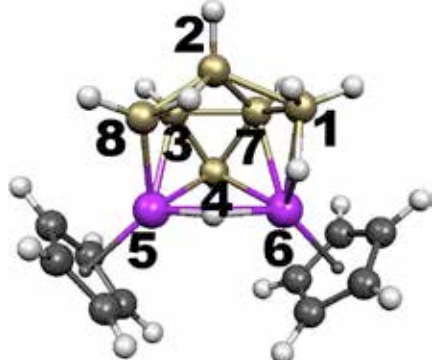
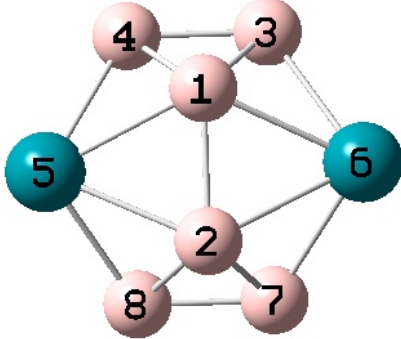
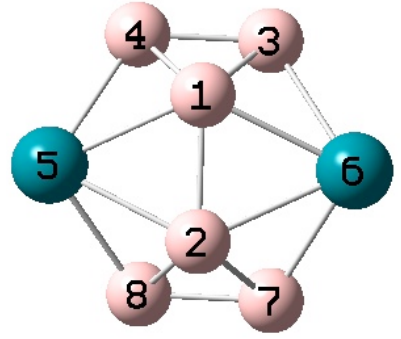
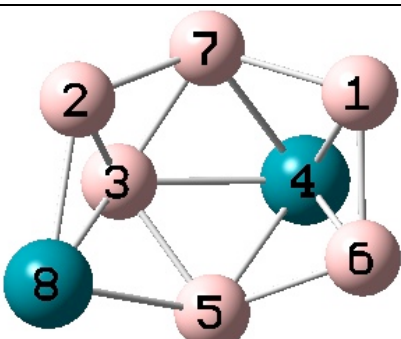
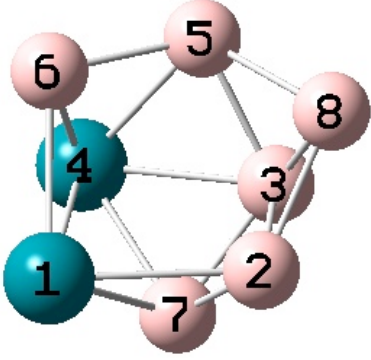
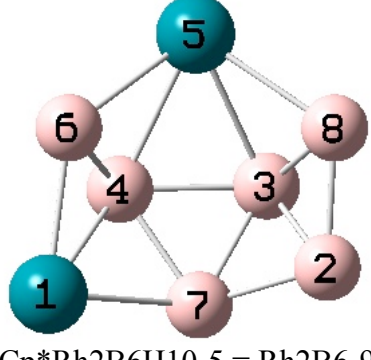
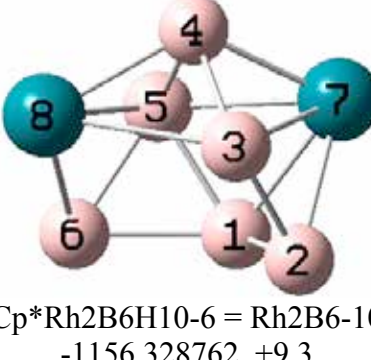
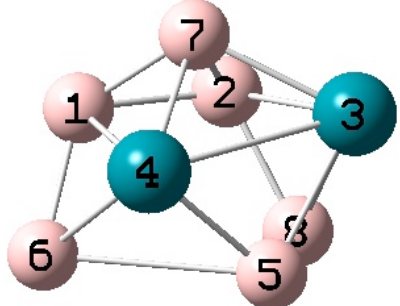
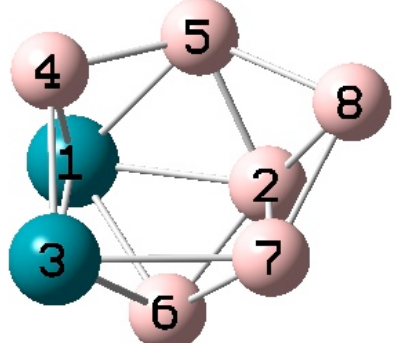
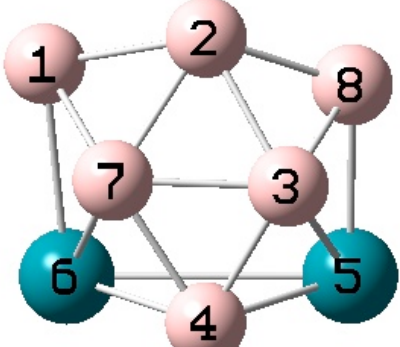
	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Rh</td><td>2.764718</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.176797</td><td>2.237030</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.237804</td><td>3.174273</td><td>1.836748</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.304432</td><td>3.306827</td><td>1.820616</td><td>1.825502</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.227610</td><td>3.666826</td><td>2.929214</td><td>1.724083</td><td>1.803636</td></tr><tr><td>7 B</td><td>2.119507</td><td>2.110114</td><td>1.728035</td><td>1.726745</td><td>2.945469</td></tr><tr><td>8 B</td><td>3.676484</td><td>2.239576</td><td>1.723980</td><td>2.940724</td><td>1.808974</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.033938</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.071629</td><td>3.039884</td><td>0.000000</td><td></td><td></td></tr></table> Rh1-H-B6 Rh1-H 1.72 B6-H 1.34 Rh2-H-B8 Rh2-H 1.72 B8-H 1.34 B5-H-B6 B5-H 1.47 B6-H 1.24 B5-H-B8 B5-H 1.50 B8-H 1.24		1	2	3	4	5	1 Rh	0.000000					2 Rh	2.764718	0.000000				3 B	3.176797	2.237030	0.000000			4 B	2.237804	3.174273	1.836748	0.000000		5 B	3.304432	3.306827	1.820616	1.825502	0.000000	6 B	2.227610	3.666826	2.929214	1.724083	1.803636	7 B	2.119507	2.110114	1.728035	1.726745	2.945469	8 B	3.676484	2.239576	1.723980	2.940724	1.808974		6	7	8			6 B	0.000000					7 B	3.033938	0.000000				8 B	3.071629	3.039884	0.000000		
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Table 8B. Distance table for the lowest-lying $\text{Cp}^*\text{Rh}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Rh2B6H10-1 = Rh2B6-1 -1156.343580 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.869143</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.769136</td><td>3.062263</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.769198</td><td>3.062247</td><td>1.718391</td><td>0.000000</td><td></td></tr><tr><td>5 Rh</td><td>2.209473</td><td>2.207641</td><td>3.366983</td><td>2.164359</td><td>0.000000</td></tr><tr><td>6 Rh</td><td>2.209455</td><td>2.207658</td><td>2.164306</td><td>3.366919</td><td>3.871075</td></tr><tr><td>7 B</td><td>3.002310</td><td>1.734253</td><td>3.278043</td><td>3.688650</td><td>3.312245</td></tr><tr><td>8 B</td><td>3.002316</td><td>1.734227</td><td>3.688779</td><td>3.277991</td><td>2.127307</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.127332</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.312268</td><td>1.665056</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.869143	0.000000				3 B	1.769136	3.062263	0.000000			4 B	1.769198	3.062247	1.718391	0.000000		5 Rh	2.209473	2.207641	3.366983	2.164359	0.000000	6 Rh	2.209455	2.207658	2.164306	3.366919	3.871075	7 B	3.002310	1.734253	3.278043	3.688650	3.312245	8 B	3.002316	1.734227	3.688779	3.277991	2.127307		6	7	8			6 Rh	0.000000					7 B	2.127332	0.000000				8 B	3.312268	1.665056	0.000000		
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 Cp*Rh2B6H10-2 = Rh2B6-2 -1156.341444 +1.3	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.860346</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.778344</td><td>3.039611</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.724926</td><td>3.024085</td><td>1.692014</td><td>0.000000</td><td></td></tr><tr><td>5 Rh</td><td>2.222061</td><td>2.198460</td><td>3.310097</td><td>2.113736</td><td>0.000000</td></tr><tr><td>6 Rh</td><td>2.198480</td><td>2.222039</td><td>2.171463</td><td>3.354487</td><td>3.867336</td></tr><tr><td>7 B</td><td>3.024070</td><td>1.724934</td><td>3.297187</td><td>3.774608</td><td>3.354409</td></tr><tr><td>8 B</td><td>3.039657</td><td>1.778349</td><td>3.622829</td><td>3.297291</td><td>2.171452</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><td></td><td></td></tr><tr><td>6 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.113731</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.310113</td><td>1.691955</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.860346	0.000000				3 B	1.778344	3.039611	0.000000			4 B	1.724926	3.024085	1.692014	0.000000		5 Rh	2.222061	2.198460	3.310097	2.113736	0.000000	6 Rh	2.198480	2.222039	2.171463	3.354487	3.867336	7 B	3.024070	1.724934	3.297187	3.774608	3.354409	8 B	3.039657	1.778349	3.622829	3.297291	2.171452		6	7	8			6 Rh	0.000000					7 B	2.113731	0.000000				8 B	3.310113	1.691955	0.000000		
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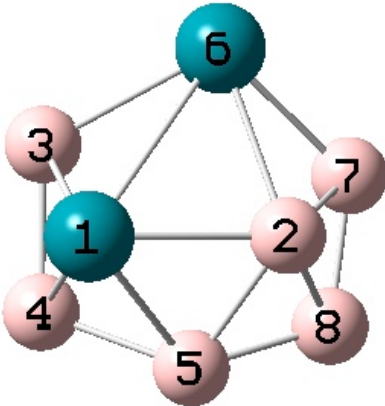
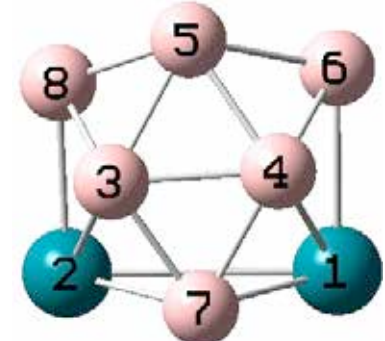
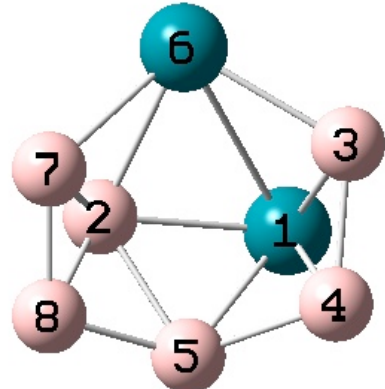
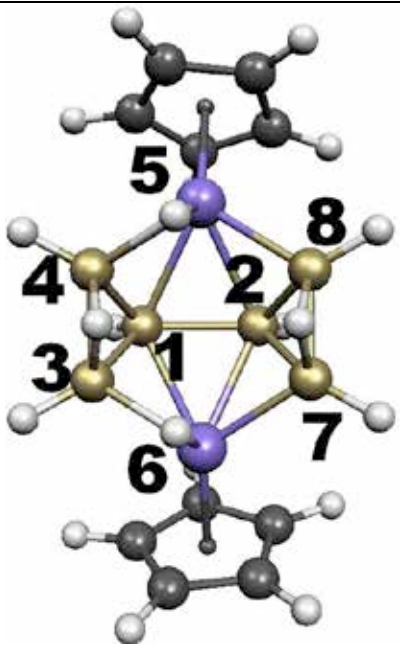
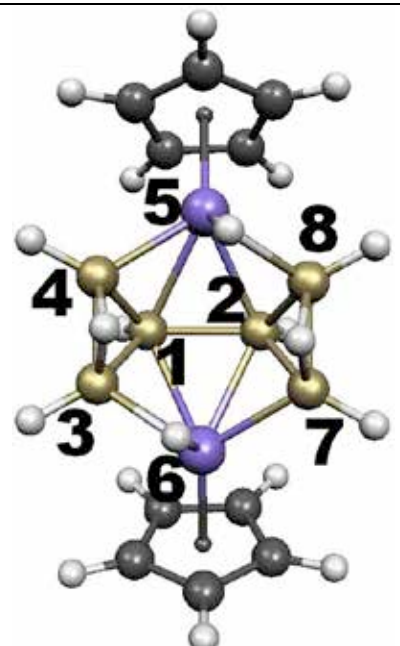
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 Cp*Rh2B6H10-11 = Rh2B6-11 -1156.319042 +15.4	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Rh</td><td>2.935693</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.236630</td><td>2.232884</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.220354</td><td>3.176422</td><td>1.818532</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.369593</td><td>3.292541</td><td>1.784096</td><td>1.748159</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.281484</td><td>3.740997</td><td>3.025124</td><td>1.780007</td><td>1.901870</td></tr><tr><td>7 B</td><td>2.097353</td><td>2.116991</td><td>1.740917</td><td>1.756879</td><td>2.922064</td></tr><tr><td>8 B</td><td>3.708174</td><td>2.185948</td><td>1.735565</td><td>2.836910</td><td>1.756328</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.108889</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.029978</td><td>3.000085</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Rh	0.000000					2 Rh	2.935693	0.000000				3 B	3.236630	2.232884	0.000000			4 B	2.220354	3.176422	1.818532	0.000000		5 B	3.369593	3.292541	1.784096	1.748159	0.000000	6 B	2.281484	3.740997	3.025124	1.780007	1.901870	7 B	2.097353	2.116991	1.740917	1.756879	2.922064	8 B	3.708174	2.185948	1.735565	2.836910	1.756328		6	7	8			6 B	0.000000					7 B	3.108889	0.000000				8 B	3.029978	3.000085	0.000000		
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 Cp*Rh2B6H10-12 = Rh2B6-7 -1156.317836 +16.2	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.220045</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.085845</td><td>3.022625</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.102979</td><td>2.996401</td><td>1.777004</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.181795</td><td>1.888809</td><td>2.965194</td><td>1.829139</td><td>0.000000</td></tr><tr><td>6 Rh</td><td>2.790874</td><td>2.225046</td><td>2.120824</td><td>3.313422</td><td>3.409862</td></tr><tr><td>7 B</td><td>3.617674</td><td>1.783121</td><td>3.391303</td><td>3.551510</td><td>2.794125</td></tr><tr><td>8 B</td><td>3.428225</td><td>1.721080</td><td>3.828653</td><td>3.186811</td><td>1.744423</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Rh</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.172403</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.344060</td><td>1.670138</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Rh	0.000000					2 B	2.220045	0.000000				3 B	2.085845	3.022625	0.000000			4 B	2.102979	2.996401	1.777004	0.000000		5 B	2.181795	1.888809	2.965194	1.829139	0.000000	6 Rh	2.790874	2.225046	2.120824	3.313422	3.409862	7 B	3.617674	1.783121	3.391303	3.551510	2.794125	8 B	3.428225	1.721080	3.828653	3.186811	1.744423		6	7	8			6 Rh	0.000000					7 B	2.172403	0.000000				8 B	3.344060	1.670138	0.000000		
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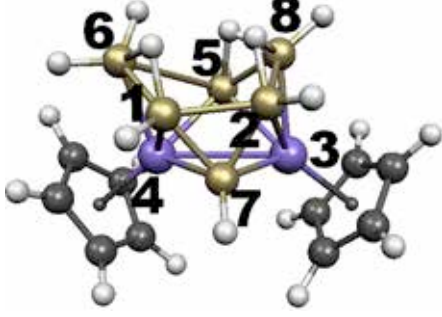
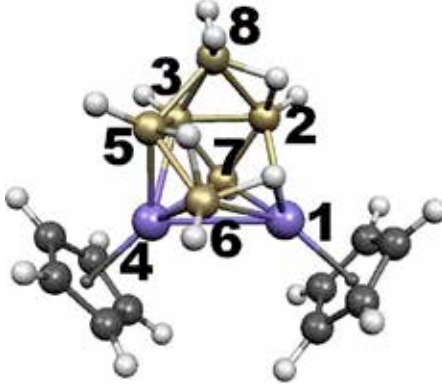
Table 8C. Energy ranking for all of the $\text{Cp}_2\text{Rh}_2\text{B}_6\text{H}_{10}$ optimized structures:

