Supporting information

Novel Non-spherical Deltahedra in Tritungstaboranes Related to the Experimentally Known $Cp^*_3W_3(H)B_8H_8$

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Gaussian 09, Revision E.01,
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 S1A. Initial $Cp_3W_3(H)B_2H_2$ structures, 13 structures.

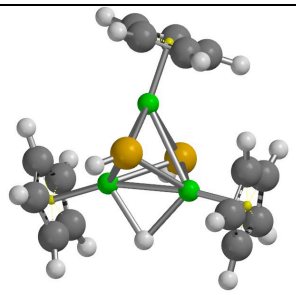 Trigonal bipyramid (13)

Table S1B. Distance table for the lowest-lying $Cp_3W_3(H)B_2H_2$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.
For clarity only the atoms of the cluster framework and the extra H atom are presented.

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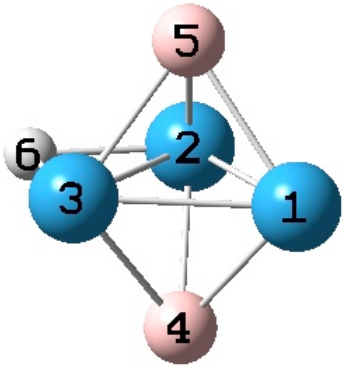
<td> 

1. -833.4208275 0.0 C_{2v}</td>
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		1	2	3	4	5
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2	W	2.528219	0.000000			
3	W	2.525083	2.567552	0.000000		
4	B	2.214111	2.259919	2.223785	0.000000	
5	B	2.248018	2.230987	2.217268	3.365642	0.000000
6	H	3.528273	1.845458	1.884068	2.657037	2.669243

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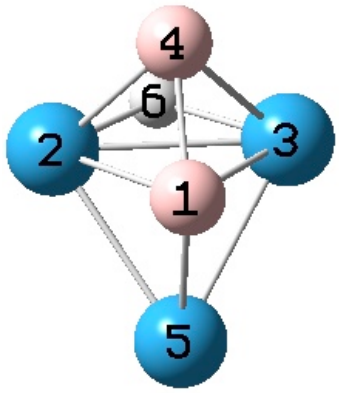
<td> 

2. -833.4069387 +8.7 C_S</td>
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3	W	2.301645	2.568376	0.000000		
4	B	1.757948	2.171043	2.179226	0.000000	
5	W	2.116828	2.533289	2.537798	3.387630	0.000000
6	H	3.313204	1.856886	1.912194	2.729485	3.132911

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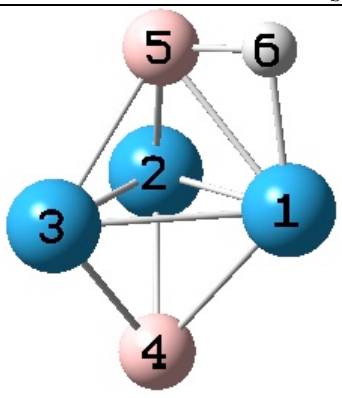
<td> 

3. -833.3990899 +13.6 C_1</td>
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		1	2	3	4	5
1	W	0.000000				
2	W	2.549187	0.000000			
3	W	2.541396	2.547517	0.000000		
4	B	2.348572	2.177537	2.149758	0.000000	
5	B	2.254243	2.239072	2.294653	3.388315	0.000000
6	H	1.797635	3.061474	3.017871	3.788733	1.355713

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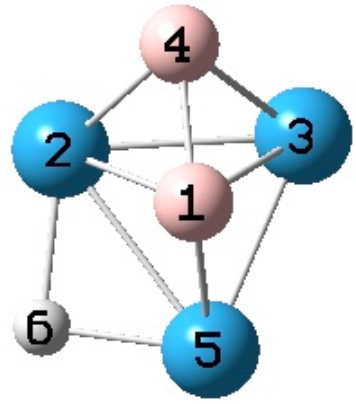

4. -833.3912758 +18.5 C_1

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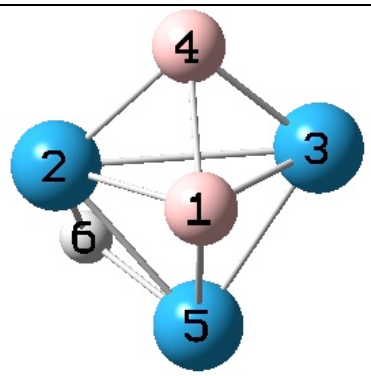
1 B	0.000000				
2 W	2.391783	0.000000			
3 W	2.370191	2.531681	0.000000		
4 B	1.720094	2.178039	2.197100	0.000000	
5 W	2.108906	2.647736	2.492652	3.353451	0.000000
6 H	2.832688	1.873232	3.378197	3.614434	1.845061



5. -833.3733413 +29.8 C_1

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1 B	0.000000				
2 W	2.170813	0.000000			
3 W	2.155750	2.971241	0.000000		
4 B	1.908902	2.152804	2.102759	0.000000	
5 W	2.459433	2.514644	2.465142	3.479865	0.000000
6 H	3.281092	1.868552	3.148508	3.439965	1.848803

Table S1C. Energy ranking for all of the $Cp_3W_3(H)B_2H_2$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	05v-TrigPiPyr--W3----a4	-833.2107874	0.00
2	05v-TrigPiPyr--W3----a1	-833.2106958	0.06
3	05v-TrigPiPyr--W3----b4	-833.1989470	7.43
4	05v-TrigPiPyr--W3----a2	-833.1962942	9.09
5	05v-TrigPiPyr--W3----a3	-833.1960856	9.23
6	05v-TrigPiPyr--W3----b1	-833.1831180	17.36
7	05v-TrigPiPyr--W3----b2	-833.1705766	25.23
8	05v-TrigPiPyr--W3----c3	-833.1704894	25.29
9	05v-TrigPiPyr--W3----b3	-833.1489648	38.79
10	05v-TrigPiPyr--W3----c2	-833.1269875	52.59
11	05v-TrigPiPyr--W3----c4	-833.1262432	53.05
12	05v-TrigPiPyr--W3----c1_r-12	-833.1212001	56.22
13	05v-TrigPiPyr--W3----c1_i-12	-833.1210071	56.34

Table S2A. Initial $Cp_3W_3(H)B_3H_3$ structures, 30 structures.