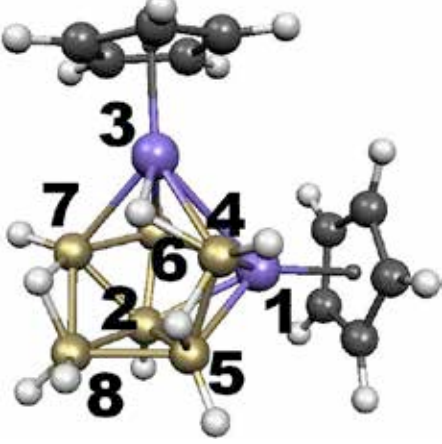
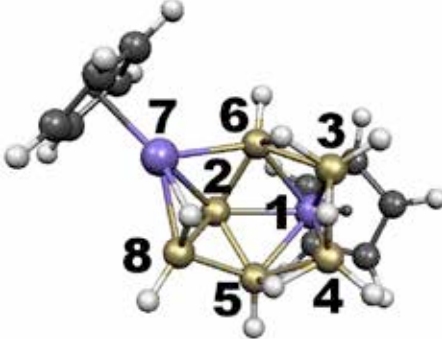
Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	025_hexagonal-b4-_Rh	-763.65783312	0.00
2	091_closoTTP-A-a3_Rh	-763.65783075	0.00
3	022_hexagonal-b3_Rh	-763.65683362	0.63
4	132_closoTTP-A-i1_Rh	-763.65669442	0.71
5	113_closoTTP-A-f-1_Rh	-763.65644873	0.87
6	144_closoTTP-A-k3_Rh	-763.65618618	1.03
7	023_hexagonal-b3-_Rh	-763.65536946	1.55
8	137_closoTTP-A-j1_Rh	-763.65302316	3.02
9	041_hexagonal-c12_Rh	-763.65260919	3.28
10	042_hexagonal-c13_Rh	-763.65244439	3.38
11	031_hexagonal-c02_Rh	-763.64898619	5.55
12	048_hexagonal-d05_Rh	-763.64899078	5.55
13	116_closoTTP-A-f3_Rh	-763.64799763	6.17
14	140_closoTTP-A-j4_Rh -i45	-763.64821902	6.03
15	012_hexagonal-a1_Rh -i45	-763.64821602	6.03
16	001_B7Mo2-1F_a_Rh	-763.64716076	6.70
17	147_closoTTP-A-l1_Rh	-763.64716019	6.70
18	12b-001_B7Mo2-1F_a_Rh	-763.64670541	6.98
19	157_closoTTP-A-m1_Rh -i28	-763.64548623	7.75
20	118_closoTTP-A-f4_Rh	-763.64478255	8.19
21	159_closoTTP-A-m3_Rh	-763.64313781	9.22
22	108_closoTTP-A-e2_Rh	-763.64220083	9.81
23	152_closoTTP-A-l-3_Rh	-763.64075444	10.72
24	086_hexagonal-f13_Rh	-763.63787485	12.52
25	085_hexagonal-f12_Rh	-763.63787391	12.52
26	088_hexagonal-f15_Rh	-763.63700919	13.07
27	162_closoTTP-A-n2_Rh -i42	-763.63668426	13.27
28	164_closoTTP-A-n3_Rh	-763.63668268	13.27
29	099_closoTTP-A-c3_Rh	-763.63606587	13.66
30	076_hexagonal-f03_Rh	-763.63606559	13.66
31	079_hexagonal-f06_Rh	-763.63570356	13.89
32	075_hexagonal-f02_Rh	-763.63465629	14.54
33	100_closoTTP-A-c4_Rh	-763.63465619	14.54
34	159_closoTTP-A-m3_Rh	-763.63302552	15.57
35	143_closoTTP-A-k2_Rh	-763.63285222	15.68
36	146_closoTTP-A-k5_Rh	-763.63027831	17.29
37	095_closoTTP-A-b4_Rh	-763.62985193	17.56
38	138_closoTTP-A-j2_Rh	-763.62981050	17.58

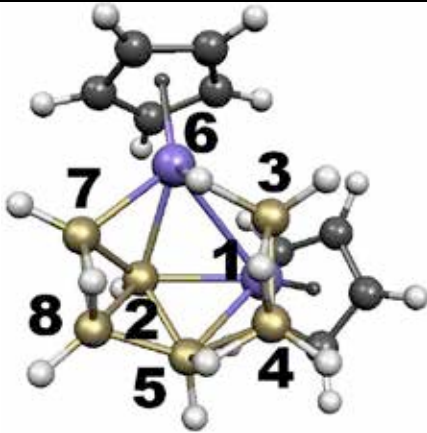
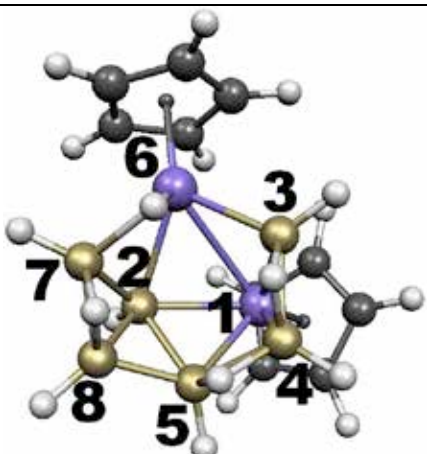
39	094_closoTTP-A-b3_Rh	-763.62590050	20.04
40	089_closoTTP-A-a1_Rh -i18	-763.62553515	20.27
41	018_hexagonal-b1_Rh -i17	-763.62553345	20.27
42	108_closoTTP-A-e2_Rh	-763.62435109	21.01
43	127_closoTTP-A-h1_Rh	-763.62135123	22.89
44	8Ir-9-106_Rh	-763.61827926	24.82
45	092_closoTTP-A-b1_Rh	-763.61673968	25.79
46	093_closoTTP-A-b2_Rh	-763.61673852	25.79
47	097_closoTTP-A-c1_Rh	-763.60798220	31.28
48	098_closoTTP-A-c2_Rh	-763.60774054	31.43
49	096_closoTTP-A-b5_Rh	-763.58330118	46.77