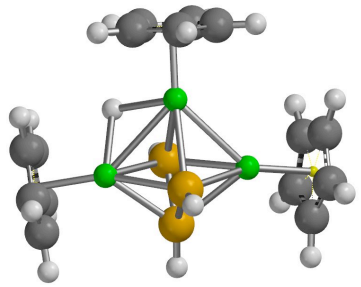
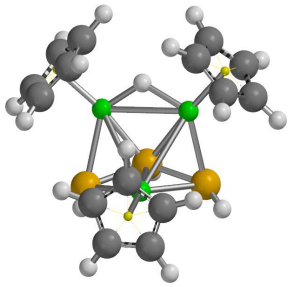
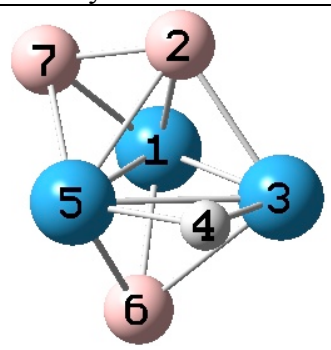
 Octahedron (18)	 Bicapped tetrahedron (12)

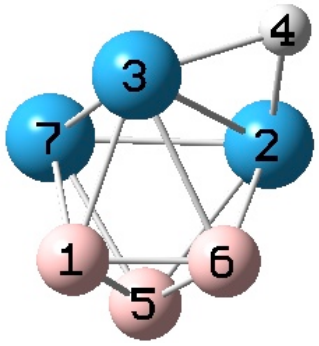
Table S2B. Distance table for the lowest-lying $Cp_3W_3(H)B_3H_3$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



1. -858.9000002 0.0 C_S

		1	2	3	4	5
1	W	0.000000				
2	B	2.362674	0.000000			
3	W	2.503148	2.169479	0.000000		
4	H	3.734822	2.680419	1.881132	0.000000	
5	W	2.894315	2.348627	2.554740	1.851585	0.000000
6	B	2.203626	3.304362	2.314407	2.799055	2.147816
7	B	2.145723	1.742744	3.292409	3.550167	2.176281

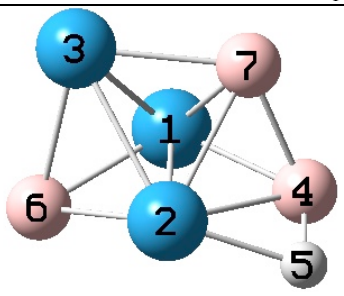
		6	7
6	B	0.000000	
7	B	3.165498	0.000000



2. -858.8944597 +3.5 C_1

		1	2	3	4	5
1	B	0.000000				
2	W	3.103180	0.000000			
3	W	2.236155	2.605478	0.000000		
4	H	3.584758	1.843030	1.894200	0.000000	
5	B	1.692153	2.321363	3.086090	3.634350	0.000000
6	B	1.718140	2.245141	2.359244	2.769146	1.731268
7	W	2.392284	2.490988	2.504672	3.296883	2.244967

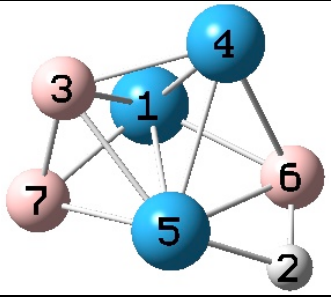
		6	7
6	B	0.000000	
7	W	3.108975	0.000000



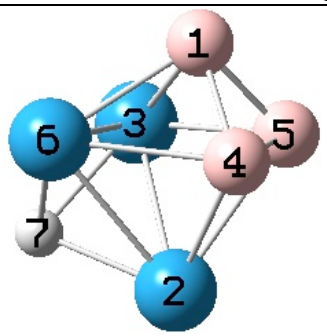
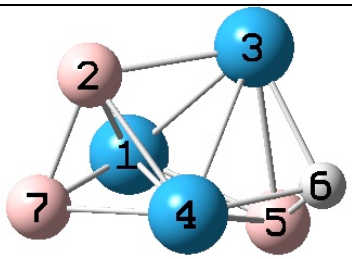
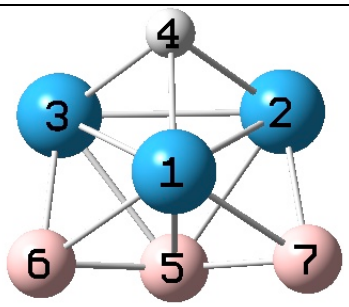
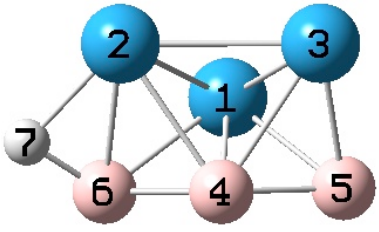
3. -858.8923123 +4.8 C_1

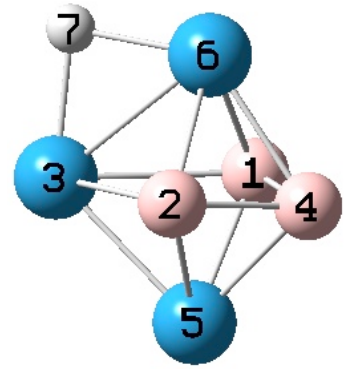
		1	2	3	4	5
1	W	0.000000				
2	W	2.737377	0.000000			
3	W	2.500369	2.532899	0.000000		
4	B	2.180817	2.226325	3.508758	0.000000	
5	H	3.122175	1.879705	3.983668	1.265779	0.000000
6	B	2.190458	2.217770	2.278435	3.379389	3.583271
7	B	2.284077	2.298928	2.198636	1.908816	2.627560