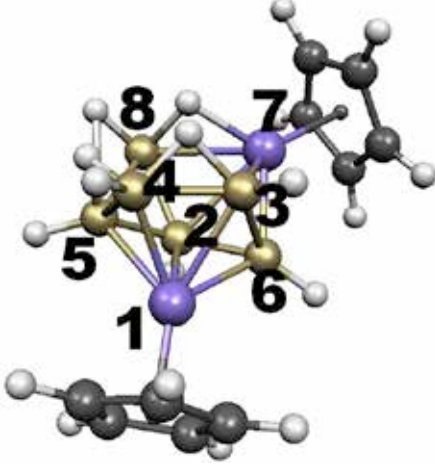
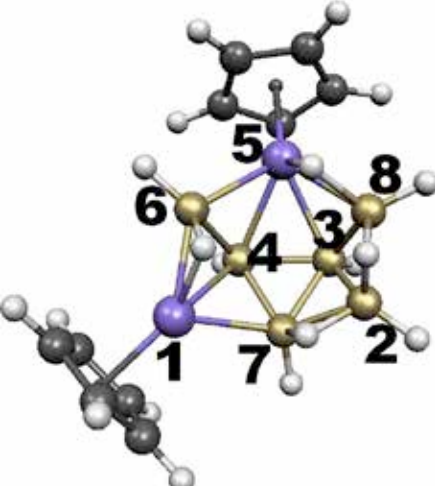
Table 9A. Distance table for the lowest-lying $\text{Cp}_2\text{Ir}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.877866</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.744933</td><td>3.044935</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.744933</td><td>3.044935</td><td>1.686910</td><td>0.000000</td><td></td></tr><tr><td>5 Ir</td><td>2.235595</td><td>2.228373</td><td>3.336351</td><td>2.140256</td><td>0.000000</td></tr><tr><td>6 Ir</td><td>2.235595</td><td>2.228373</td><td>2.140256</td><td>3.336351</td><td>3.883160</td></tr><tr><td>7 B</td><td>3.040167</td><td>1.738880</td><td>3.313814</td><td>3.714227</td><td>3.318735</td></tr><tr><td>8 B</td><td>3.040167</td><td>1.738880</td><td>3.714227</td><td>3.313814</td><td>2.129805</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.129805</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.318735</td><td>1.668212</td><td>0.000000</td><td></td><td></td></tr></table> Ir5-H-B4 Ir5-H 1.62 B4-H 1.65 Ir6-H-B3 Ir6-H 1.62 B3-H 1.65 B3-H-B4 B3-H 1.34 B4-H 1.34 B7-H-B8 B7-H 1.34 B8-H 1.34		1	2	3	4	5	1 B	0.000000					2 B	1.877866	0.000000				3 B	1.744933	3.044935	0.000000			4 B	1.744933	3.044935	1.686910	0.000000		5 Ir	2.235595	2.228373	3.336351	2.140256	0.000000	6 Ir	2.235595	2.228373	2.140256	3.336351	3.883160	7 B	3.040167	1.738880	3.313814	3.714227	3.318735	8 B	3.040167	1.738880	3.714227	3.313814	2.129805		6	7	8			6 Ir	0.000000					7 B	2.129805	0.000000				8 B	3.318735	1.668212	0.000000		
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 3. -750.995275 +3.0 C1 WBI 0.34	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.985827</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Ir</td><td>3.291144</td><td>2.208252</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Ir</td><td>2.209082</td><td>3.114341</td><td>2.735297</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.088801</td><td>2.862468</td><td>2.125693</td><td>2.112014</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.814127</td><td>3.198869</td><td>4.005616</td><td>2.206008</td><td>2.707879</td></tr><tr><td>7 B</td><td>1.725589</td><td>1.729953</td><td>2.105056</td><td>2.115875</td><td>2.980136</td></tr><tr><td>8 B</td><td>3.037317</td><td>1.825490</td><td>2.111209</td><td>3.286711</td><td>1.808223</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td></tr><tr><td>7 B</td><td>3.153851</td><td>0.000000</td><td></td></tr><tr><td>8 B</td><td>3.248243</td><td>2.965800</td><td>0.000000</td></tr></table> B1-H-B6 B1-H 1.28 B6-H 1.36 B2-H-B8 B2-H 1.30 B8-H 1.32 B5-H-B8 B5-H 1.35 B8-H 1.28 B6-H 1.2		1	2	3	4	5	1 B	0.000000					2 B	1.985827	0.000000				3 Ir	3.291144	2.208252	0.000000			4 Ir	2.209082	3.114341	2.735297	0.000000		5 B	3.088801	2.862468	2.125693	2.112014	0.000000	6 B	1.814127	3.198869	4.005616	2.206008	2.707879	7 B	1.725589	1.729953	2.105056	2.115875	2.980136	8 B	3.037317	1.825490	2.111209	3.286711	1.808223		6	7	8	6 B	0.000000			7 B	3.153851	0.000000		8 B	3.248243	2.965800	0.000000
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5 B	2.207049	1.877003	2.970452	1.836356	0.000000																																																																																																		
6 Ir	2.746044	2.242496	2.149420	3.388229	3.448230																																																																																																		
7 B	3.605071	1.763224	3.357790	3.607795	2.843432																																																																																																		
8 B	3.438860	1.717430	3.729131	3.136427	1.752109																																																																																																		
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7 B	2.167068	0.000000																																																																																																					
8 B	3.322265	1.656019	0.000000																																																																																																				
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 9. -750.986944 +8.3 C1 WBI 0.09	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.255108</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.235640</td><td>2.670586</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.096500</td><td>2.890251</td><td>1.828412</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.164262</td><td>1.763121</td><td>2.804823</td><td>1.836292</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.057124</td><td>1.808814</td><td>1.824411</td><td>3.042584</td><td>2.979495</td></tr><tr><td>7 Ir</td><td>3.625350</td><td>2.281404</td><td>2.291751</td><td>3.468598</td><td>3.323167</td></tr><tr><td>8 B</td><td>3.538150</td><td>1.760157</td><td>3.198841</td><td>3.045767</td><td>1.915629</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Ir</td><td>2.059678</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.143340</td><td>2.312493</td><td>0.000000</td><td></td><td></td></tr></table> Ir7-H-B8 Ir7-H 1.66 B8-H 1.44 B3-H-B4 B3-H 1.31 B4-H 1.31 B4-H-B5 B3-H 1.28 B5-H 1.34 B8-H 1.2		1	2	3	4	5	1 Ir	0.000000					2 B	2.255108	0.000000				3 B	2.235640	2.670586	0.000000			4 B	2.096500	2.890251	1.828412	0.000000		5 B	2.164262	1.763121	2.804823	1.836292	0.000000	6 B	2.057124	1.808814	1.824411	3.042584	2.979495	7 Ir	3.625350	2.281404	2.291751	3.468598	3.323167	8 B	3.538150	1.760157	3.198841	3.045767	1.915629		6	7	8			6 B	0.000000					7 Ir	2.059678	0.000000				8 B	3.143340	2.312493	0.000000		
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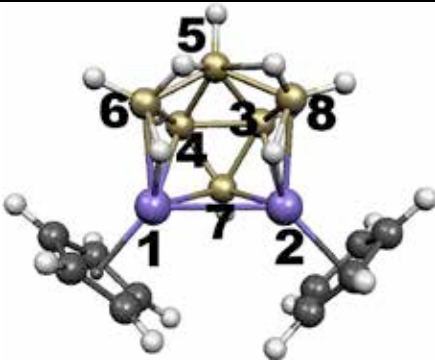
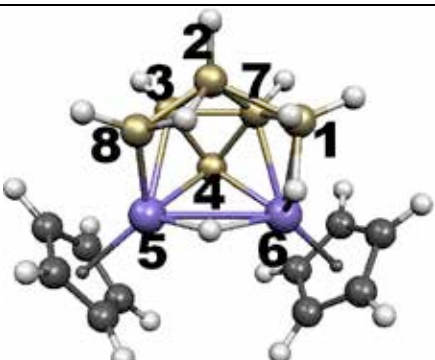
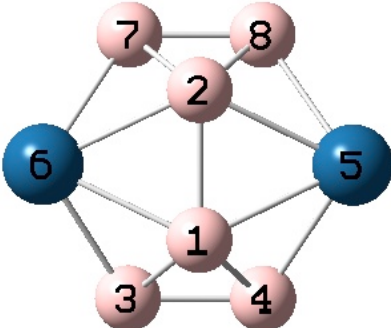
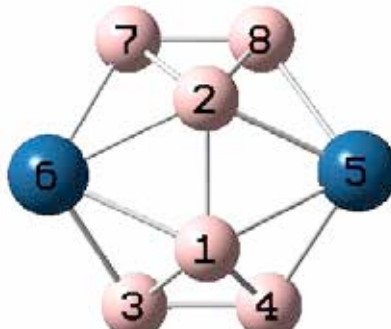
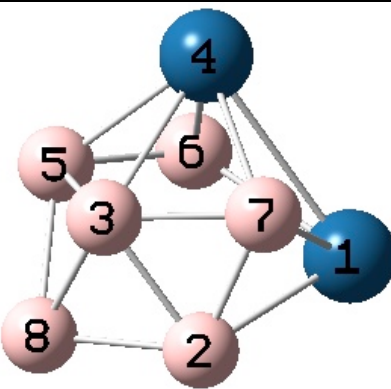
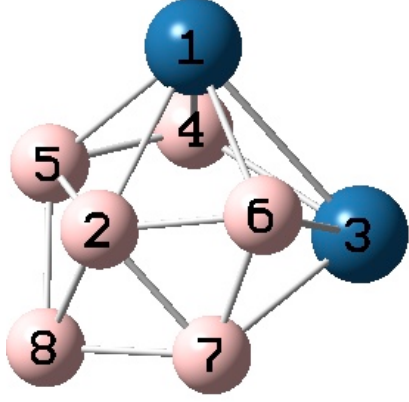
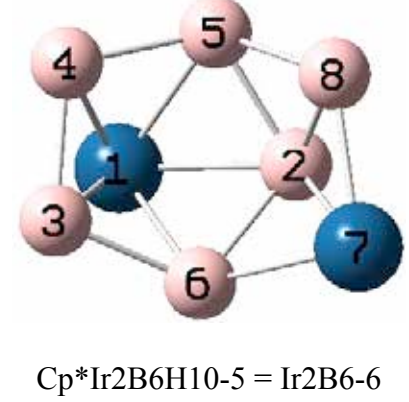
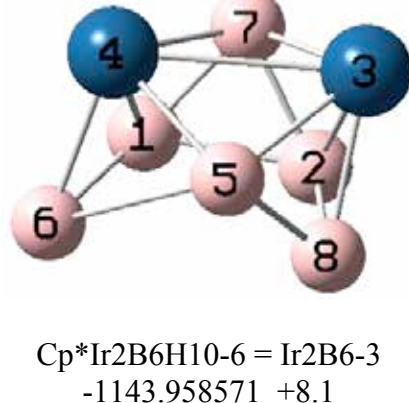
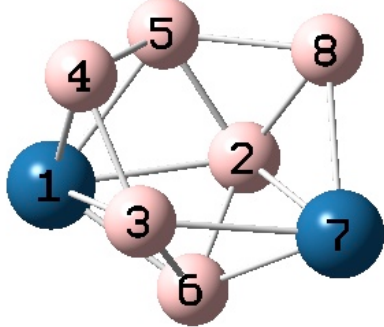
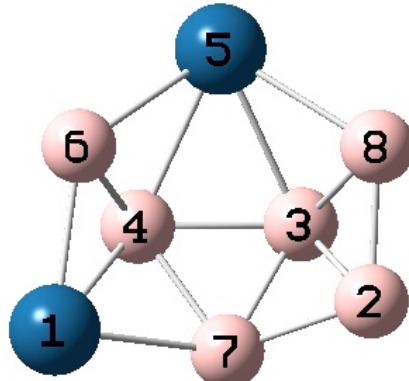
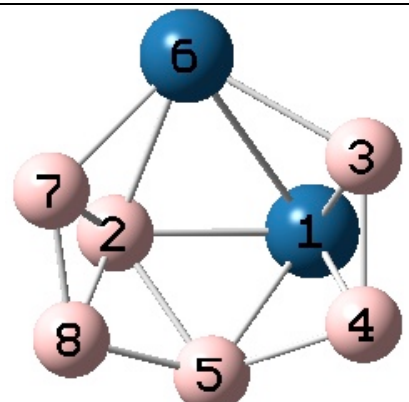
 11. -750.980590 +12.3 C1 WBI 0.41	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 Ir</td><td>2.814666</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.167053</td><td>2.239197</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.263650</td><td>3.226899</td><td>1.835778</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.275825</td><td>3.351725</td><td>1.752689</td><td>1.785606</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.192041</td><td>3.673783</td><td>2.845842</td><td>1.719818</td><td>1.753523</td></tr><tr><td>7 B</td><td>2.124600</td><td>2.107063</td><td>1.756210</td><td>1.735171</td><td>2.911711</td></tr><tr><td>8 B</td><td>3.728966</td><td>2.291728</td><td>1.768082</td><td>3.051911</td><td>1.919394</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.991264</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.086219</td><td>3.119057</td><td>0.000000</td><td></td><td></td></tr></table> Ir1-H-B6 Ir1-H 1.67 B6-H 1.45 Ir2-H-B8 Ir2-H 1.67 B8-H 1.44 B5-H-B6 B5-H 1.32 B6-H 1.29 B8-H 1.20		1	2	3	4	5	1 Ir	0.000000					2 Ir	2.814666	0.000000				3 B	3.167053	2.239197	0.000000			4 B	2.263650	3.226899	1.835778	0.000000		5 B	3.275825	3.351725	1.752689	1.785606	0.000000	6 B	2.192041	3.673783	2.845842	1.719818	1.753523	7 B	2.124600	2.107063	1.756210	1.735171	2.911711	8 B	3.728966	2.291728	1.768082	3.051911	1.919394		6	7	8			6 B	0.000000					7 B	2.991264	0.000000				8 B	3.086219	3.119057	0.000000		
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Table 9B. Distance table for the lowest-lying $\text{Cp}^*\text{Ir}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Ir2B6H10-1 = Ir2B6-1 -1143.971459 0.0	<table><tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.881866</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.749000</td><td>3.046697</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.749068</td><td>3.046730</td><td>1.700525</td><td>0.000000</td><td></td></tr><tr><td>5 Ir</td><td>2.235210</td><td>2.225829</td><td>3.353765</td><td>2.150577</td><td>0.000000</td></tr><tr><td>6 Ir</td><td>2.235311</td><td>2.225792</td><td>2.150478</td><td>3.353695</td><td>3.894526</td></tr><tr><td>7 B</td><td>3.040914</td><td>1.737388</td><td>3.308455</td><td>3.713524</td><td>3.330136</td></tr><tr><td>8 B</td><td>3.040880</td><td>1.737380</td><td>3.713664</td><td>3.308397</td><td>2.138687</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.138682</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.330130</td><td>1.673070</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.881866	0.000000				3 B	1.749000	3.046697	0.000000			4 B	1.749068	3.046730	1.700525	0.000000		5 Ir	2.235210	2.225829	3.353765	2.150577	0.000000	6 Ir	2.235311	2.225792	2.150478	3.353695	3.894526	7 B	3.040914	1.737388	3.308455	3.713524	3.330136	8 B	3.040880	1.737380	3.713664	3.308397	2.138687		6	7	8			6 Ir	0.000000					7 B	2.138682	0.000000				8 B	3.330130	1.673070	0.000000		
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 Cp*Ir2B6H10-8 = Ir2B6-10 -1143.953288 +11.4	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.571057</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.490708</td><td>1.740116</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.185400</td><td>2.934391</td><td>1.825379</td><td>0.000000</td><td></td></tr><tr><td>5 Ir</td><td>3.827154</td><td>3.342489</td><td>2.235279</td><td>2.218227</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.074564</td><td>3.699650</td><td>3.099190</td><td>1.825465</td><td>2.175168</td></tr><tr><td>7 B</td><td>2.219576</td><td>1.785691</td><td>1.788316</td><td>1.787072</td><td>3.370021</td></tr><tr><td>8 B</td><td>4.165720</td><td>1.728745</td><td>1.757943</td><td>3.001946</td><td>2.154164</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.969438</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.340447</td><td>2.878290</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Ir	0.000000					2 B	3.571057	0.000000				3 B	3.490708	1.740116	0.000000			4 B	2.185400	2.934391	1.825379	0.000000		5 Ir	3.827154	3.342489	2.235279	2.218227	0.000000	6 B	2.074564	3.699650	3.099190	1.825465	2.175168	7 B	2.219576	1.785691	1.788316	1.787072	3.370021	8 B	4.165720	1.728745	1.757943	3.001946	2.154164		6	7	8			6 B	0.000000					7 B	2.969438	0.000000				8 B	3.340447	2.878290	0.000000		
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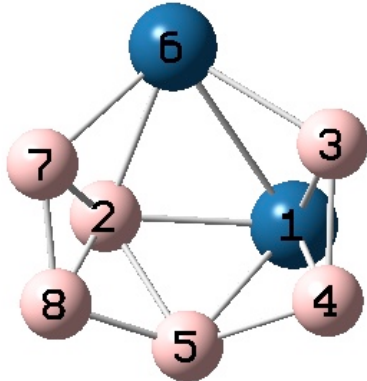
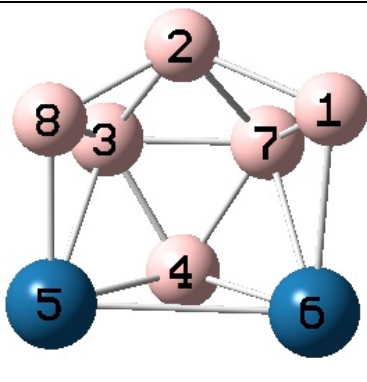
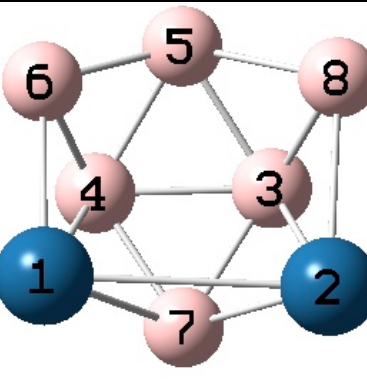
 Cp*Ir2B6H10-10 = Ir2B6-7 -1143.946084 +15.9	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.257909</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.116500</td><td>3.032259</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.101091</td><td>3.035470</td><td>1.816452</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.210375</td><td>1.877132</td><td>2.955064</td><td>1.836230</td><td>0.000000</td></tr><tr><td>6 Ir</td><td>2.832490</td><td>2.244747</td><td>2.214358</td><td>3.476111</td><td>3.469830</td></tr><tr><td>7 B</td><td>3.634848</td><td>1.758709</td><td>3.370581</td><td>3.662208</td><td>2.832950</td></tr><tr><td>8 B</td><td>3.452634</td><td>1.742075</td><td>3.695934</td><td>3.139753</td><td>1.738834</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.149580</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.308838</td><td>1.638172</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Ir	0.000000					2 B	2.257909	0.000000				3 B	2.116500	3.032259	0.000000			4 B	2.101091	3.035470	1.816452	0.000000		5 B	2.210375	1.877132	2.955064	1.836230	0.000000	6 Ir	2.832490	2.244747	2.214358	3.476111	3.469830	7 B	3.634848	1.758709	3.370581	3.662208	2.832950	8 B	3.452634	1.742075	3.695934	3.139753	1.738834		6	7	8			6 Ir	0.000000					7 B	2.149580	0.000000				8 B	3.308838	1.638172	0.000000		
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 Cp*Ir2B6H10-11 = Ir2B6-12 -1143.945511 +16.3	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.903879</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.077333</td><td>1.784383</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.204528</td><td>2.929925</td><td>1.734644</td><td>0.000000</td><td></td></tr><tr><td>5 Ir</td><td>3.859776</td><td>3.240080</td><td>2.248795</td><td>2.090712</td><td>0.000000</td></tr><tr><td>6 Ir</td><td>2.339411</td><td>3.331731</td><td>3.258610</td><td>2.168111</td><td>2.939174</td></tr><tr><td>7 B</td><td>1.786664</td><td>1.769424</td><td>1.803844</td><td>1.782643</td><td>3.168102</td></tr><tr><td>8 B</td><td>3.149711</td><td>1.739382</td><td>1.708375</td><td>2.937802</td><td>2.109134</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Ir</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.238626</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.672744</td><td>2.824909</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.903879	0.000000				3 B	3.077333	1.784383	0.000000			4 B	3.204528	2.929925	1.734644	0.000000		5 Ir	3.859776	3.240080	2.248795	2.090712	0.000000	6 Ir	2.339411	3.331731	3.258610	2.168111	2.939174	7 B	1.786664	1.769424	1.803844	1.782643	3.168102	8 B	3.149711	1.739382	1.708375	2.937802	2.109134		6	7	8			6 Ir	0.000000					7 B	2.238626	0.000000				8 B	3.672744	2.824909	0.000000		
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Table 9C. Energy ranking for all of the $\text{Cp}_2\text{Ir}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	023_hexagonal-b3- Ir-B3LYP	-751.0956273	0.00
2	091_closoTTP-A-a3 Ir-B3LYP	-751.0955799	0.03
3	026_hexagonal-b5 Ir-B3LYP	-751.0955799	0.03
4	020_hexagonal-b2 Ir-B3LYP	-751.0955798	0.03
5	022_hexagonal-b3 Ir-B3LYP	-751.0955798	0.03
6	027_hexagonal-b5- Ir-B3LYP	-751.0955798	0.03
7	024_hexagonal-b4 Ir-B3LYP	-751.0955797	0.03
8	025_hexagonal-b4- Ir-B3LYP	-751.0947533	0.55
9	140_closoTTP-A-j4 Ir-B3LYP-i56	-751.0848964	6.73
10	012_hexagonal-a1 Ir-B3LYP-i56	-751.0848941	6.74
11	141_closoTTP-A-j5-Ir-B3LYP	-751.0848273	6.78
12	139_closoTTP-A-j3 Ir-B3LYP	-751.0848245	6.78
13	062_hexagonal-e04 Ir-B3LYP	-751.0808963	9.24
14	061_hexagonal-e03 Ir-B3LYP	-751.0808963	9.24
15	145_closoTTP-A-k4 Ir-B3LYP	-751.0808962	9.24
16	066_hexagonal-e08 Ir-B3LYP	-751.0808962	9.24
17	151_closoTTP-A-l3 Ir-B3LYP	-751.0808961	9.24
18	146_closoTTP-A-k5 Ir-B3LYP	-751.0808961	9.24
19	065_hexagonal-e07 Ir-B3LYP	-751.080896	9.24
20	072_hexagonal-e14 Ir-B3LYP	-751.0808956	9.24
21	144_closoTTP-A-k3 Ir-B3LYP	-751.0808955	9.24
22	063_hexagonal-e05 Ir-B3LYP	-751.0808952	9.24
23	073_hexagonal-e15 Ir-B3LYP	-751.0808944	9.25
24	067_hexagonal-e09 Ir-B3LYP	-751.0808805	9.25
25	043_hexagonal-c14 Ir-B3LYP	-751.0770123	11.68
26	032_hexagonal-c03 Ir-B3LYP	-751.0770123	11.68
27	041_hexagonal-c12 Ir-B3LYP	-751.0770123	11.68
28	040_hexagonal-c11 Ir-B3LYP	-751.0770122	11.68
29	035_hexagonal-c06 Ir-B3LYP	-751.0770122	11.68
30	042_hexagonal-c13 Ir-B3LYP	-751.0770122	11.68
31	031_hexagonal-c02 Ir-B3LYP	-751.0770121	11.68
32	037_hexagonal-c08 Ir-B3LYP	-751.077012	11.68
33	036_hexagonal-c07 Ir-B3LYP	-751.0770119	11.68
34	033_hexagonal-c04 Ir-B3LYP	-751.0770118	11.68
35	092_closoTTP-A-b1 Ir-B3LYP	-751.0770118	11.68
36	136_closoTTP-A-i5 Ir-B3LYP	-751.0746677	13.15
37	122_closoTTP-A-g1 Ir-B3LYP	-751.0746676	13.15
38	058_hexagonal-d15 Ir-B3LYP	-751.0746676	13.15
39	132_closoTTP-A-i1 Ir-B3LYP	-751.0746676	13.15
40	047_hexagonal-d04 Ir-B3LYP	-751.0746675	13.15
41	123_closoTTP-A-g2 Ir-B3LYP	-751.0746675	13.15

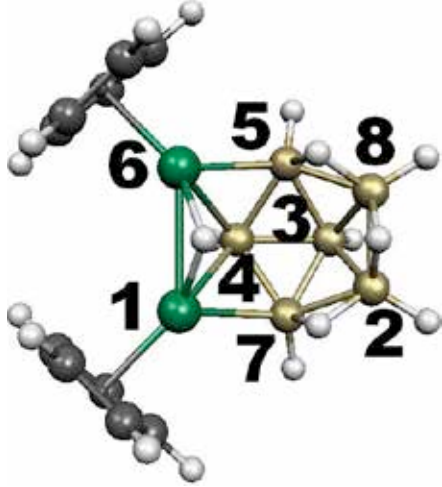
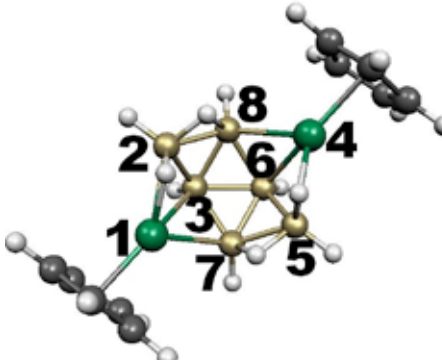
42	133_closoTTP-A-i2_Ir-B3LYP	-751.0746674	13.15
43	048_hexagonal-d05_Ir-B3LYP	-751.0746674	13.15
44	102_closoTTP-A-d1_Ir-B3LYP	-751.0689247	16.76
45	155_closoTTP-A-l5_Ir-B3LYP	-751.0689243	16.76
46	103_closoTTP-A-d2_Ir-B3LYP	-751.0689243	16.76
47	153_closoTTP-A-l4_Ir-B3LYP	-751.0687355	16.87
48	059_hexagonal-e01_Ir-B3LYP	-751.068094	17.28
49	147_closoTTP-A-l1_Ir-B3LYP	-751.0680937	17.28
50	148_closoTTP-A-l-1_Ir-B3LYP	-751.0680924	17.28
51	149_closoTTP-A-l2_Ir-B3LYP	-751.0680905	17.28
52	150_closoTTP-A-l-2_Ir-B3LYP	-751.0680875	17.28
53	001_B7Mo2-1F_a_Ir-B3LYP	-751.0676632	17.55
54	121_closoTTP-A-f-5_Ir-B3LYP	-751.0656106	18.84
55	118_closoTTP-A-f4_Ir-B3LYP	-751.0656105	18.84
56	116_closoTTP-A-f3_Ir-B3LYP	-751.065609	18.84
57	104_closoTTP-A-d3_Ir-B3LYP	-751.0656087	18.84
58	156_closoTTP-A-l-5_Ir-B3LYP	-751.064662	19.43
59	152_closoTTP-A-l-3_Ir-B3LYP	-751.064662	19.43
60	154_closoTTP-A-l-4_Ir-B3LYP	-751.0646616	19.43
61	158_closoTTP-A-m2_Ir-B3LYP	-751.0624443	20.82
62	157_closoTTP-A-m1_Ir-B3LYP-i431	-751.0624411	20.82
63	106_closoTTP-A-d5_Ir-B3LYP	-751.061604	21.35
64	044_hexagonal-d01_Ir-B3LYP_CC_xqc	-751.0615264	21.40
65	052_hexagonal-d09_Ir-B3LYP	-751.0615232	21.40
66	142_closoTTP-A-k1_Ir-B3LYP	-751.0610751	21.68
67	071_hexagonal-e13_Ir-B3LYP	-751.061073	21.68
68	143_closoTTP-A-k2_Ir-B3LYP	-751.0610546	21.69
69	157_closoTTP-A-m1_Ir-B3LYP-i10-i433	-751.0609589	21.75
70	137_closoTTP-A-j1_Ir-B3LYP-i39-i17	-751.0609315	21.77
71	094_closoTTP-A-b3_Ir-B3LYP	-751.0608898	21.80
72	138_closoTTP-A-j2_Ir-B3LYP	-751.0608898	21.80
73	095_closoTTP-A-b4_Ir-B3LYP	-751.0606747	21.93
74	159_closoTTP-A-m3_Ir-B3LYP	-751.0601912	22.24
75	177_closoTTP-A-p3_Ir-B3LYP	-751.0585188	23.29
76	085_hexagonal-f12_Ir-B3LYP	-751.0581097	23.54
77	084_hexagonal-f11_Ir-B3LYP	-751.0580964	23.55
78	082_hexagonal-f09_Ir-B3LYP	-751.0580963	23.55
79	074_hexagonal-f01_Ir-B3LYP	-751.0580958	23.55
80	081_hexagonal-f08_Ir-B3LYP	-751.0580956	23.55
81	075_hexagonal-f02_Ir-B3LYP	-751.0580954	23.55
82	100_closoTTP-A-c4_Ir-B3LYP	-751.0580386	23.59
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84	077_hexagonal-f04_Ir-B3LYP	-751.0577413	23.77