		6	7
6	B	0.000000	
7	B	3.342575	0.000000



		1	2	3	4	5
1	W	0.000000				
2	H	3.090633	0.000000			
3	B	2.260466	3.766618	0.000000		
4	W	2.522989	3.108675	2.183345	0.000000	
5	W	2.805305	1.833491	2.327073	2.524994	0.000000
6	B	2.203984	1.313740	3.379739	2.383067	2.276051
7	B	2.118455	3.386184	1.785296	3.382952	2.192873

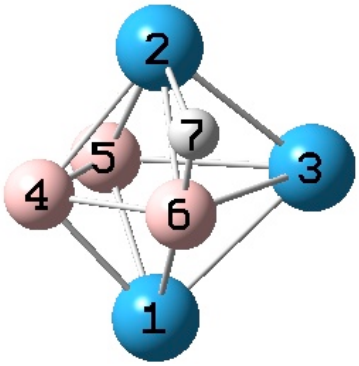
4. -858.8922286 +4.9 C_1	6 7 7 B 3.299606 0.000000
 5. -858.8870446 +8.1 C_1	1 2 3 4 5 1 B 0.000000 2 W 3.100155 0.000000 3 W 2.364459 2.562541 0.000000 4 B 1.722653 2.214132 3.104008 0.000000 5 B 1.722407 2.358190 2.217255 1.722483 0.000000 6 W 2.214224 2.563676 2.563285 2.360749 3.099747 7 H 3.308628 1.955240 1.953451 3.308108 3.306226 6 7 6 W 0.000000 7 H 1.957526 0.000000
 6. -858.8870373 +8.2 C_1	1 2 3 4 5 1 W 0.000000 2 B 2.304554 0.000000 3 W 2.514542 2.215387 0.000000 4 W 2.809347 2.246710 2.586109 0.000000 5 B 2.157761 3.361747 2.383925 2.329493 0.000000 6 H 3.068910 3.291940 2.002809 1.933903 1.415813 7 B 2.121117 1.838090 3.428336 2.128762 3.238664 6 7 6 H 0.000000 7 B 3.631805 0.000000
 7. -858.8851149 +9.3 C_S	1 2 3 4 5 1 W 0.000000 2 W 2.618285 0.000000 3 W 2.630518 2.672223 0.000000 4 H 1.933730 2.016756 2.018929 0.000000 5 B 2.288459 2.283757 2.290983 2.984862 0.000000 6 B 2.241095 3.564485 2.052142 3.169889 1.802515 7 B 2.233457 2.052677 3.572850 3.174394 1.799714 6 7 6 B 0.000000 7 B 3.189488 0.000000
 8. -858.8711488 +18.1 C_1	1 2 3 4 5 1 W 0.000000 2 W 2.608254 0.000000 3 W 2.520564 2.578518 0.000000 4 B 2.327160 2.306830 2.299217 0.000000 5 B 2.250291 3.530097 2.080273 1.748642 0.000000 6 B 2.250651 2.186022 3.537421 1.776501 3.082255 7 H 3.071922 1.830513 4.028326 2.619257 4.131795 6 7 6 B 0.000000 7 H 1.290654 0.000000



9. -858.8681750 +20.0 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	2.875407	0.000000			
3 W	2.499511	2.495254	0.000000		
4 B	1.894827	1.897655	3.273244	0.000000	
5 W	2.207583	2.208168	2.463632	2.098927	0.000000
6 W	2.172057	2.169821	2.556992	2.192862	3.289656
7 H	2.985950	2.995701	1.838035	3.680371	3.864100

	6	7
6 W	0.000000	
7 H	1.821616	0.000000



10. -858.8619556 +23.9 C_1

	1	2	3	4	5
1 W	0.000000				
2 W	3.253526	0.000000			
3 W	2.537849	2.534185	0.000000		
4 B	2.133388	2.208529	3.378696	0.000000	
5 B	2.144254	2.234143	2.471374	1.909570	0.000000
6 B	2.069142	2.115535	2.542586	1.867111	2.764097
7 H	3.311191	1.964588	3.138145	2.557185	3.530183

	6	7
6 B	0.000000	
7 H	1.260314	0.000000

Table S2C. Energy ranking for all of the $Cp_3W_3(H)B_3H_3$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	06v-02-BicappTd----29	-858.6719920	0.00
2	06v-02-BicappTd----30	-858.6719908	0.00
3	06v-02-BicappTd----25	-858.6719817	0.01
4	06v-02-BicappTd----28	-858.6688481	1.97
5	06v-01-Oh----13	-858.6658017	3.88
6	06v-01-Oh----3	-858.6658010	3.88
7	06v-02-BicappTd----27	-858.6657983	3.89
8	06v-01-Oh----11	-858.6650908	4.33
9	06v-02-BicappTd----26	-858.6605532	7.18
10	06v-02-BicappTd----23	-858.6596692	7.73
11	06v-02-BicappTd----22	-858.6596666	7.73
12	06v-01-Oh----12	-858.6570925	9.35
13	06v-02-BicappTd----24	-858.6536754	11.49
14	06v-02-BicappTd----21	-858.6440813	17.51
15	06v-01-Oh----6	-858.6404974	19.76
16	06v-01-Oh----17	-858.6404972	19.76
17	06v-01-Oh----15	-858.6404969	19.76
18	06v-01-Oh----4	-858.6404949	19.76
19	06v-01-Oh----16	-858.6356056	22.83
20	06v-01-Oh----18	-858.6356005	22.84
21	06v-01-Oh----7	-858.6332726	24.30
22	06v-01-Oh----9	-858.6332540	24.31
23	06v-01-Oh----8	-858.6332395	24.32
24	06v-02-BicappTd----19	-858.6298701	26.43
25	06v-02-BicappTd----20	-858.6295087	26.66
26	06v-01-Oh----1	-858.6263585	28.64
27	06v-01-Oh----2	-858.6263548	28.64
28	06v-01-Oh----14	-858.6263527	28.64
29	06v-01-Oh----10	-858.5952495	48.16
30	06v-01-Oh----5	-858.5828458	55.94

Table S3A. Initial $Cp_3W_3(H)B_4H_4$ structures, 85 structures.