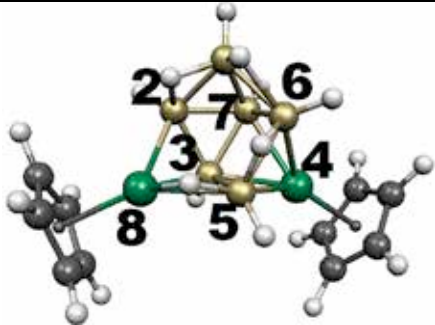
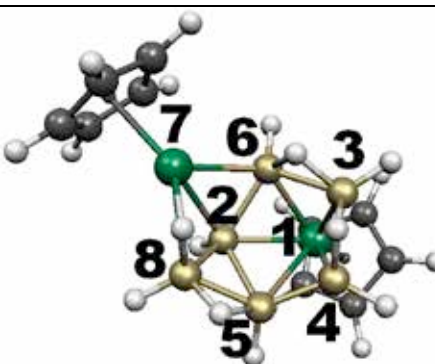
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88	079_hexagonal-f06_Ir-B3LYP	-751.0577311	23.78
89	018_hexagonal-b1_Ir-B3LYP	-751.0553907	25.25
90	089_closoTTP-A-a1_Ir-B3LYP	-751.055361	25.27
91	034_hexagonal-c05_Ir-B3LYP	-751.0547468	25.65
92	107_closoTTP-A-e1_Ir-B3LYP	-751.0533069	26.56
93	086_hexagonal-f13_Ir-B3LYP	-751.0533064	26.56
94	134_closoTTP-A-i3_Ir-B3LYP	-751.0525053	27.06
95	053_hexagonal-d10_Ir-B3LYP	-751.0525051	27.06
96	051_hexagonal-d08_Ir-B3LYP	-751.0525051	27.06
97	054_hexagonal-d11_Ir-B3LYP	-751.0525051	27.06
98	056_hexagonal-d13_Ir-B3LYP	-751.0525051	27.06
99	055_hexagonal-d12_Ir-B3LYP	-751.052505	27.06
100	135_closoTTP-A-i4_Ir-B3LYP	-751.052505	27.06
101	057_hexagonal-d14_Ir-B3LYP	-751.0525049	27.06
102	046_hexagonal-d03_Ir-B3LYP	-751.0525049	27.06
103	160_closoTTP-A-n1_Ir-B3LYP	-751.0508453	28.10
104	168_closoTTP-A-n5_Ir-B3LYP	-751.0498867	28.70
105	186_closoTTP-B-i_Ir-B3LYP_CC_xqc	-751.0494389	28.98
106	162_closoTTP-A-n2_Ir-B3LYP	-751.0494216	28.99
107	015_hexagonal-a4_Ir-B3LYP-i314-i19	-751.048958	29.29
108	015_hexagonal-a4_Ir-B3LYP-i314	-751.0489563	29.29
109	166_closoTTP-A-n4_Ir-B3LYP	-751.0483007	29.70
110	164_closoTTP-A-n3_Ir-B3LYP	-751.0483004	29.70
111	007_B7Mo2-1F_b3-Ir-B3LYP_CC_xqc	-751.0479321	29.93
112	098_closoTTP-A-c2_Ir-B3LYP	-751.0478139	30.00
113	097_closoTTP-A-c1_Ir-B3LYP	-751.0478139	30.00
114	126_closoTTP-A-g5_Ir-B3LYP	-751.0478138	30.00
115	178_closoTTP-B-a_Ir-B3LYP-i31-i168	-751.0474886	30.21
116	178_closoTTP-B-a_Ir-B3LYP-i26-i167	-751.047485	30.21
117	173_closoTTP-A-o4_Ir-B3LYP	-751.0469	30.58
118	108_closoTTP-A-e2_Ir-B3LYP	-751.0468962	30.58
119	127_closoTTP-A-h1_Ir-B3LYP	-751.0464955	30.83
120	070_hexagonal-e12_Ir-B3LYP	-751.0459811	31.15
121	013_hexagonal-a2_Ir-B3LYP	-751.0459148	31.20
122	112_closoTTP-A-f1_Ir-B3LYP	-751.0456749	31.35
123	124_closoTTP-A-g3_Ir-B3LYP	-751.0444137	32.14
124	125_closoTTP-A-g4_Ir-B3LYP	-751.0444132	32.14
125	114_closoTTP-A-f2_Ir-B3LYP	-751.0435635	32.67
126	119_closoTTP-A-f-4_Ir-B3LYP	-751.0435324	32.69
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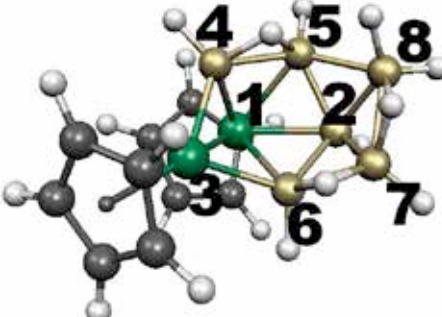
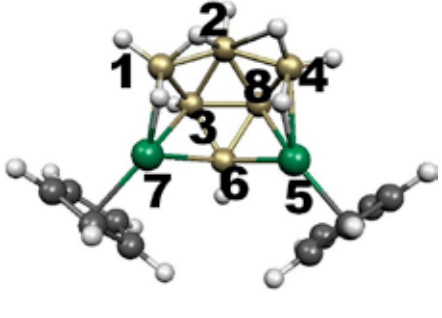
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131	174_closoTTP-A-o5_Ir-B3LYP	-751.0377603	36.31
132	170_closoTTP-A-o1_Ir-B3LYP	-751.0377601	36.31
133	109_closoTTP-A-e3_Ir-B3LYP	-751.0369549	36.82
134	111_closoTTP-A-e5_Ir-B3LYP	-751.0369547	36.82
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137	183_closoTTP-B-f_Ir-B3LYP	-751.0360204	37.40
138	130_closoTTP-A-h4_Ir-B3LYP	-751.03575	37.57
139	131_closoTTP-A-h5_Ir-B3LYP	-751.0351498	37.95
140	017_hexagonal-a6_Ir-B3LYP-i63	-751.0346332	38.27
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143	049_hexagonal-d06_Ir-B3LYP	-751.0334475	39.02
144	069_hexagonal-e11_Ir-B3LYP	-751.0333547	39.08
145	129_closoTTP-A-h3_Ir-B3LYP	-751.033084	39.25
146	175_closoTTP-A-p1_Ir-B3LYP	-751.0329849	39.31
147	068_hexagonal-e10_Ir-B3LYP	-751.0321335	39.84
148	039_hexagonal-c10_Ir-B3LYP	-751.0305028	40.87
149	172_closoTTP-A-o3_Ir-B3LYP	-751.029522	41.48
150	038_hexagonal-c09_Ir-B3LYP-i23	-751.0293505	41.59
151	030_hexagonal-c01_Ir-B3LYP-i21	-751.0293501	41.59
152	030_hexagonal-c01_Ir-B3LYP-i28	-751.0293501	41.59
153	115_closoTTP-A-f-2_Ir-B3LYP	-751.02843	42.17
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155	163_closoTTP-A-n-2_Ir-B3LYP	-751.0267024	43.25
156	064_hexagonal-e06_Ir-B3LYP	-751.0261816	43.58
157	120_closoTTP-A-f5_Ir-B3LYP	-751.0249932	44.32
158	016_hexagonal-a5_Ir-B3LYP	-751.0239503	44.98
159	009_B7Mo2-1F_c-_Ir-B3LYP	-751.0223815	45.96
160	167_closoTTP-A-n-4_Ir-B3LYP	-751.0194276	47.82
161	187_closoTTP-B-j_Ir-B3LYP	-751.0190242	48.07
162	060_hexagonal-e02_Ir-B3LYP	-751.0179203	48.76
163	179_closoTTP-B-b_Ir-B3LYP	-751.0178066	48.83
164	180_closoTTP-B-c_Ir-B3LYP	-751.0170891	49.28
165	171_closoTTP-A-o2_Ir-B3LYP	-751.0151688	50.49
166	090_closoTTP-A-a2_Ir-B3LYP	-751.0147486	50.75
167	184_closoTTP-B-g_Ir-B3LYP	-751.013839	51.32
168	080_hexagonal-f07_Ir-B3LYP	-751.0121737	52.37
169	128_closoTTP-A-h2_Ir-B3LYP	-751.0116898	52.67
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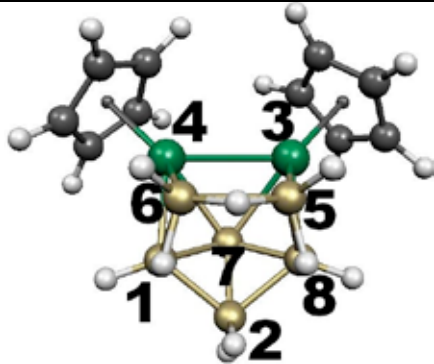
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174	185_closoTTP-B-h_Ir-B3LYP	-751.00614	56.15
175	093_closoTTP-A-b2_Ir-B3LYP	-751.0050489	56.84
176	011_B7Mo2-1F_d-Ir-B3LYP	-751.0049701	56.89
177	096_closoTTP-A-b5_Ir-B3LYP	-751.004627	57.10
178	181_closoTTP-B-d_Ir-B3LYP	-751.0041832	57.38
179	021_hexagonal-b2-Ir-B3LYP	-751.0038893	57.57
180	165_closoTTP-A-n-3_Ir-B3LYP	-751.0026697	58.33
181	161_closoTTP-A-n-1_Ir-B3LYP	-751.0026694	58.33
182	003_B7Mo2-1F_b1_Ir-B3LYP	-750.9981815	61.15
183	004_B7Mo2-1F_b2_Ir-B3LYP	-750.9981806	61.15
184	006_B7Mo2-1F_b3_Ir-B3LYP-cont	-750.9981793	61.15
185	182_closoTTP-B-e_Ir-B3LYP	-750.9965336	62.18
186	101_closoTTP-A-c5_Ir-B3LYP	-750.9910234	65.64
187	002_B7Mo2-1F_b1-Ir-B3LYP	-750.9805134	72.24
188	019_hexagonal-b1-Ir-B3LYP-i76	-750.977111	74.37
189	028_hexagonal-b6_Ir-B3LYP	-750.9757122	75.25
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192	017_hexagonal-a6_Ir-B3LYP-i139	-750.9575967	86.62

Table 10A. Distance table for the lowest-lying $\text{Cp}_2\text{Pd}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.538067</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.460369</td><td>1.735040</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.182319</td><td>2.898726</td><td>1.794785</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.500687</td><td>2.855941</td><td>1.775715</td><td>1.799012</td><td>0.000000</td></tr><tr><td>6 Pd</td><td>2.622553</td><td>4.137442</td><td>3.460351</td><td>2.182355</td><td>2.175729</td></tr><tr><td>7 B</td><td>2.175729</td><td>1.767723</td><td>1.775715</td><td>1.799028</td><td>2.867734</td></tr><tr><td>8 B</td><td>4.137585</td><td>1.754556</td><td>1.735034</td><td>2.898726</td><td>1.767720</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.500622</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.537976</td><td>2.855955</td><td>0.000000</td><td></td><td></td></tr></table> Pd1-H- Pd6 Pd1-H 1.73 Pd6-H 1.73 B2-H-B7 B2-H 1.30 B7-H 1.35 B2-H-B8 B2-H 1.33 B8-H 1.33 B5-H-B8 B5-H 1.35 B8-H 1.30		1	2	3	4	5	1 Pd	0.000000					2 B	3.538067	0.000000				3 B	3.460369	1.735040	0.000000			4 B	2.182319	2.898726	1.794785	0.000000		5 B	3.500687	2.855941	1.775715	1.799012	0.000000	6 Pd	2.622553	4.137442	3.460351	2.182355	2.175729	7 B	2.175729	1.767723	1.775715	1.799028	2.867734	8 B	4.137585	1.754556	1.735034	2.898726	1.767720		6	7	8			6 Pd	0.000000					7 B	3.500622	0.000000				8 B	3.537976	2.855955	0.000000		
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	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.210401</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.214414</td><td>1.751988</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Pd</td><td>4.521384</td><td>3.499523</td><td>3.416519</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.499542</td><td>3.684651</td><td>2.943523</td><td>2.210407</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.416523</td><td>2.943523</td><td>1.775903</td><td>2.214417</td><td>1.751982</td></tr><tr><td>7 B</td><td>2.209049</td><td>2.991621</td><td>1.812057</td><td>3.381315</td><td>1.754086</td></tr><tr><td>8 B</td><td>3.381313</td><td>1.754083</td><td>1.753366</td><td>2.209059</td><td>2.991633</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.753377</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.812057</td><td>2.881657</td><td>0.000000</td><td></td><td></td></tr></table> Pd1-H-B2 Pd1-H 1.72 B2-H 1.34 Pd4-H-B5 Pd2-H 1.72 B5-H 1.34 B2-H-B8 B2-H 1.31 B8-H 1.35 B5-H-B7 B5-H 1.31 B7-H 1.35		1	2	3	4	5	1 Pd	0.000000					2 B	2.210401	0.000000				3 B	2.214414	1.751988	0.000000			4 Pd	4.521384	3.499523	3.416519	0.000000		5 B	3.499542	3.684651	2.943523	2.210407	0.000000	6 B	3.416523	2.943523	1.775903	2.214417	1.751982	7 B	2.209049	2.991621	1.812057	3.381315	1.754086	8 B	3.381313	1.754083	1.753366	2.209059	2.991633		6	7	8			6 B	0.000000					7 B	1.753377	0.000000				8 B	1.812057	2.881657	0.000000		
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7 B	1.753377	0.000000																																																																													
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8 B	2.948172	1.842915	0.000000																																																																												
 6. -797.973889 +20.9 C₁ WBI 0.07	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.755183</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.748719</td><td>1.802359</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.172719</td><td>1.889758</td><td>3.071648</td><td>0.000000</td><td></td></tr><tr><td>5 Pd</td><td>4.017496</td><td>3.404677</td><td>3.393793</td><td>2.259546</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.953152</td><td>2.870827</td><td>1.760314</td><td>3.057516</td><td>2.128257</td></tr><tr><td>7 Pd</td><td>2.198641</td><td>3.364418</td><td>2.210038</td><td>4.103579</td><td>3.633553</td></tr><tr><td>8 B</td><td>2.873054</td><td>1.750682</td><td>1.798510</td><td>1.795009</td><td>2.190920</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Pd</td><td>2.152734</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.753947</td><td>3.348647</td><td>0.000000</td><td></td><td></td></tr></table> Pd7-H-B1 Pd7-H 1.72 B1-H 1.34 Pd5-H-B4 Pd 5-H1.70 B4-H 1.35 B1-H-B2 B1-H 1.29 B2-H 1.33 B4-H 1.20		1	2	3	4	5	1 B	0.000000					2 B	1.755183	0.000000				3 B	1.748719	1.802359	0.000000			4 B	3.172719	1.889758	3.071648	0.000000		5 Pd	4.017496	3.404677	3.393793	2.259546	0.000000	6 B	2.953152	2.870827	1.760314	3.057516	2.128257	7 Pd	2.198641	3.364418	2.210038	4.103579	3.633553	8 B	2.873054	1.750682	1.798510	1.795009	2.190920		6	7	8			6 B	0.000000					7 Pd	2.152734	0.000000				8 B	1.753947	3.348647	0.000000		
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7. -797.973829 +21.0 C_S
WBI 0.29

	1	2	3	4	5
1 B	0.000000				
2 B	1.848569	0.000000			
3 Pd	3.479457	3.529997	0.000000		
4 Pd	2.180275	3.528350	2.598651	0.000000	
5 B	3.017997	3.019732	2.078869	3.107987	0.000000
6 B	1.818828	3.019999	3.104996	2.078438	2.050872
7 B	1.767856	1.678999	2.234428	2.233781	2.665550
8 B	2.828561	1.849614	2.181343	3.479384	1.818660

	6	7	8
6 B	0.000000		
7 B	2.665471	0.000000	
8 B	3.018175	1.766686	0.000000

B1-H-B6

B1-H 1.33

B6-H 1.29

B5-H-B8

B5-H 1.29

B8-H 1.33

B5-H-B6

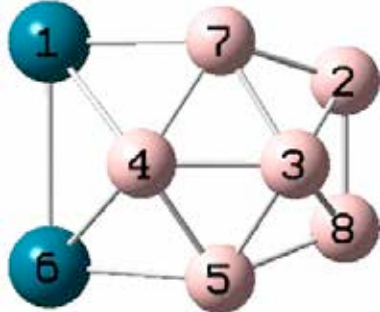
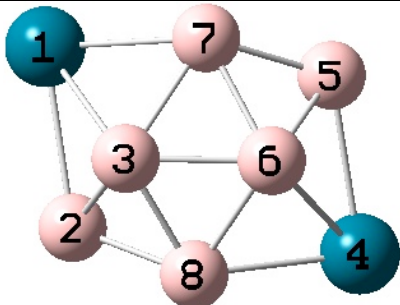
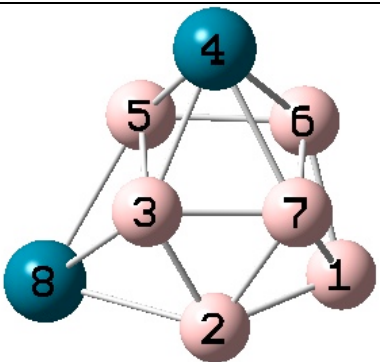
B5-H 1.29

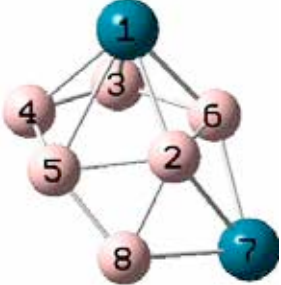
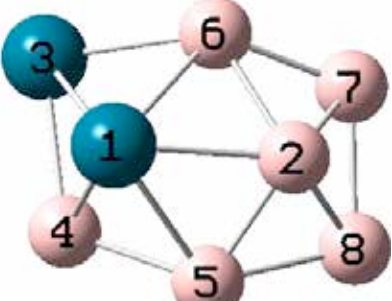
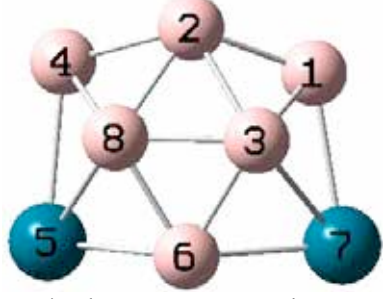
B6-H 1.29

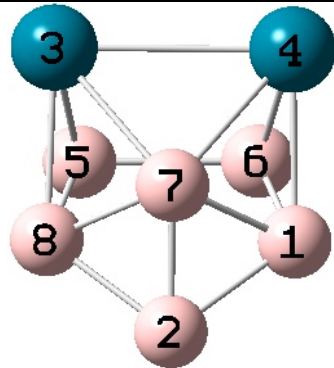
B2-H

1.20

Table 10B. Distance table for the lowest-lying $\text{Cp}^*\text{Pd}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Pd2B6H10-1 = Pd2B6-1 -1190.963725 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.533917</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.481790</td><td>1.732235</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.186936</td><td>2.900216</td><td>1.819264</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.514105</td><td>2.845584</td><td>1.762588</td><td>1.787277</td><td>0.000000</td></tr><tr><td>6 Pd</td><td>2.685559</td><td>4.144517</td><td>3.480415</td><td>2.194868</td><td>2.175765</td></tr><tr><td>7 B</td><td>2.182355</td><td>1.765629</td><td>1.766862</td><td>1.787501</td><td>2.840751</td></tr><tr><td>8 B</td><td>4.147115</td><td>1.757621</td><td>1.732874</td><td>2.902845</td><td>1.765537</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.522158</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.527983</td><td>2.850114</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pd	0.000000					2 B	3.533917	0.000000				3 B	3.481790	1.732235	0.000000			4 B	2.186936	2.900216	1.819264	0.000000		5 B	3.514105	2.845584	1.762588	1.787277	0.000000	6 Pd	2.685559	4.144517	3.480415	2.194868	2.175765	7 B	2.182355	1.765629	1.766862	1.787501	2.840751	8 B	4.147115	1.757621	1.732874	2.902845	1.765537		6	7	8			6 Pd	0.000000					7 B	3.522158	0.000000				8 B	3.527983	2.850114	0.000000		
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8 B	3.527983	2.850114	0.000000																																																																												
 Cp*Pd2B6H10-2 = Pd2B6-2 -1190.951766 +7.5	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.212362</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.211303</td><td>1.763473</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Pd</td><td>4.566431</td><td>3.501627</td><td>3.424130</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.501676</td><td>3.648805</td><td>2.940746</td><td>2.212324</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.424053</td><td>2.940683</td><td>1.775044</td><td>2.211375</td><td>1.763470</td></tr><tr><td>7 B</td><td>2.210024</td><td>2.977391</td><td>1.803911</td><td>3.392951</td><td>1.760810</td></tr><tr><td>8 B</td><td>3.392939</td><td>1.760796</td><td>1.749936</td><td>2.210168</td><td>2.977435</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.749998</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.803842</td><td>2.870736</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pd	0.000000					2 B	2.212362	0.000000				3 B	2.211303	1.763473	0.000000			4 Pd	4.566431	3.501627	3.424130	0.000000		5 B	3.501676	3.648805	2.940746	2.212324	0.000000	6 B	3.424053	2.940683	1.775044	2.211375	1.763470	7 B	2.210024	2.977391	1.803911	3.392951	1.760810	8 B	3.392939	1.760796	1.749936	2.210168	2.977435		6	7	8			6 B	0.000000					7 B	1.749998	0.000000				8 B	1.803842	2.870736	0.000000		
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 Cp*Pd2B6H10-3 = Pd2B6-3 -1190.942109 +13.6	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.847943</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.917854</td><td>1.757811</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Pd</td><td>3.542729</td><td>3.417065</td><td>2.090322</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.021280</td><td>2.819733</td><td>2.037014</td><td>2.168911</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.871568</td><td>2.775353</td><td>2.635350</td><td>2.153839</td><td>1.935359</td></tr><tr><td>7 B</td><td>1.762072</td><td>1.785300</td><td>1.778617</td><td>2.184327</td><td>2.671896</td></tr><tr><td>8 Pd</td><td>3.489643</td><td>2.224221</td><td>2.129831</td><td>3.797682</td><td>2.267770</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.770645</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 Pd</td><td>3.595329</td><td>3.394326</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.847943	0.000000				3 B	2.917854	1.757811	0.000000			4 Pd	3.542729	3.417065	2.090322	0.000000		5 B	3.021280	2.819733	2.037014	2.168911	0.000000	6 B	1.871568	2.775353	2.635350	2.153839	1.935359	7 B	1.762072	1.785300	1.778617	2.184327	2.671896	8 Pd	3.489643	2.224221	2.129831	3.797682	2.267770		6	7	8			6 B	0.000000					7 B	1.770645	0.000000				8 Pd	3.595329	3.394326	0.000000		
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 Cp*Pd2B6H10-4 = Pd2B6-4 -1190.940771 +14.4	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.197443</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.118020</td><td>2.910364</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.164038</td><td>2.769036</td><td>1.806105</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.521364</td><td>1.883066</td><td>2.935364</td><td>1.658263</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.147746</td><td>1.828103</td><td>1.843941</td><td>2.888710</td><td>3.022833</td></tr><tr><td>7 Pd</td><td>3.956836</td><td>2.185017</td><td>3.570851</td><td>4.054950</td><td>3.437060</td></tr><tr><td>8 B</td><td>3.604428</td><td>1.759267</td><td>3.670485</td><td>3.053452</td><td>1.751363</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Pd</td><td>2.202981</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.042832</td><td>2.233247</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pd	0.000000					2 B	2.197443	0.000000				3 B	2.118020	2.910364	0.000000			4 B	2.164038	2.769036	1.806105	0.000000		5 B	2.521364	1.883066	2.935364	1.658263	0.000000	6 B	2.147746	1.828103	1.843941	2.888710	3.022833	7 Pd	3.956836	2.185017	3.570851	4.054950	3.437060	8 B	3.604428	1.759267	3.670485	3.053452	1.751363		6	7	8			6 B	0.000000					7 Pd	2.202981	0.000000				8 B	3.042832	2.233247	0.000000		
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 Cp*Pd2B6H10-5 = Pd2B6-5 -1190.937374 +16.5	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pd</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.181581</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 Pd</td><td>2.626414</td><td>3.417334</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.110513</td><td>2.918294</td><td>2.050596</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.204456</td><td>1.755455</td><td>3.353912</td><td>1.839216</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.287045</td><td>1.829930</td><td>2.114316</td><td>2.838651</td><td>2.844115</td></tr><tr><td>7 B</td><td>3.512408</td><td>1.738993</td><td>3.501677</td><td>3.661015</td><td>2.923193</td></tr><tr><td>8 B</td><td>3.588707</td><td>1.763653</td><td>4.147887</td><td>3.305639</td><td>1.909887</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.775965</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.953333</td><td>1.844407</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pd	0.000000					2 B	2.181581	0.000000				3 Pd	2.626414	3.417334	0.000000			4 B	2.110513	2.918294	2.050596	0.000000		5 B	2.204456	1.755455	3.353912	1.839216	0.000000	6 B	2.287045	1.829930	2.114316	2.838651	2.844115	7 B	3.512408	1.738993	3.501677	3.661015	2.923193	8 B	3.588707	1.763653	4.147887	3.305639	1.909887		6	7	8			6 B	0.000000					7 B	1.775965	0.000000				8 B	2.953333	1.844407	0.000000		
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8 B	2.953333	1.844407	0.000000																																																																												
 Cp*Pd2B6H10-6 = Pd2B6-6 -1190.935887 +17.5	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.762049</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.762769</td><td>1.782508</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>3.152848</td><td>1.894696</td><td>3.080166</td><td>0.000000</td><td></td></tr><tr><td>5 Pd</td><td>3.964603</td><td>3.391284</td><td>3.402506</td><td>2.258498</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.920731</td><td>2.866686</td><td>1.771805</td><td>3.084261</td><td>2.147896</td></tr><tr><td>7 Pd</td><td>2.182717</td><td>3.384065</td><td>2.204507</td><td>4.181839</td><td>3.703714</td></tr><tr><td>8 B</td><td>2.857600</td><td>1.745460</td><td>1.784370</td><td>1.818482</td><td>2.193042</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Pd</td><td>2.150448</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.755900</td><td>3.362199</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.762049	0.000000				3 B	1.762769	1.782508	0.000000			4 B	3.152848	1.894696	3.080166	0.000000		5 Pd	3.964603	3.391284	3.402506	2.258498	0.000000	6 B	2.920731	2.866686	1.771805	3.084261	2.147896	7 Pd	2.182717	3.384065	2.204507	4.181839	3.703714	8 B	2.857600	1.745460	1.784370	1.818482	2.193042		6	7	8			6 B	0.000000					7 Pd	2.150448	0.000000				8 B	1.755900	3.362199	0.000000		
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6 B	2.920731	2.866686	1.771805	3.084261	2.147896																																																																										
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8 B	1.755900	3.362199	0.000000																																																																												



Cp*Pd2B6H10-7 = Pd2B6-7
-1190.922438 +25.9

	1	2	3	4	5
1 B	0.000000				
2 B	1.820582	0.000000			
3 Pd	3.491967	3.516696	0.000000		
4 Pd	2.181564	3.517730	2.682696	0.000000	
5 B	3.000309	3.025691	2.075982	3.145301	0.000000
6 B	1.833553	3.026330	3.086515	2.078041	2.011513
7 B	1.774781	1.695670	2.221481	2.219436	2.669208
8 B	2.789787	1.822476	2.182275	3.506434	1.828895
	6	7	8		
6 B	0.000000				
7 B	2.652465	0.000000			
8 B	2.987835	1.776381	0.000000		

Table 10C. Energy ranking for all of the $\text{Cp}_2\text{Pd}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	171_closoTTP-A-o2_Pd-B3LYP	-798.073523	0.00
2	170_closoTTP-A-o1_Pd-B3LYP	-798.073523	0.00
3	185_closoTTP-B-h_Pd-B3LYP	-798.073522	0.00
4	186_closoTTP-B-i_Pd-B3LYP	-798.054236	12.10
5	146_closoTTP-A-k5_Pd-B3LYP	-798.049536	15.05
6	105_closoTTP-A-d4_Pd-B3LYP	-798.049536	15.05
7	104_closoTTP-A-d3_Pd-B3LYP	-798.049535	15.05
8	136_closoTTP-A-i5_Pd-B3LYP	-798.049535	15.05
9	103_closoTTP-A-d2_Pd-B3LYP	-798.049535	15.05
10	184_closoTTP-B-g_Pd-B3LYP	-798.049535	15.05
11	132_closoTTP-A-i1_Pd-B3LYP	-798.049517	15.06
12	127_closoTTP-A-h1_Pd-B3LYP	-798.045457	17.61
13	101_closoTTP-A-c5_Pd-B3LYP	-798.045457	17.61
14	128_closoTTP-A-h2_Pd-B3LYP	-798.045457	17.61
15	097_closoTTP-A-c1_Pd-B3LYP	-798.045457	17.61
16	180_closoTTP-B-c_Pd-B3LYP	-798.045453	17.61
17	140_closoTTP-A-j4_Pd-B3LYP	-798.042001	19.78
18	061_hexagonal-e03_Pd-B3LYP	-798.041869	19.86
19	065_hexagonal-e07_Pd-B3LYP	-798.041868	19.86
20	071_hexagonal-e13_Pd-B3LYP	-798.041868	19.86
21	072_hexagonal-e14_Pd-B3LYP	-798.041868	19.86
22	047_hexagonal-d04_Pd-B3LYP	-798.041707	19.96
23	048_hexagonal-d05_Pd-B3LYP	-798.041156	20.31
24	182_closoTTP-B-e_Pd-B3LYP	-798.040821	20.52
25	157_closoTTP-A-m1_Pd-B3LYP-i249	-798.040820	20.52
26	107_closoTTP-A-e1_Pd-B3LYP	-798.040820	20.52
27	102_closoTTP-A-d1_Pd-B3LYP	-798.039959	21.06
28	106_closoTTP-A-d5_Pd-B3LYP	-798.039959	21.06
29	133_closoTTP-A-i2_Pd-B3LYP	-798.039868	21.12
30	076_hexagonal-f03_Pd-B3LYP	-798.039743	21.20
31	129_closoTTP-A-h3_Pd-B3LYP	-798.039742	21.20
32	077_hexagonal-f04_Pd-B3LYP	-798.039742	21.20
33	080_hexagonal-f07_Pd-B3LYP	-798.039742	21.20
34	079_hexagonal-f06_Pd-B3LYP	-798.039742	21.20
35	081_hexagonal-f08_Pd-B3LYP	-798.039742	21.20
36	075_hexagonal-f02_Pd-B3LYP	-798.039742	21.20
37	156_closoTTP-A-l-5_Pd-B3LYP	-798.038597	21.92
38	151_closoTTP-A-l3_Pd-B3LYP	-798.038577	21.93
39	042_hexagonal-c13_Pd-B3LYP	-798.037586	22.55
40	040_hexagonal-c11_Pd-B3LYP	-798.037585	22.55
41	041_hexagonal-c12_Pd-B3LYP	-798.037585	22.55