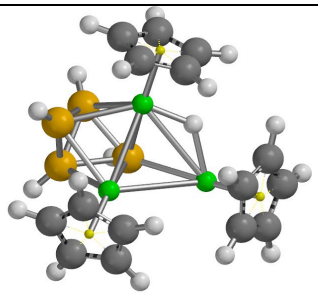
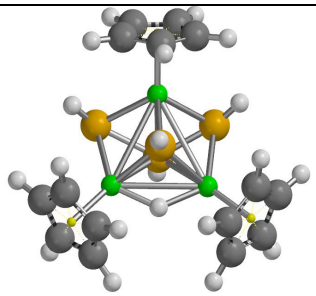
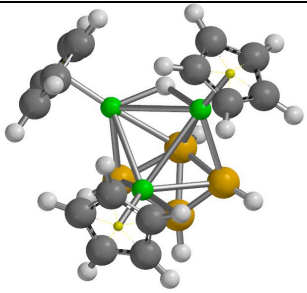
 Capped octahedron (51)	 Tricapped tetrahedron (14)	 Pentagonal bipyramid (21)

Table S3B. Distance table for the lowest-lying $Cp_3W_3(H)B_4H_4$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

<table>
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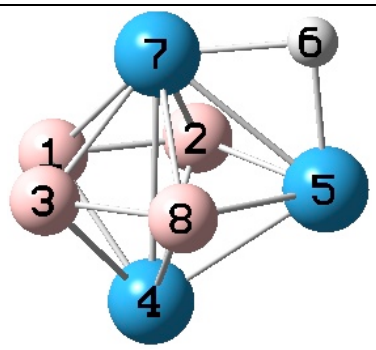
<td> 

1. -884.4134176 0.0 C_S</td>
<td>
<table>
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<tr><td>6</td><td>H</td><td>3.666699</td><td>2.762527</td><td>3.678144</td><td>3.753303</td><td>1.826661</td></tr>
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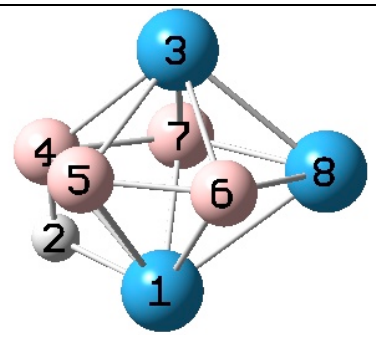
<td> 

2. -884.3874361 +16.3 C_1</td>
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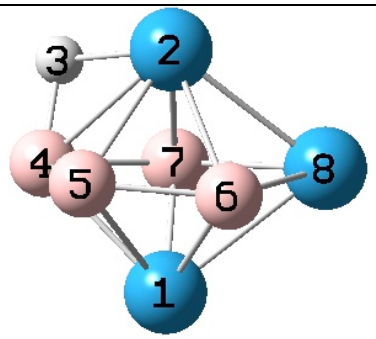
<td> 

3. -884.3853102 +17.6 C_1</td>
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<tr><td>8</td><td>W</td><td>2.496465</td><td>2.523855</td><td>3.546253</td><td>3.464095</td><td>3.446557</td></tr>
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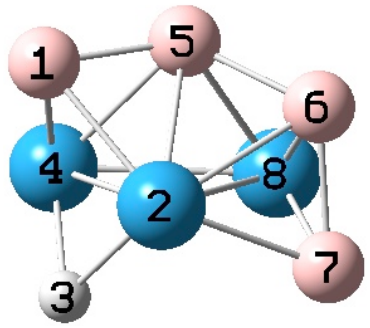
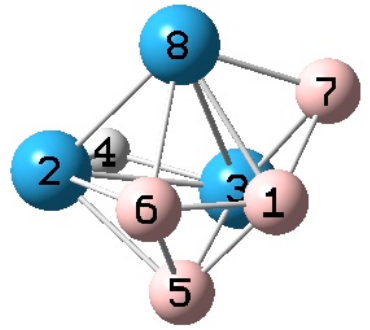


4. -884.3835879 +18.7 C_1

	1	2	3	4	5
1	B	0.000000			
2	W	2.183313	0.000000		
3	H	2.747606	1.896007	0.000000	
4	W	2.097647	2.621638	1.871257	0.000000
5	B	1.785031	2.297522	3.234054	2.301273	0.000000
6	B	3.187544	2.248213	3.650951	3.472700	1.800541
7	B	4.029161	2.267172	3.038299	3.579639	3.080832
8	W	3.615090	2.982891	3.191584	2.582148	2.289082

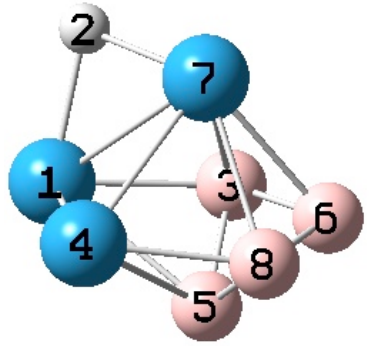
	6	7	8
6	B	0.000000	
7	B	1.856339	0.000000
8	W	2.116212	2.058934	0.000000



5. -884.3800945 +20.9 C_1

	1	2	3	4	5
1	B	0.000000			
2	W	3.120863	0.000000		
3	W	2.355268	2.605519	0.000000	
4	H	3.692284	1.848334	1.852425	0.000000
5	B	1.768962	2.330101	2.229940	3.050601	0.000000
6	B	1.723314	2.293034	3.154139	3.680577	1.703798
7	B	1.818527	3.643884	2.138927	3.513564	3.152937
8	W	2.330393	2.500940	2.884863	3.204199	3.154589