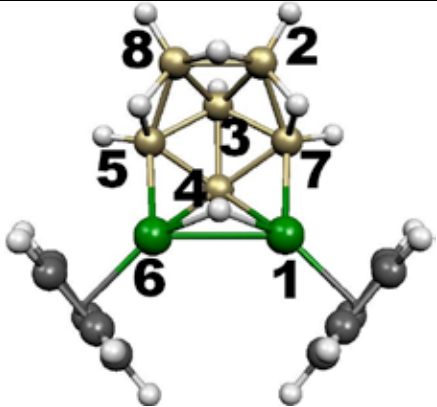
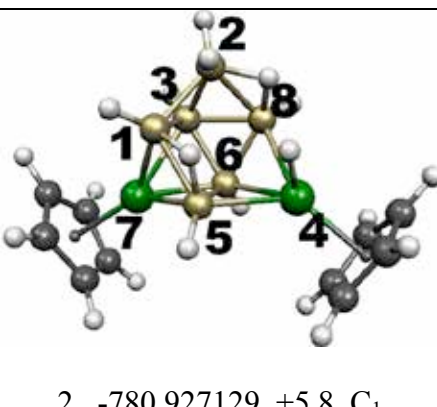
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44	014_hexagonal-a3_Pd-B3LYP	-798.037519	22.59
45	144_closoTTP-A-k3_Pd-B3LYP	-798.037461	22.63
46	181_closoTTP-B-d_Pd-B3LYP	-798.037460	22.63
47	145_closoTTP-A-k4_Pd-B3LYP	-798.037459	22.63
48	024_hexagonal-b4_Pd-B3LYP-i199	-798.035711	23.73
49	090_closoTTP-A-a2_Pd-B3LYP	-798.035413	23.91
50	091_closoTTP-A-a3_Pd-B3LYP	-798.035368	23.94
51	153_closoTTP-A-l4_Pd-B3LYP	-798.035289	23.99
52	093_closoTTP-A-b2_Pd-B3LYP	-798.035063	24.13
53	092_closoTTP-A-b1_Pd-B3LYP	-798.035063	24.13
54	158_closoTTP-A-m2_Pd-B3LYP	-798.034713	24.35
55	078_hexagonal-f05_Pd-B3LYP	-798.034476	24.50
56	082_hexagonal-f09_Pd-B3LYP	-798.034436	24.53
57	121_closoTTP-A-f-5_Pd-B3LYP	-798.032569	25.70
58	159_closoTTP-A-m3_Pd-B3LYP	-798.032020	26.04
59	060_hexagonal-e02_Pd-B3LYP	-798.031944	26.09
60	064_hexagonal-e06_Pd-B3LYP	-798.031943	26.09
61	019_hexagonal-b1-_Pd-B3LYP-i32	-798.031642	26.28
62	021_hexagonal-b2-_Pd-B3LYP	-798.031641	26.28
63	019_hexagonal-b1-_Pd-B3LYP-i350	-798.031641	26.28
64	018_hexagonal-b1_Pd-B3LYP	-798.031640	26.28
65	020_hexagonal-b2_Pd-B3LYP	-798.031640	26.28
66	029_hexagonal-b6-_Pd-B3LYP-i311-i356	-798.031640	26.28
67	089_closoTTP-A-a1_Pd-B3LYP-i33.log	-798.031639	26.28
68	089_closoTTP-A-a1_Pd-B3LYP-i215	-798.031639	26.28
69	019_hexagonal-b1-_Pd-B3LYP-i54	-798.031638	26.28
70	052_hexagonal-d09_Pd-B3LYP	-798.030976	26.70
71	063_hexagonal-e05_Pd-B3LYP	-798.029452	27.65
72	073_hexagonal-e15_Pd-B3LYP	-798.029361	27.71
73	062_hexagonal-e04_Pd-B3LYP	-798.029360	27.71
74	088_hexagonal-f15_Pd-B3LYP	-798.028724	28.11
75	085_hexagonal-f12_Pd-B3LYP	-798.028723	28.11
76	087_hexagonal-f14_Pd-B3LYP	-798.028723	28.11
77	066_hexagonal-e08_Pd-B3LYP	-798.028215	28.43
78	067_hexagonal-e09_Pd-B3LYP	-798.028215	28.43
79	032_hexagonal-c03_Pd-B3LYP	-798.027636	28.79
80	033_hexagonal-c04_Pd-B3LYP	-798.027636	28.79
81	049_hexagonal-d06_Pd-B3LYP	-798.027499	28.88
82	123_closoTTP-A-g2_Pd-B3LYP	-798.027498	28.88
83	098_closoTTP-A-c2_Pd-B3LYP	-798.027498	28.88
84	131_closoTTP-A-h5_Pd-B3LYP	-798.027498	28.88

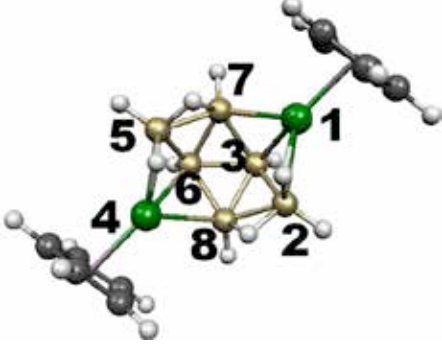
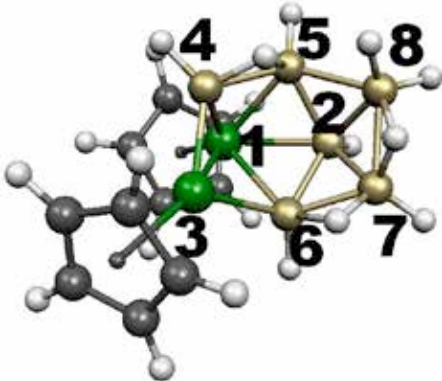
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88	059_hexagonal-e01_Pd-B3LYP	-798.027142	29.10
89	147_closoTTP-A-l1_Pd-B3LYP	-798.027139	29.11
90	022_hexagonal-b3_Pd-B3LYP	-798.027033	29.17
91	028_hexagonal-b6_Pd-B3LYP	-798.027030	29.17
92	055_hexagonal-d12_Pd-B3LYP	-798.026095	29.76
93	034_hexagonal-c05_Pd-B3LYP	-798.026056	29.79
94	027_hexagonal-b5-_Pd-B3LYP	-798.025633	30.05
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96	054_hexagonal-d11_Pd-B3LYP	-798.025526	30.12
97	135_closoTTP-A-i4_Pd-B3LYP	-798.025526	30.12
98	138_closoTTP-A-j2_Pd-B3LYP	-798.025008	30.44
99	137_closoTTP-A-j1_Pd-B3LYP	-798.025008	30.44
100	069_hexagonal-e11_Pd-B3LYP	-798.024332	30.87
101	070_hexagonal-e12_Pd-B3LYP	-798.024332	30.87
102	124_closoTTP-A-g3_Pd-B3LYP	-798.023470	31.41
103	039_hexagonal-c10_Pd-B3LYP	-798.023469	31.41
104	154_closoTTP-A-l-4_Pd-B3LYP	-798.022618	31.94
105	057_hexagonal-d14_Pd-B3LYP	-798.022215	32.20
106	056_hexagonal-d13_Pd-B3LYP	-798.022208	32.20
107	155_closoTTP-A-l5_Pd-B3LYP	-798.021638	32.56
108	086_hexagonal-f13_Pd-B3LYP	-798.021588	32.59
109	118_closoTTP-A-f4_Pd-B3LYP	-798.021142	32.87
110	113_closoTTP-A-f-1_Pd-B3LYP	-798.021141	32.87
111	051_hexagonal-d08_Pd-B3LYP	-798.020982	32.97
112	084_hexagonal-f11_Pd-B3LYP	-798.020711	33.14
113	162_closoTTP-A-n2_Pd-B3LYP	-798.020004	33.58
114	164_closoTTP-A-n3_Pd-B3LYP	-798.020004	33.58
115	163_closoTTP-A-n-2_Pd-B3LYP	-798.020004	33.58
116	165_closoTTP-A-n-3_Pd-B3LYP	-798.020004	33.58
117	005_B7Mo2-1F b2-_Pd-B3LYP	-798.019424	33.95
118	015_hexagonal-a4_Pd-B3LYP	-798.019036	34.19
119	095_closoTTP-A-b4_Pd-B3LYP	-798.018343	34.63
120	074_hexagonal-f01_Pd-B3LYP	-798.017519	35.14
121	045_hexagonal-d02_Pd-B3LYP	-798.017445	35.19
122	178_closoTTP-B-a_Pd-B3LYP-i193	-798.017216	35.33
123	111_closoTTP-A-e5_Pd-B3LYP	-798.016899	35.53
124	044_hexagonal-d01_Pd-B3LYP	-798.016852	35.56
125	167_closoTTP-A-n-4_Pd-B3LYP	-798.016257	35.93
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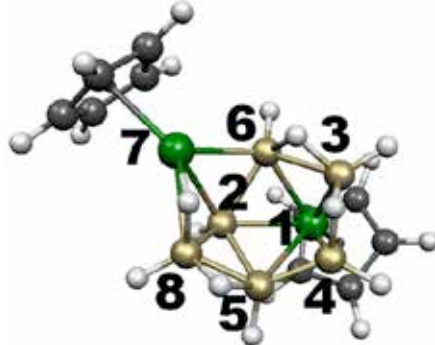
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131	013_hexagonal-a2 Pd-B3LYP-i21	-798.011933	38.65
132	114_closoTTP-A-f2 Pd-B3LYP	-798.011402	38.98
133	116_closoTTP-A-f3 Pd-B3LYP	-798.011402	38.98
134	119_closoTTP-A-f-4 Pd-B3LYP	-798.011402	38.98
135	178_closoTTP-B-a Pd-B3LYP-i254	-798.011079	39.18
136	173_closoTTP-A-o4 Pd-B3LYP	-798.010852	39.33
137	174_closoTTP-A-o5 Pd-B3LYP	-798.009713	40.04
138	148_closoTTP-A-l-1 Pd-B3LYP	-798.009338	40.28
139	149_closoTTP-A-l2 Pd-B3LYP	-798.009337	40.28
140	117_closoTTP-A-f-3 Pd-B3LYP	-798.008901	40.55
141	031_hexagonal-c02 Pd-B3LYP	-798.008326	40.91
142	002_B7Mo2-1F b1- Pd-B3LYP	-798.008180	41.00
143	008_B7Mo2-1F c Pd-B3LYP	-798.008161	41.01
144	112_closoTTP-A-f1 Pd-B3LYP	-798.008161	41.02
145	011_B7Mo2-1F d- Pd-B3LYP	-798.008160	41.02
146	108_closoTTP-A-e2 Pd-B3LYP	-798.007750	41.27
147	109_closoTTP-A-e3 Pd-B3LYP	-798.007749	41.27
148	122_closoTTP-A-g1 Pd-B3LYP	-798.007677	41.32
149	139_closoTTP-A-j3 Pd-B3LYP	-798.007673	41.32
150	141_closoTTP-A-j5-Pd-B3LYP	-798.007673	41.32
151	094_closoTTP-A-b3 Pd-B3LYP	-798.007673	41.32
152	012_hexagonal-a1 Pd-B3LYP-i22	-798.007523	41.42
153	016_hexagonal-a5 Pd-B3LYP	-798.007518	41.42
154	169_closoTTP-A-n-5 Pd-B3LYP	-798.006760	41.89
155	152_closoTTP-A-l-3 Pd-B3LYP	-798.006547	42.03
156	125_closoTTP-A-g4 Pd-B3LYP	-798.006287	42.19
157	134_closoTTP-A-i3 Pd-B3LYP	-798.006278	42.20
158	161_closoTTP-A-n-1 Pd-B3LYP-i58	-798.006107	42.30
159	096_closoTTP-A-b5 Pd-B3LYP	-798.005860	42.46
160	037_hexagonal-c08 Pd-B3LYP	-798.005684	42.57
161	036_hexagonal-c07 Pd-B3LYP	-798.005684	42.57
162	035_hexagonal-c06 Pd-B3LYP	-798.005684	42.57
163	168_closoTTP-A-n5 Pd-B3LYP	-798.004827	43.11
164	177_closoTTP-A-p3 Pd-B3LYP	-798.004827	43.11
165	187_closoTTP-B-j Pd-B3LYP	-798.004819	43.11
166	142_closoTTP-A-k1 Pd-B3LYP	-798.004470	43.33
167	143_closoTTP-A-k2 Pd-B3LYP	-798.004045	43.60
168	030_hexagonal-c01 Pd-B3LYP	-798.003273	44.08
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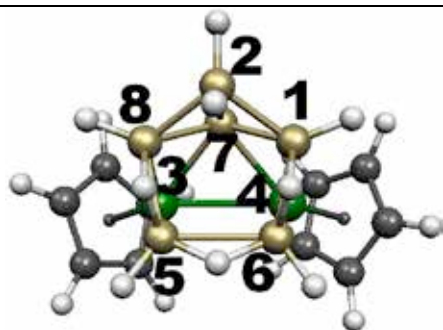
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173	058_hexagonal-d15_Pd-B3LYP	-798.000607	45.76
174	001_B7Mo2-1F_a_Pd-B3LYP	-798.000556	45.79
175	038_hexagonal-c09_Pd-B3LYP	-798.000323	45.93
176	175_closoTTP-A-p1_Pd-B3LYP-i113	-797.999451	46.48
177	176_closoTTP-A-p2_Pd-B3LYP	-797.999450	46.48
178	172_closoTTP-A-o3_Pd-B3LYP	-797.996301	48.46
179	083_hexagonal-f10_Pd-B3LYP	-797.995955	48.67
180	110_closoTTP-A-e4_Pd-B3LYP	-797.995955	48.67
181	160_closoTTP-A-n1_Pd-B3LYP-i29	-797.992434	50.88
182	053_hexagonal-d10_Pd-B3LYP	-797.991651	51.38
183	179_closoTTP-B-b_Pd-B3LYP_CC_xqc	-797.990854	51.88
184	150_closoTTP-A-l-2_Pd-B3LYP	-797.989673	52.62
185	009_B7Mo2-1F_c_Pd-B3LYP	-797.981605	57.68
186	025_hexagonal-b4_Pd-B3LYP	-797.981571	57.70
187	006_B7Mo2-1F_b3_Pd-B3LYP	-797.980590	58.32
188	183_closoTTP-B-f_Pd-B3LYP	-797.980301	58.50
189	007_B7Mo2-1F_b3_Pd-B3LYP	-797.973705	62.64
190	010_B7Mo2-1F_d_Pd-B3LYP_CC_xqc	-797.973227	62.94
191	017_hexagonal-a6_Pd-B3LYP-i62	-797.972154	63.61
192	004_B7Mo2-1F_b2_Pd-B3LYP	-797.952248	76.10

Table 11A. Distance table for the lowest-lying $\text{Cp}_2\text{Pt}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), symmetry and WBI.

 1. -780.936426 0.0 C_s WBI 0.32	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.551109</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.430301</td><td>1.734084</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.178323</td><td>2.948253</td><td>1.804452</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.518999</td><td>2.870864</td><td>1.781659</td><td>1.843457</td><td>0.000000</td></tr><tr><td>6 Pt</td><td>2.675641</td><td>4.160078</td><td>3.430306</td><td>2.178338</td><td>2.150254</td></tr><tr><td>7 B</td><td>2.150236</td><td>1.775318</td><td>1.781659</td><td>1.843464</td><td>2.900137</td></tr><tr><td>8 B</td><td>4.160127</td><td>1.755138</td><td>1.734078</td><td>2.948253</td><td>1.775314</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.518977</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.551098</td><td>2.870874</td><td>0.000000</td><td></td><td></td></tr></table> Pt1-H- Pt5 Pt1-H 1.75 Pt5-H 1.75 B2-H-B7 B2-H 1.29 B7-H 1.37 B8-H-B5 B8-H 1.29 B5-H 1.37 B2-H-B8 B2-H 1.33 B8-H 1.33		1	2	3	4	5	1 Pt	0.000000					2 B	3.551109	0.000000				3 B	3.430301	1.734084	0.000000			4 B	2.178323	2.948253	1.804452	0.000000		5 B	3.518999	2.870864	1.781659	1.843457	0.000000	6 Pt	2.675641	4.160078	3.430306	2.178338	2.150254	7 B	2.150236	1.775318	1.781659	1.843464	2.900137	8 B	4.160127	1.755138	1.734078	2.948253	1.775314		6	7	8			6 Pt	0.000000					7 B	3.518977	0.000000				8 B	3.551098	2.870874	0.000000		
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 2. -780.927129 +5.8 C₁ WBI 0.07	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.892127</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.797002</td><td>1.776292</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Pt</td><td>3.486473</td><td>3.472296</td><td>3.387823</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.904246</td><td>3.084846</td><td>2.641890</td><td>2.211355</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.620576</td><td>2.954126</td><td>1.778378</td><td>2.178105</td><td>1.968641</td></tr><tr><td>7 Pt</td><td>2.140939</td><td>3.546055</td><td>2.166329</td><td>3.836032</td><td>2.125948</td></tr><tr><td>8 B</td><td>2.777762</td><td>1.894189</td><td>1.800691</td><td>2.217819</td><td>2.816303</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Pt</td><td>2.115655</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.765679</td><td>3.436656</td><td>0.000000</td><td></td><td></td></tr></table> B1-H-B5 B1-H 1.31 B5-H 1.31 B2-H-B8 B2-H 1.31 B8-H 1.31 Pt4-H 1.6 B2-H 1.2		1	2	3	4	5	1 B	0.000000					2 B	1.892127	0.000000				3 B	1.797002	1.776292	0.000000			4 Pt	3.486473	3.472296	3.387823	0.000000		5 B	1.904246	3.084846	2.641890	2.211355	0.000000	6 B	2.620576	2.954126	1.778378	2.178105	1.968641	7 Pt	2.140939	3.546055	2.166329	3.836032	2.125948	8 B	2.777762	1.894189	1.800691	2.217819	2.816303		6	7	8			6 B	0.000000					7 Pt	2.115655	0.000000				8 B	1.765679	3.436656	0.000000		
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7 Pt	2.115655	0.000000																																																																													
8 B	1.765679	3.436656	0.000000																																																																												