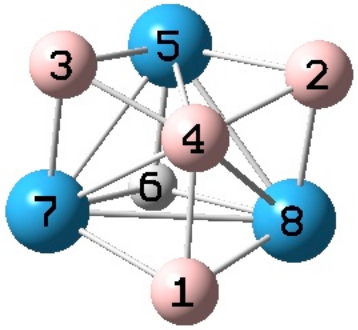
	6	7	8
6	B	0.000000	
7	B	3.136705	0.000000
8	W	2.258318	2.106675	0.000000



6. -884.3756694 +23.7 C_1

	1	2	3	4	5
1	W	0.000000			
2	H	1.859137	0.000000		
3	B	2.148747	2.642039	0.000000	
4	W	2.500410	3.202355	3.411358	0.000000	
5	B	2.383779	3.536891	1.795528	2.410339	0.000000
6	B	3.321398	3.608519	1.690798	3.316469	1.754439
7	W	2.631610	1.898656	2.374816	2.548655	2.815530
8	B	3.398701	3.868430	2.805461	2.134057	1.761290

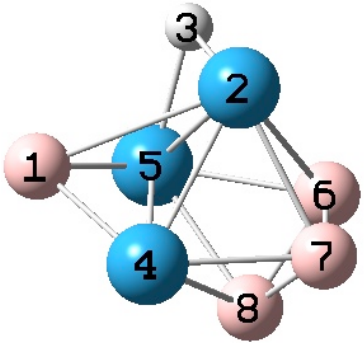
	6	7	8
6	B	0.000000	
7	W	2.310056	0.000000
8	B	1.694039	2.353113	0.000000



7. -884.3717846 +26.1 C_{3v}

		1	2	3	4	5
1	B	0.000000				
2	B	3.125502	0.000000			
3	B	3.125531	3.152113	0.000000		
4	B	1.894832	1.850010	1.850019	0.000000	
5	W	3.419233	2.210850	2.210822	2.309158	0.000000
6	H	2.812007	3.175327	3.175306	2.916723	1.905364
7	W	2.128330	3.714190	2.055078	2.350187	2.611357
8	W	2.128300	2.055052	3.714233	2.350187	2.611436

		6	7	8
6	H	0.000000		
7	W	2.050544	0.000000	
8	W	2.050667	3.036716	0.000000



8. -884.3661218 +29.7 C_S

		1	2	3	4	5
1	B	0.000000				
2	W	2.751335	0.000000			
3	H	2.747100	1.869969	0.000000		
4	W	2.101245	2.506410	3.616867	0.000000	
5	W	2.127041	2.595695	1.861047	2.879199	0.000000
6	B	3.758943	2.365220	2.691954	3.162204	2.255458
7	B	3.754579	2.339627	3.611204	2.259782	3.151695
8	B	3.270314	3.064036	3.569390	2.294422	2.275532

		6	7	8
6	B	0.000000		
7	B	1.691904	0.000000	
8	B	1.714226	1.689401	0.000000

Table S3C. Energy ranking for all of the $Cp_3W_3(H)B_4H_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	07v-03-PentBipyr------76_i-10	-884.1568914	0.00
2	07v-03-PentBipyr------76_r-10	-884.1568424	0.03
3	07v-01-CapOh------31	-884.1567898	0.06
4	07v-03-PentBipyr------72	-884.1566890	0.13
5	07v-01-CapOh------45	-884.1379021	11.92
6	07v-01-CapOh------13	-884.1379013	11.92
7	07v-01-CapOh------46	-884.1378964	11.92
8	07v-01-CapOh------47	-884.1378932	11.92
9	07v-01-CapOh------39_i-18	-884.1360155	13.10
10	07v-03-PentBipyr------73	-884.1359375	13.15
11	07v-03-PentBipyr------75	-884.1359353	13.15
12	07v-01-CapOh------39_r-18	-884.1359092	13.17
13	07v-03-PentBipyr------74	-884.1358976	13.17
14	07v-03-PentBipyr------71	-884.1346817	13.94
15	07v-03-PentBipyr------67	-884.1333530	14.77
16	07v-03-PentBipyr------68	-884.1333484	14.77
17	07v-03-PentBipyr------65	-884.1333467	14.77
18	07v-01-CapOh------49	-884.1291945	17.38
19	07v-01-CapOh------21	-884.1291934	17.38
20	07v-01-CapOh------50	-884.1291914	17.38
21	07v-01-CapOh------24	-884.1291866	17.39
22	07v-01-CapOh------25	-884.1290329	17.48
23	07v-01-CapOh------22	-884.1290123	17.49
24	07v-01-CapOh------27	-884.1289434	17.54
25	07v-01-CapOh------26	-884.1287814	17.64
26	07v-02-TricapTd------61	-884.1275129	18.44
27	07v-02-TricapTd------64	-884.1275128	18.44
28	07v-02-TricapTd------62	-884.1275127	18.44
29	07v-02-TricapTd------63	-884.1275099	18.44
30	07v-01-CapOh------5	-884.1253746	19.78
31	07v-01-CapOh------6	-884.1253746	19.78
32	07v-01-CapOh------18	-884.1253379	19.80
33	07v-01-CapOh------17	-884.1253350	19.80
34	07v-01-CapOh------19	-884.1253340	19.80
35	07v-01-CapOh------48	-884.1253330	19.80
36	07v-01-CapOh------15	-884.1253312	19.80
37	07v-01-CapOh------7	-884.1252798	19.84
38	07v-01-CapOh------8	-884.1252798	19.84

39	07v-02-TricapTd------55_r-23	-884.1252128	19.88
40	07v-02-TricapTd------55_i-23	-884.1247850	20.15
41	07v-03-PentBipyr------83	-884.1223725	21.66
42	07v-01-CapOh------20	-884.1216826	22.09
43	07v-02-TricapTd------60	-884.1216385	22.12
44	07v-01-CapOh------16	-884.1202466	23.00
45	07v-01-CapOh------28	-884.1197253	23.32
46	07v-01-CapOh------4	-884.1194879	23.47
47	07v-03-PentBipyr------77	-884.1194847	23.47
48	07v-03-PentBipyr------78	-884.1194847	23.47
49	07v-02-TricapTd------54	-884.1170760	24.98
50	07v-02-TricapTd------53	-884.1170702	24.99
51	07v-01-CapOh------32	-884.1107239	28.97
52	07v-02-TricapTd------59	-884.1101733	29.32
53	07v-01-CapOh------12	-884.1086561	30.27
54	07v-02-TricapTd------56	-884.1024315	34.17
55	07v-02-TricapTd------57	-884.1024308	34.18
56	07v-02-TricapTd------58	-884.1024308	34.18
57	07v-01-CapOh------10	-884.1023290	34.24
58	07v-01-CapOh------9	-884.1023290	34.24
59	07v-01-CapOh------11	-884.1023283	34.24
60	07v-01-CapOh------1	-884.0994020	36.08
61	07v-01-CapOh------2	-884.0994019	36.08
62	07v-01-CapOh------30	-884.0988491	36.42
63	07v-01-CapOh------29	-884.0988465	36.42
64	07v-01-CapOh------41	-884.0972441	37.43
65	07v-01-CapOh------44	-884.0972416	37.43
66	07v-01-CapOh------40	-884.0965467	37.87
67	07v-01-CapOh------37	-884.0943074	39.27
68	07v-01-CapOh------38	-884.0943074	39.27
69	07v-01-CapOh------14	-884.0942992	39.28
70	07v-03-PentBipyr------69	-884.0907013	41.54
71	07v-03-PentBipyr------70	-884.0906969	41.54
72	07v-01-CapOh------3	-884.0890508	42.57
73	07v-01-CapOh------43	-884.0727298	52.81
74	07v-03-PentBipyr------66	-884.0717772	53.41
75	07v-01-CapOh------51	-884.0648444	57.76
76	07v-03-PentBipyr------84	-884.0640754	58.24
77	07v-03-PentBipyr------80	-884.0628227	59.03
78	07v-01-CapOh------23	-884.0599352	60.84
79	07v-01-CapOh------42	-884.0588003	61.55

80	07v-01-CapOh------33	-884.0575719	62.32
81	07v-01-CapOh------34	-884.0575679	62.33
82	07v-01-CapOh------36	-884.0549301	63.98
83	07v-01-CapOh------35	-884.0548808	64.01
84	07v-03-PentBipyr------81	-884.0431613	71.37
85	07v-03-PentBipyr------82	-884.0431613	71.37
86	07v-03-PentBipyr------79	-884.0366953	75.43
87	07v-01-CapOh------52	-884.0353867	76.25

Table S4A. Initial $Cp_3W_3(H)B_5H_5$ structures, 279 structures.

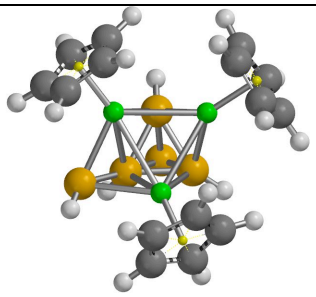
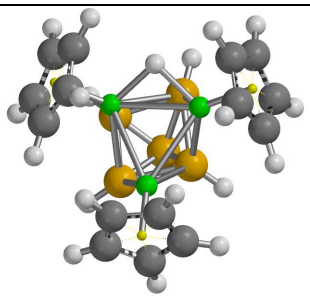
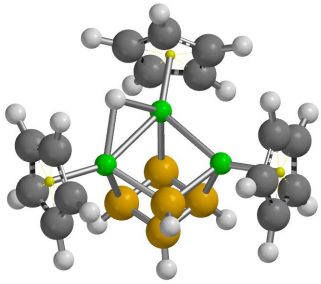
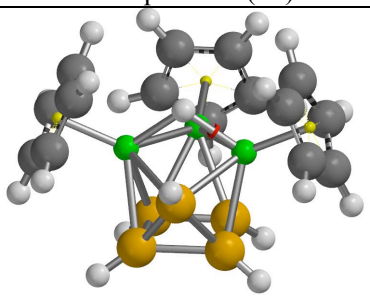
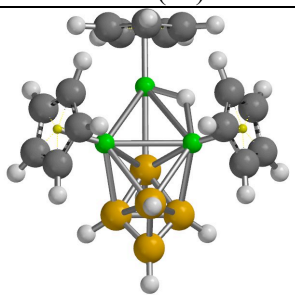
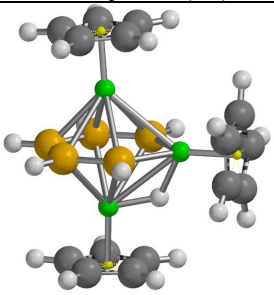
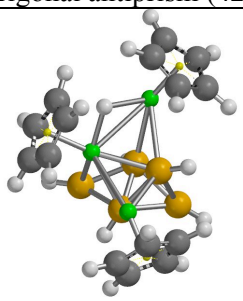
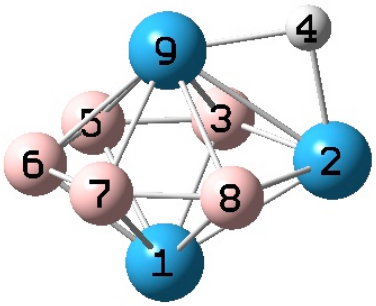
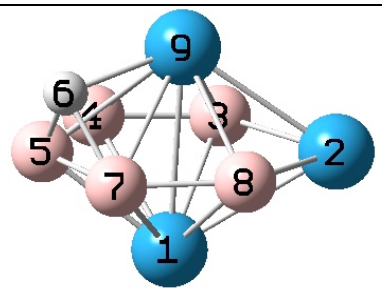
Initial structures	 Dicapped octahedron (70)
 Bisdisphenoid (54)	 Cube (24)
 Antiprism (26)	 Trigonal antiprism (42)
 Hexagonal bipyramid (24)	 All capped tetrahedron (39)

Table S4B. Distance table for the lowest-lying $Cp_3W_3(H)B_5H_5$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