 3. -780.919855 +10.4 C₂ WBI 0.03	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.195618</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.219141</td><td>1.734508</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 Pt</td><td>4.502924</td><td>3.531295</td><td>3.415057</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.531295</td><td>3.736269</td><td>2.959675</td><td>2.195615</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.415046</td><td>2.959672</td><td>1.780204</td><td>2.219142</td><td>1.734498</td></tr><tr><td>7 B</td><td>2.194560</td><td>2.988974</td><td>1.830815</td><td>3.363974</td><td>1.756415</td></tr><tr><td>8 B</td><td>3.363984</td><td>1.756424</td><td>1.762459</td><td>2.194577</td><td>2.988983</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.762457</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.830810</td><td>2.882111</td><td>0.000000</td><td></td><td></td></tr></table> Pt1-H- B2 Pt1-H 1.68 B2-H 1.42 Pt4-H-B5 Pt4-H 1.68 B5-H 1.42 B2-H-B8 B2-H 1.30 B8-H 1.38 B5-H-B7 B5-H 1.29 B7-H 1.67		1	2	3	4	5	1 Pt	0.000000					2 B	2.195618	0.000000				3 B	2.219141	1.734508	0.000000			4 Pt	4.502924	3.531295	3.415057	0.000000		5 B	3.531295	3.736269	2.959675	2.195615	0.000000	6 B	3.415046	2.959672	1.780204	2.219142	1.734498	7 B	2.194560	2.988974	1.830815	3.363974	1.756415	8 B	3.363984	1.756424	1.762459	2.194577	2.988983		6	7	8			6 B	0.000000					7 B	1.762457	0.000000				8 B	1.830810	2.882111	0.000000		
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 6. -780.911072 +15.9 C₁ WBI 0.07	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.196113</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.112960</td><td>2.969369</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.174286</td><td>2.785778</td><td>1.822194</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.549982</td><td>1.891096</td><td>2.957427</td><td>1.654005</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.160784</td><td>1.910810</td><td>1.853388</td><td>2.909808</td><td>3.060548</td></tr><tr><td>7 Pt</td><td>3.918124</td><td>2.201748</td><td>3.568501</td><td>4.033149</td><td>3.415407</td></tr><tr><td>8 B</td><td>3.590508</td><td>1.737892</td><td>3.705258</td><td>3.062444</td><td>1.740784</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td></tr><tr><td>7 Pt</td><td>2.176675</td><td>0.000000</td><td></td></tr><tr><td>8 B</td><td>3.061391</td><td>2.224430</td><td>0.000000</td></tr></table> Pt7-H-B8 Pt7-H 1.69 B8-H 1.41 B3-H-B4 B3-H 1.30 B4-H 1.33 B3-H-B6 B3-H 1.30 B6-H 1.32 B5-H-B8 B5-H 1.44 B8-H 1.26		1	2	3	4	5	1 Pt	0.000000					2 B	2.196113	0.000000				3 B	2.112960	2.969369	0.000000			4 B	2.174286	2.785778	1.822194	0.000000		5 B	2.549982	1.891096	2.957427	1.654005	0.000000	6 B	2.160784	1.910810	1.853388	2.909808	3.060548	7 Pt	3.918124	2.201748	3.568501	4.033149	3.415407	8 B	3.590508	1.737892	3.705258	3.062444	1.740784		6	7	8	6 B	0.000000			7 Pt	2.176675	0.000000		8 B	3.061391	2.224430	0.000000
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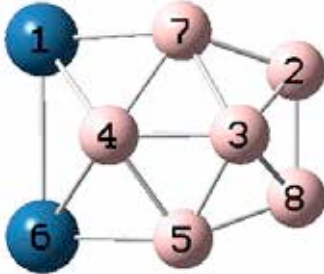
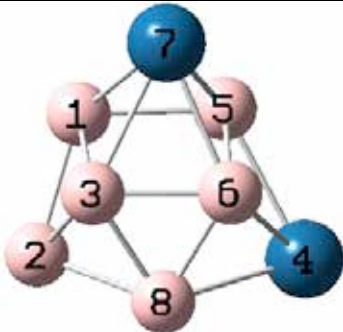
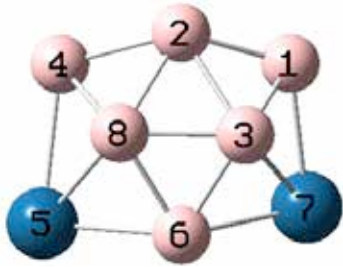


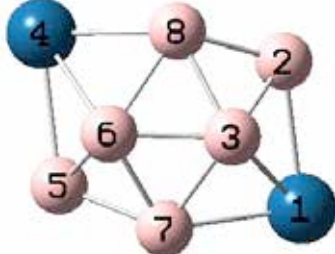
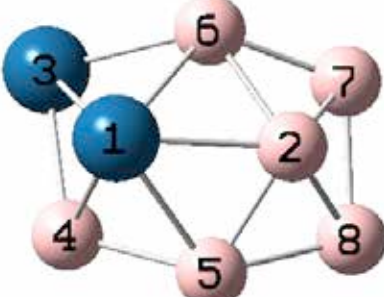
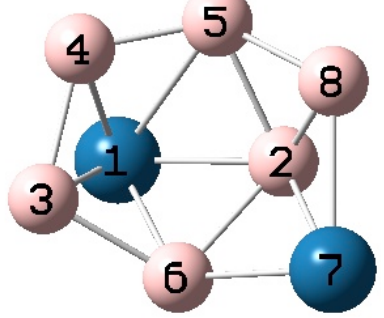
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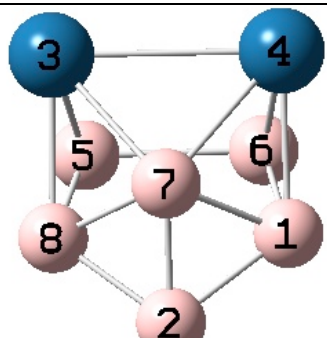
	1	2	3	4	5	
1 B	0.000000					
2 B	1.832265	0.000000				
3 Pt	3.504971	3.517525	0.000000			
4 Pt	2.176739	3.513909	2.660328	0.000000		
5 B	3.091911	3.051010	2.076524	3.180469	0.000000	
6 B	1.841505	3.052481	3.179216	2.076063	2.180342	
7 B	1.792964	1.694089	2.241521	2.239518	2.737039	
8 B	2.832307	1.833506	2.178622	3.502779	1.841031	
	6	7	8			
6 B	0.000000					
7 B	2.738642	0.000000				
8 B	3.093768	1.790125	0.000000			

B1-H-B6 B1-H 1.33 B6-H 1.29
B8-H-B5 B8-H 1.33 B5-H 1.29
B5-H-B6 B5-H 1.30 B6-H 1.30
B2-H 1.20

Table 11B. Distance table for the lowest-lying $\text{Cp}^*\text{Pt}_2\text{B}_6\text{H}_{10}$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.) and relative energy (kcal/mol).

 Cp*Pt2B6H10-1 = Pt2B6-1 -1173.892811 0.0	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.553375</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>3.448897</td><td>1.730020</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.183913</td><td>2.948800</td><td>1.819975</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.519939</td><td>2.870266</td><td>1.772778</td><td>1.830773</td><td>0.000000</td></tr><tr><td>6 Pt</td><td>2.723346</td><td>4.193925</td><td>3.452360</td><td>2.187522</td><td>2.149961</td></tr><tr><td>7 B</td><td>2.159973</td><td>1.771999</td><td>1.775068</td><td>1.830262</td><td>2.877236</td></tr><tr><td>8 B</td><td>4.154922</td><td>1.758784</td><td>1.733908</td><td>2.946859</td><td>1.777338</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.545105</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.556595</td><td>2.860174</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pt	0.000000					2 B	3.553375	0.000000				3 B	3.448897	1.730020	0.000000			4 B	2.183913	2.948800	1.819975	0.000000		5 B	3.519939	2.870266	1.772778	1.830773	0.000000	6 Pt	2.723346	4.193925	3.452360	2.187522	2.149961	7 B	2.159973	1.771999	1.775068	1.830262	2.877236	8 B	4.154922	1.758784	1.733908	2.946859	1.777338		6	7	8			6 Pt	0.000000					7 B	3.545105	0.000000				8 B	3.556595	2.860174	0.000000		
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 Cp*Pt2B6H10-6 = Pt2B6-6 -1173.877066 +9.9	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 Pt</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.200671</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.115152</td><td>2.966985</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.179120</td><td>2.805579</td><td>1.819584</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.507964</td><td>1.875973</td><td>2.934943</td><td>1.655051</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.167358</td><td>1.896292</td><td>1.860120</td><td>2.920460</td><td>3.032950</td></tr><tr><td>7 Pt</td><td>3.931343</td><td>2.193551</td><td>3.595188</td><td>4.073212</td><td>3.431705</td></tr><tr><td>8 B</td><td>3.594046</td><td>1.745912</td><td>3.700587</td><td>3.074447</td><td>1.757973</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 Pt</td><td>2.181087</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.054551</td><td>2.236691</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 Pt	0.000000					2 B	2.200671	0.000000				3 B	2.115152	2.966985	0.000000			4 B	2.179120	2.805579	1.819584	0.000000		5 B	2.507964	1.875973	2.934943	1.655051	0.000000	6 B	2.167358	1.896292	1.860120	2.920460	3.032950	7 Pt	3.931343	2.193551	3.595188	4.073212	3.431705	8 B	3.594046	1.745912	3.700587	3.074447	1.757973		6	7	8			6 B	0.000000					7 Pt	2.181087	0.000000				8 B	3.054551	2.236691	0.000000		
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8 B	3.054551	2.236691	0.000000																																																																												



Cp*Pt2B6H10-7 = Pt2B6-7
-1173.858508 +21.5

	1	2	3	4	5
1 B	0.000000				
2 B	1.805272	0.000000			
3 Pt	3.515589	3.505114	0.000000		
4 Pt	2.176099	3.499059	2.731460	0.000000	
5 B	3.060389	3.055818	2.077144	3.192699	0.000000
6 B	1.855226	3.058813	3.167911	2.077172	2.123478
7 B	1.806418	1.714497	2.225991	2.221478	2.738132
8 B	2.789916	1.808686	2.178206	3.515865	1.850904
	6	7	8		
6 B	0.000000				
7 B	2.734396	0.000000			
8 B	3.057770	1.801585	0.000000		

Table 11C. Energy ranking for all of the $\text{Cp}_2\text{Pt}_2\text{B}_6\text{H}_{10}$ optimized structures:

Nr.	Name	Energy (a.u.)	ΔE (kcal/mol)
1	170_closoTTP-A-o1_Pt-B3LYP	-781.0187487	0.00
2	185_closoTTP-B-h_Pt-B3LYP	-781.0187486	0.00
3	027_hexagonal-b5-_Pt-B3LYP	-781.0140701	2.94
4	186_closoTTP-B-i_Pt-B3LYP	-781.0119703	4.25
5	158_closoTTP-A-m2_Pt-B3LYP	-781.0098774	5.57
6	151_closoTTP-A-l3_Pt-B3LYP	-781.0085402	6.41
7	156_closoTTP-A-l-5_Pt-B3LYP	-781.0085034	6.43
8	154_closoTTP-A-l-4_Pt-B3LYP	-781.008494	6.43
9	152_closoTTP-A-l-3_Pt-B3LYP	-781.0084899	6.44
10	103_closoTTP-A-d2_Pt-B3LYP	-781.0069031	7.43
11	133_closoTTP-A-i2_Pt-B3LYP	-781.0069027	7.43
12	102_closoTTP-A-d1_Pt-B3LYP	-781.0069025	7.43
13	104_closoTTP-A-d3_Pt-B3LYP	-781.0069017	7.43
14	106_closoTTP-A-d5_Pt-B3LYP	-781.0068692	7.45
15	047_hexagonal-d04_Pt-B3LYP	-781.0041386	9.17
16	048_hexagonal-d05_Pt-B3LYP	-781.0039838	9.27
17	184_closoTTP-B-g_Pt-B3LYP	-781.0036843	9.45
18	136_closoTTP-A-i5_Pt-B3LYP	-781.0036843	9.45
19	105_closoTTP-A-d4_Pt-B3LYP	-781.003684	9.45
20	132_closoTTP-A-i1_Pt-B3LYP	-781.0036836	9.45
21	121_closoTTP-A-f-5_Pt-B3LYP	-781.0018151	10.63
22	146_closoTTP-A-k5_Pt-B3LYP	-781.0015771	10.78
23	061_hexagonal-e03_Pt-B3LYP	-781.001343	10.92
24	032_hexagonal-c03_Pt-B3LYP	-781.0013178	10.94
25	071_hexagonal-e13_Pt-B3LYP	-781.0012708	10.97
26	072_hexagonal-e14_Pt-B3LYP	-781.0012708	10.97
27	142_closoTTP-A-k1_Pt-B3LYP	-781.0012706	10.97
28	065_hexagonal-e07_Pt-B3LYP	-781.0012701	10.97
29	181_closoTTP-B-d_Pt-B3LYP	-781.000314	11.57
30	145_closoTTP-A-k4_Pt-B3LYP	-781.0003135	11.57
31	144_closoTTP-A-k3_Pt-B3LYP	-781.0003131	11.57
32	079_hexagonal-f06_Pt-B3LYP	-781.000179	11.65
33	075_hexagonal-f02_Pt-B3LYP	-781.000179	11.65
34	074_hexagonal-f01_Pt-B3LYP	-781.000179	11.65
35	100_closoTTP-A-c4_Pt-B3LYP	-781.0001789	11.65
36	076_hexagonal-f03_Pt-B3LYP	-781.0001789	11.65
37	085_hexagonal-f12_Pt-B3LYP	-781.0001789	11.65
38	082_hexagonal-f09_Pt-B3LYP	-781.0001789	11.65
39	088_hexagonal-f15_Pt-B3LYP	-781.0001789	11.65
40	077_hexagonal-f04_Pt-B3LYP	-781.0001788	11.65
41	078_hexagonal-f05_Pt-B3LYP	-781.0001786	11.65

42	081_hexagonal-f08_Pt-B3LYP	-781.0001785	11.65
43	080_hexagonal-f07_Pt-B3LYP	-781.0001779	11.65
44	099_closoTTP-A-c3_Pt-B3LYP	-781.0001722	11.66
45	024_hexagonal-b4_Pt-B3LYP	-780.9976892	13.22
46	155_closoTTP-A-l5_Pt-B3LYP	-780.9959351	14.32
47	066_hexagonal-e08_Pt-B3LYP	-780.9959343	14.32
48	067_hexagonal-e09_Pt-B3LYP	-780.9959342	14.32
49	153_closoTTP-A-l4_Pt-B3LYP	-780.9958901	14.34
50	060_hexagonal-e02_Pt-B3LYP	-780.9958894	14.34
51	059_hexagonal-e01_Pt-B3LYP	-780.9958894	14.34
52	064_hexagonal-e06_Pt-B3LYP	-780.9958891	14.34
53	068_hexagonal-e10_Pt-B3LYP	-780.9958887	14.34
54	069_hexagonal-e11_Pt-B3LYP	-780.9958881	14.35
55	070_hexagonal-e12_Pt-B3LYP	-780.9958865	14.35
56	147_closoTTP-A-l1_Pt-B3LYP	-780.9957649	14.42
57	062_hexagonal-e04_Pt-B3LYP	-780.9952299	14.76
58	014_hexagonal-a3_Pt-B3LYP	-780.9949309	14.95
59	183_closoTTP-B-f_Pt-B3LYP-i57	-780.9948128	15.02
60	090_closoTTP-A-a2_Pt-B3LYP	-780.9948115	15.02
61	091_closoTTP-A-a3_Pt-B3LYP	-780.9948111	15.02
62	183_closoTTP-B-f_Pt-B3LYP-19	-780.9948108	15.02
63	042_hexagonal-c13_Pt-B3LYP	-780.993394	15.91
64	040_hexagonal-c11_Pt-B3LYP	-780.9933931	15.91
65	041_hexagonal-c12_Pt-B3LYP	-780.9933929	15.91
66	043_hexagonal-c14_Pt-B3LYP	-780.9933926	15.91
67	021_hexagonal-b2_Pt-B3LYP	-780.9933023	15.97
68	026_hexagonal-b5_Pt-B3LYP	-780.9930229	16.14
69	051_hexagonal-d08_Pt-B3LYP	-780.9930167	16.15
70	023_hexagonal-b3-_Pt-B3LYP-i334	-780.9925603	16.43
71	022_hexagonal-b3_Pt-B3LYP	-780.9925556	16.44
72	028_hexagonal-b6_Pt-B3LYP	-780.9925552	16.44
73	019_hexagonal-b1-_Pt-B3LYP-i414	-780.9917049	16.97
74	020_hexagonal-b2_Pt-B3LYP	-780.9917046	16.97
75	019_hexagonal-b1-_Pt-B3LYP-i19	-780.9917044	16.97
76	089_closoTTP-A-a1_Pt-B3LYP-i85	-780.9917032	16.97
77	019_hexagonal-b1-_Pt-B3LYP-i53.	-780.991703	16.97
78	018_hexagonal-b1_Pt-B3LYP	-780.9917027	16.97
79	089_closoTTP-A-a1_Pt-B3LYP-i14	-780.9917025	16.97
80	063_hexagonal-e05_Pt-B3LYP	-780.9907415	17.57
81	140_closoTTP-A-j4_Pt-B3LYP-i59	-780.9903217	17.84
82	139_closoTTP-A-j3_Pt-B3LYP	-780.9903215	17.84
83	092_closoTTP-A-b1_Pt-B3LYP	-780.9902873	17.86
84	093_closoTTP-A-b2_Pt-B3LYP	-780.9902848	17.86