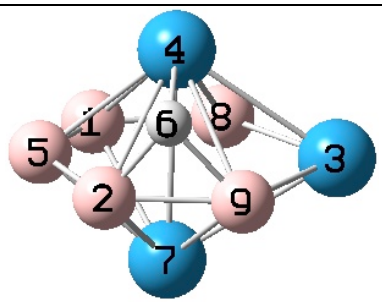
1. -909.9017965 0.0 C_S

		1	2	3	4	5
1	W	0.000000				
2	W	2.570516	0.000000			
3	B	2.354573	2.177299	0.000000		
4	H	3.683048	1.835867	2.660206	0.000000	
5	B	2.257162	3.406632	1.699429	3.582432	0.000000
6	B	2.162464	3.857918	3.016230	3.983625	1.711689
7	B	2.257552	3.407273	3.624171	3.583986	3.019493
8	B	2.353843	2.178391	3.392969	2.663119	3.623453
9	W	2.890665	2.628187	2.378235	1.851573	2.289306
		6	7	8	9	
7	B	1.712584	0.000000			
8	B	3.016006	1.698787	0.000000		
9	W	2.299362	2.289240	2.378213	0.000000	



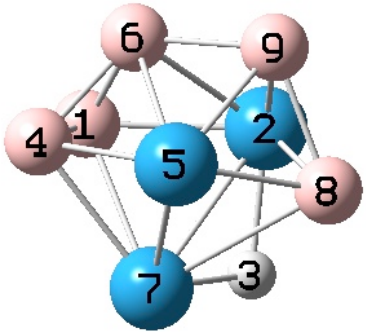
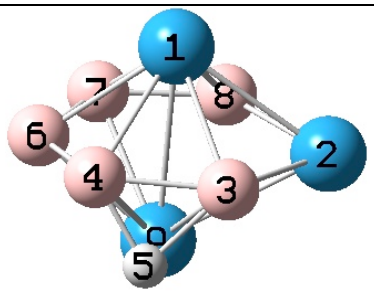
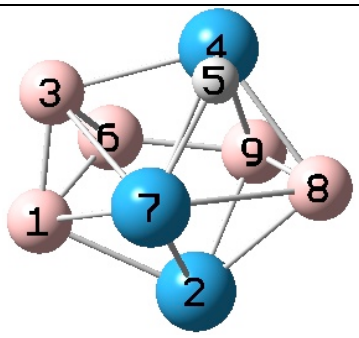
2. -909.8894068 +7.8 (C_S)

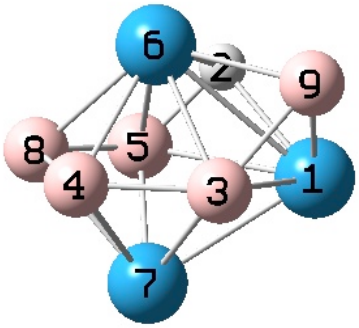
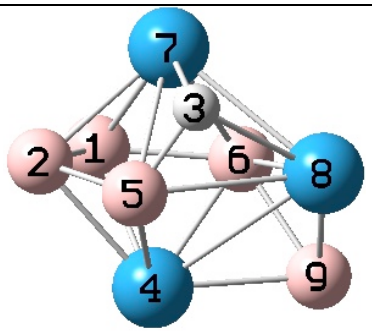
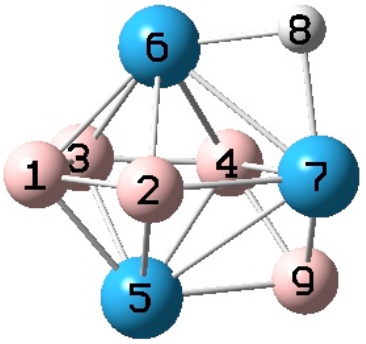
		1	2	3	4	5
1	W	0.000000				
2	W	2.585605	0.000000			
3	B	2.322669	2.179033	0.000000		
4	B	2.275757	3.450613	1.720849	0.000000	
5	B	2.207266	3.937440	3.031897	1.698107	0.000000
6	H	3.016164	3.997449	3.634420	2.667849	1.423349
7	B	2.233426	3.474112	3.657763	3.062275	1.787966
8	B	2.346637	2.188149	3.363207	3.622459	3.069942
9	W	2.815147	2.550488	2.299382	2.261027	2.345847
		6	7	8	9	
6	H	0.000000				
7	B	1.442629	0.000000			
8	B	2.684948	1.722333	0.000000		
9	W	1.919738	2.387013	2.308625	0.000000	

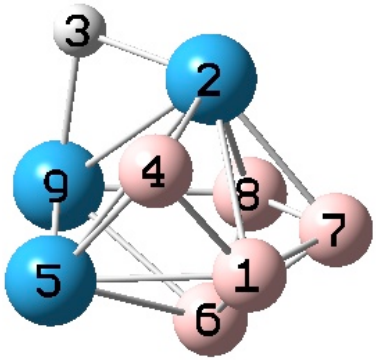


3. -909.8873349 +9.1 (C_S)

		1	2	3	4	5
1	B	0.000000				
2	B	3.028608	0.000000			
3	W	3.424306	3.492618	0.000000		
4	W	2.277562	2.405334	2.581447	0.000000	
5	B	1.699450	1.698456	3.874061	2.236143	0.000000
6	H	3.562070	1.397333	3.155722	1.916630	2.573192
7	W	2.238565	2.236850	2.580318	2.850151	2.234875
8	B	1.717124	3.654196	2.158372	2.301716	3.009074
9	B	3.648627	1.799716	2.181846	2.435371	3.051552
		6	7	8	9	
6	H	0.000000				
7	W	3.047672	0.000000			