85	033_hexagonal-c04_Pt-B3LYP	-780.989319	18.47
86	034_hexagonal-c05_Pt-B3LYP-i19	-780.9886929	18.86
87	180_closoTTP-B-c_Pt-B3LYP	-780.9866989	20.11
88	127_closoTTP-A-h1_Pt-B3LYP	-780.9866988	20.11
89	097_closoTTP-A-c1_Pt-B3LYP	-780.9866988	20.11
90	030_hexagonal-c01_Pt-B3LYP	-780.9863084	20.36
91	095_closoTTP-A-b4_Pt-B3LYP	-780.9862942	20.37
92	138_closoTTP-A-j2_Pt-B3LYP	-780.9861	20.49
93	137_closoTTP-A-j1_Pt-B3LYP	-780.9860975	20.49
94	128_closoTTP-A-h2_Pt-B3LYP	-780.9824959	22.75
95	159_closoTTP-A-m3_Pt-B3LYP	-780.9814107	23.43
96	052_hexagonal-d09_Pt-B3LYP	-780.9796437	24.54
97	031_hexagonal-c02_Pt-B3LYP	-780.9786732	25.15
98	163_closoTTP-A-n-2_Pt-B3LYP	-780.9780421	25.54
99	165_closoTTP-A-n-3_Pt-B3LYP	-780.9780416	25.54
100	126_closoTTP-A-g5_Pt-B3LYP	-780.9780216	25.56
101	166_closoTTP-A-n4_Pt-B3LYP	-780.9776784	25.77
102	164_closoTTP-A-n3_Pt-B3LYP	-780.9776784	25.77
103	162_closoTTP-A-n2_Pt-B3LYP	-780.977678	25.77
104	143_closoTTP-A-k2_Pt-B3LYP	-780.9774883	25.89
105	178_closoTTP-B-a_Pt-B3LYP	-780.977041	26.17
106	169_closoTTP-A-n-5_Pt-B3LYP	-780.9759819	26.84
107	167_closoTTP-A-n-4_Pt-B3LYP	-780.9759749	26.84
108	160_closoTTP-A-n1_Pt-B3LYP	-780.9756106	27.07
109	113_closoTTP-A-f-1_Pt-B3LYP	-780.975608	27.07
110	118_closoTTP-A-f4_Pt-B3LYP	-780.975481	27.15
111	131_closoTTP-A-h5_Pt-B3LYP	-780.975263	27.29
112	098_closoTTP-A-c2_Pt-B3LYP	-780.975263	27.29
113	049_hexagonal-d06_Pt-B3LYP	-780.9752608	27.29
114	130_closoTTP-A-h4_Pt-B3LYP	-780.9752211	27.31
115	039_hexagonal-c10_Pt-B3LYP	-780.9751436	27.36
116	123_closoTTP-A-g2_Pt-B3LYP	-780.9750559	27.42
117	124_closoTTP-A-g3_Pt-B3LYP	-780.974427	27.81
118	149_closoTTP-A-l2_Pt-B3LYP	-780.9741794	27.97
119	148_closoTTP-A-l-1_Pt-B3LYP-i195	-780.9741762	27.97
120	116_closoTTP-A-f3_Pt-B3LYP	-780.9741718	27.97
121	101_closoTTP-A-c5_Pt-B3LYP	-780.9733098	28.51
122	046_hexagonal-d03_Pt-B3LYP	-780.9726411	28.93
123	087_hexagonal-f14_Pt-B3LYP	-780.9722021	29.21
124	084_hexagonal-f11_Pt-B3LYP	-780.9720684	29.29
125	111_closoTTP-A-e5_Pt-B3LYP	-780.9719649	29.36
126	054_hexagonal-d11_Pt-B3LYP	-780.9717901	29.47
127	086_hexagonal-f13_Pt-B3LYP	-780.9705978	30.22

128	055_hexagonal-d12_Pt-B3LYP	-780.9704105	30.33
129	083_hexagonal-f10_Pt-B3LYP	-780.970185	30.47
130	056_hexagonal-d13_Pt-B3LYP	-780.9696358	30.82
131	057_hexagonal-d14_Pt-B3LYP	-780.9696355	30.82
132	001_B7Mo2-1F_a_Pt-B3LYP	-780.9695713	30.86
133	002_B7Mo2-1F_b1-_Pt-B3LYP	-780.9691941	31.10
134	015_hexagonal-a4_Pt-B3LYP	-780.9688729	31.30
135	174_closoTTP-A-o5_Pt-B3LYP	-780.9675792	32.11
136	171_closoTTP-A-o2_Pt-B3LYP	-780.9675687	32.12
137	119_closoTTP-A-f-4_Pt-B3LYP	-780.9675343	32.14
138	114_closoTTP-A-f2_Pt-B3LYP	-780.967507	32.15
139	094_closoTTP-A-b3_Pt-B3LYP	-780.9667683	32.62
140	157_closoTTP-A-m1_Pt-B3LYP	-780.9662434	32.95
141	004_B7Mo2-1F_b2_Pt-B3LYP	-780.9661382	33.01
142	112_closoTTP-A-f1_Pt-B3LYP	-780.9661297	33.02
143	117_closoTTP-A-f-3_Pt-B3LYP	-780.9661293	33.02
144	044_hexagonal-d01_Pt-B3LYP	-780.9658727	33.18
145	141_closoTTP-A-j5-Pt-B3LYP	-780.9658541	33.19
146	096_closoTTP-A-b5_Pt-B3LYP	-780.965852	33.19
147	045_hexagonal-d02_Pt-B3LYP	-780.964975	33.74
148	122_closoTTP-A-g1_Pt-B3LYP	-780.9648786	33.80
149	135_closoTTP-A-i4_Pt-B3LYP	-780.9646165	33.97
150	053_hexagonal-d10_Pt-B3LYP	-780.9644955	34.04
151	073_hexagonal-e15_Pt-B3LYP	-780.9637522	34.51
152	173_closoTTP-A-o4_Pt-B3LYP	-780.963606	34.60
153	037_hexagonal-c08_Pt-B3LYP	-780.9622064	35.48
154	035_hexagonal-c06_Pt-B3LYP	-780.9622054	35.48
155	036_hexagonal-c07_Pt-B3LYP	-780.9622053	35.48
156	110_closoTTP-A-e4_Pt-B3LYP	-780.9608422	36.34
157	161_closoTTP-A-n-1_Pt-B3LYP	-780.959477	37.19
158	120_closoTTP-A-f5_Pt-B3LYP	-780.9585516	37.77
159	115_closoTTP-A-f-2_Pt-B3LYP	-780.9585504	37.77
160	016_hexagonal-a5_Pt-B3LYP	-780.9585335	37.79
161	179_closoTTP-B-b_Pt-B3LYP	-780.9582024	37.99
162	012_hexagonal-a1_Pt-B3LYP-i23	-780.9580705	38.08
163	109_closoTTP-A-e3_Pt-B3LYP	-780.9564068	39.12
164	013_hexagonal-a2_Pt-B3LYP	-780.9561176	39.30
165	129_closoTTP-A-h3_Pt-B3LYP	-780.9561134	39.30
166	134_closoTTP-A-i3_Pt-B3LYP	-780.9552912	39.82
167	175_closoTTP-A-p1_Pt-B3LYP-i415	-780.9552912	39.82
168	176_closoTTP-A-p2_Pt-B3LYP	-780.9552749	39.83
169	108_closoTTP-A-e2_Pt-B3LYP	-780.9539758	40.65
170	008_B7Mo2-1F_c_Pt-B3LYP	-780.9538119	40.75

171	177_closoTTP-A-p3_Pt-B3LYP	-780.9532711	41.09
172	187_closoTTP-B-j_Pt-B3LYP-i248	-780.9532701	41.09
173	058_hexagonal-d15_Pt-B3LYP	-780.9528281	41.37
174	182_closoTTP-B-e_Pt-B3LYP	-780.9519866	41.89
175	038_hexagonal-c09_Pt-B3LYP	-780.9514	42.26
176	017_hexagonal-a6_Pt-B3LYP-i158	-780.9502592	42.98
177	150_closoTTP-A-l-2_Pt-B3LYP	-780.9497144	43.32
178	107_closoTTP-A-e1_Pt-B3LYP	-780.9487919	43.90
179	172_closoTTP-A-o3_Pt-B3LYP	-780.9482696	44.23
180	125_closoTTP-A-g4_Pt-B3LYP	-780.9480044	44.39
181	025_hexagonal-b4-_Pt-B3LYP	-780.9474737	44.73
182	168_closoTTP-A-n5_Pt-B3LYP	-780.9442311	46.76
183	009_B7Mo2-1F_c-_Pt-B3LYP	-780.9440879	46.85
184	005_B7Mo2-1F_b2-_Pt-B3LYP	-780.941917	48.21
185	011_B7Mo2-1F_d-_Pt-B3LYP	-780.9297803	55.83
186	140_closoTTP-A-j4_Pt-B3LYP	-780.9286015	56.57
187	007_B7Mo2-1F_b3-_Pt-B3LYP	-780.9262036	58.07
188	029_hexagonal-b6-_Pt-B3LYP	-780.9244153	59.20
189	003_B7Mo2-1F_b1_Pt-B3LYP	-780.9198735	62.05
190	010_B7Mo2-1F_d_Pt-B3LYP	-780.9100794	68.19
191	006_B7Mo2-1F_b3_Pt-B3LYP	-780.8941014	78.22

Table 12. Orbital energies and HOMO-LUMO gaps.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO Gap (kcal/mol)	HOMO/LUMO Gap (eV)
Ta2B6-1	-0.17099	-0.11503	0.05596	1.52
Ta2B6-2	-0.17199	-0.09172	0.08027	2.18
Ta2B6-3	-0.17577	-0.08941	0.08636	2.35
Ta2B6-4	-0.16416	0.08905	0.25321	6.89
Ta2B6-5	-0.18710	0.10403	0.29113	7.92
Ta2B6-6	-0.16795	0.14332	0.31127	8.47
Ta2B6-7	-0.17546	-0.08866	0.08680	2.36
Ta2B6-8	-0.15923	-0.09305	0.06618	1.80
Mo2B6-1	-0.18702	-0.08046	0.10656	2.90
Mo2B6-2	-0.19472	-0.10249	0.09223	2.51
Mo2B6-3	-0.17894	-0.10452	0.07442	2.03
Mo2B6-4	-0.17774	-0.10271	0.07503	2.04
Mo2B6-5	-0.18177	-0.11049	0.07128	1.94
Mo2B6-6	-0.19484	-0.09096	0.10388	2.83
Mo2B6-7	-0.17620	0.10724	0.28344	7.71
W2B6-1	-0.18165	-0.07130	0.11035	3.00
W2B6-2	-0.19297	-0.09438	0.09859	2.68
W2B6-3	-0.17525	-0.09689	0.07836	2.13
W2B6-4	-0.17142	-0.09418	0.07724	2.10
W2B6-5	-0.17888	-0.10250	0.07638	2.08
W2B6-6	-0.19098	-0.08217	0.10881	2.96
W2B6-7	-0.17022	-0.10173	0.06849	1.86
Re2B6-1	-0.17832	-0.05046	0.12786	3.48
Re2B6-2	-0.17864	0.06188	0.24052	6.55
Re2B6-3	-0.14401	-0.07578	0.06823	1.86
Re2B6-4	-0.15042	-0.05665	0.09377	2.55
Re2B6-5	-0.14595	-0.06918	0.07677	2.09
Re2B6-6	-0.18594	-0.08597	0.09997	2.72
Re2B6-7	-0.18589	-0.06850	0.11739	3.19
Re2B6-8	-0.18321	-0.10368	0.07953	2.16
Re2B6-9	-0.18034	-0.08695	0.09339	2.54
Re2B6-10	-0.16375	-0.09180	0.07195	1.96
Re2B6-11	-0.17468	-0.10138	0.07330	1.99
Re2B6-12	-0.13474	-0.07195	0.06279	1.71
Re2B6-13	-0.13861	-0.09707	0.04154	1.13
Ru2B6-1	-0.18308	-0.10768	0.07540	2.05
Ru2B6-2	-0.18291	-0.08047	0.10244	2.79
Ru2B6-3	-0.17762	-0.07212	0.10550	2.87
Ru2B6-4	-0.18279	-0.08221	0.10058	2.74

Ru2B6-5	-0.17730	-0.08718	0.09012	2.45
Ru2B6-6	-0.18150	-0.07512	0.10638	2.89
Ru2B6-7	-0.18515	-0.11010	0.08751	2.38
Ru2B6-8	-0.18684	-0.09933	0.07505	2.04
Ru2B6-9	-0.18284	-0.09355	0.08929	2.43
Ru2B6-10	-0.18045	-0.10387	0.07658	2.08
Ru2B6-11	-0.17696	-0.10431	0.07265	1.98
Ru2B6-12	-0.17475	-0.08635	0.08840	2.41
Os2B6-1	-0.18086	-0.06420	0.11666	3.17
Os2B6-2	-0.17809	-0.09714	0.08095	2.20
Os2B6-3	-0.17533	-0.06238	0.11295	3.07
Os2B6-4	-0.17828	-0.07066	0.10762	2.93
Os2B6-5	-0.17257	-0.07279	0.09978	2.72
Os2B6-6	-0.17984	-0.09632	0.08352	2.27
Os2B6-7	-0.17761	-0.05816	0.09943	2.71
Os2B6-8	-0.17880	-0.07937	0.11945	3.25
Os2B6-9	-0.17241	-0.09135	0.08106	2.21
Os2B6-10	-0.18318	-0.08940	0.09378	2.55
Os2B6-11	-0.18197	-0.08933	0.09264	2.52
Os2B6-12	-0.16935	-0.06834	0.10101	2.75
Rh2B6-1	-0.19065	-0.09247	0.09818	2.67
Rh2B6-2	-0.19394	-0.08690	0.10704	2.91
Rh2B6-3	-0.17779	-0.09433	0.08346	2.27
Rh2B6-4	-0.20320	-0.10818	0.09502	2.59
Rh2B6-5	-0.17750	-0.10560	0.07190	1.96
Rh2B6-6	-0.20401	-0.10375	0.10026	2.73
Rh2B6-7	-0.17857	-0.10011	0.07846	2.14
Rh2B6-8	-0.20006	-0.10094	0.09912	2.70
Rh2B6-9	-0.17930	-0.10388	0.07542	2.05
Rh2B6-10	-0.19345	0.09808	0.29153	7.93
Rh2B6-11	-0.18678	-0.10631	0.08047	2.19
Rh2B6-12	-0.18909	-0.10793	0.08116	2.21
Ir2B6-1	-0.19130	-0.05711	0.13419	3.65
Ir2B6-2	-0.19186	-0.05582	0.13604	3.70
Ir2B6-3	-0.20111	-0.08241	0.11870	3.23
Ir2B6-4	-0.20392	-0.08438	0.11954	3.25
Ir2B6-5	-0.20327	-0.08460	0.11867	3.23
Ir2B6-6	-0.17760	-0.07421	0.10339	2.81
Ir2B6-7	-0.17114	-0.08301	0.08813	2.40
Ir2B6-8	-0.17349	-0.07949	0.09400	2.56
Ir2B6-9	-0.19420	-0.07698	0.11722	3.19
Ir2B6-10	-0.17949	-0.08459	0.09490	2.58
Ir2B6-11	-0.19461	-0.08915	0.10546	2.87

Ir2B6-12	-0.18619	-0.08349	0.10270	2.79
Pd2B6-1	-0.17412	-0.13339	0.04073	1.11
Pd2B6-2	-0.17432	-0.13667	0.03765	1.02
Pd2B6-3	-0.19063	-0.10805	0.08258	2.25
Pd2B6-4	-0.18130	-0.12515	0.05615	1.53
Pd2B6-5	-0.18392	-0.12105	0.06287	1.71
Pd2B6-6	-0.18379	-0.14074	0.04305	1.17
Pd2B6-7	-0.18775	-0.12935	0.05840	1.59
Pt2B6-1	-0.17170	-0.11052	0.06118	1.66
Pt2B6-2	-0.19578	-0.08292	0.11286	3.07
Pt2B6-3	-0.17384	-0.11351	0.06033	1.64
Pt2B6-4	-0.18389	-0.10366	0.08023	2.18
Pt2B6-5	-0.18599	-0.11461	0.07138	1.94
Pt2B6-6	-0.17593	-0.09467	0.08126	2.21
Pt2B6-7	-0.18140	-0.10811	0.07329	1.99