	8 B 3.769205 2.335936 0.000000 9 B 1.488999 2.322646 3.381947 0.000000
 4. -909.8867608 +9.4 (C_S)	1 2 3 4 5 1 B 0.000000 2 W 2.192817 0.000000 3 H 2.751037 1.832779 0.000000 4 B 1.701761 3.192539 3.638114 0.000000 5 W 3.224583 3.207386 3.750237 2.205883 0.000000 6 B 1.774514 2.340168 3.635860 1.743049 2.341453 7 W 2.377938 2.592621 1.856898 2.327785 2.509599 8 B 3.614318 2.192217 2.695567 3.596900 2.164921 9 B 3.168633 2.202549 3.649695 3.119644 2.120057 6 7 8 9 6 B 0.000000 7 W 3.071148 0.000000 8 B 3.071359 2.623768 0.000000 9 B 1.839398 3.430459 1.862196 0.000000
 5. -909.8865697 +9.6 (C_S)	1 2 3 4 5 1 W 0.000000 2 W 2.567640 0.000000 3 B 2.278568 2.190175 0.000000 4 B 2.252027 3.497036 1.790158 0.000000 5 H 3.051216 3.172919 1.541403 1.380891 0.000000 6 B 2.246655 3.873081 3.044287 1.703763 2.560615 7 B 2.246692 3.418600 3.640886 3.035308 3.555118 8 B 2.303427 2.149888 3.379832 3.664397 3.791945 9 W 2.848988 2.596284 2.472077 2.396786 1.914906 6 7 8 9 6 B 0.000000 7 B 1.700767 0.000000 8 B 3.017773 1.722392 0.000000 9 W 2.219327 2.263651 2.344059 0.000000
 6. -909.8861976 +9.8 (C_S)	1 2 3 4 5 1 B 0.000000 2 W 2.202948 0.000000 3 B 1.703699 3.222713 0.000000 4 W 3.189120 3.206357 2.186109 0.000000 5 H 3.641598 3.746075 2.752566 1.832852 0.000000 6 B 1.742929 2.346530 1.777371 2.342062 3.642763 7 W 2.332012 2.508158 2.378413 2.592785 1.856725 8 B 3.593585 2.161746 3.610381 2.193730 2.692600 9 B 3.115690 2.123246 3.164118 2.199761 3.645100 6 7 8 9 6 B 0.000000 7 W 3.079640 0.000000 8 B 3.073112 2.625276 0.000000

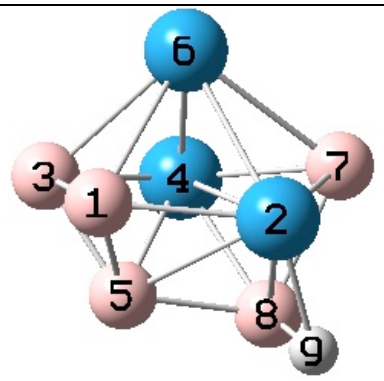
	9 B 1.839542 3.430908 1.858101 0.000000
 7. -909.8784403 +14.7 C_1	1 2 3 4 5 1 W 0.000000 2 H 1.989308 0.000000 3 B 2.350683 3.215972 0.000000 4 B 3.505131 3.504088 1.829917 0.000000 5 B 2.493800 1.474337 3.294373 3.002857 0.000000 6 W 2.786833 1.967023 2.268398 2.188202 2.405194 7 W 2.508637 3.069157 2.298108 2.166594 2.175651 8 B 3.543292 2.729252 3.054414 1.814883 1.753319 9 B 2.082662 2.760545 1.812485 3.243755 3.622177 6 7 8 9 6 W 0.000000 7 W 3.083589 0.000000 8 B 2.187314 2.196002 0.000000 9 B 2.170616 3.573952 3.935631 0.000000
 8. -909.8722074 +18.6 C_1	1 2 3 4 5 1 B 0.000000 2 B 1.806909 0.000000 3 H 3.500025 2.608758 0.000000 4 W 2.170775 2.203344 3.168821 0.000000 5 B 3.025987 1.795626 1.362170 2.212324 0.000000 6 B 1.821973 3.055178 3.401055 2.261337 3.308624 7 W 2.180282 2.160308 1.887407 3.050682 2.345190 8 W 3.516401 3.590009 2.162371 2.754769 2.554321 9 B 3.247416 3.976894 3.824787 2.183501 3.555824 6 7 8 9 6 B 0.000000 7 W 2.308903 0.000000 8 W 2.342762 2.554156 0.000000 9 B 1.828528 3.600168 2.052873 0.000000
 9. -909.8684425 +20.9 C_1	1 2 3 4 5 1 B 0.000000 2 B 1.756468 0.000000 3 B 1.902430 3.011825 0.000000 4 B 3.108005 3.210319 1.853325 0.000000 5 W 2.155649 2.297765 2.124921 2.297966 0.000000 6 W 2.223188 2.284309 2.190915 2.306660 3.124250 7 W 3.484612 2.265107 3.555085 2.430026 2.825615 8 H 3.731684 2.892020 3.678322 2.787194 3.952940 9 B 3.862973 3.371430 3.180998 1.793926 2.138924 6 7 8 9 6 W 0.000000 7 W 2.597146 0.000000 8 H 1.834363 1.826959 0.000000 9 B 3.564878 2.101574 3.464876 0.000000



10. -909.8640859 +23.7 C_1

	1	2	3	4	5
1 B	0.000000				
2 W	2.378290	0.000000			
3 H	3.802682	1.868322	0.000000		
4 B	1.855673	2.179517	3.362187	0.000000	
5 W	2.221412	2.937808	3.258433	2.076124	0.000000
6 B	1.804564	2.820558	3.544622	3.210287	2.350426
7 B	1.732957	2.248133	3.651500	3.159513	3.419692
8 B	2.847554	2.317520	2.764266	3.854025	3.473844
9 W	3.402185	2.646196	1.854399	3.630554	2.494586

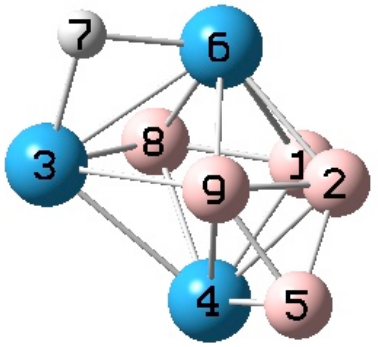
	6	7	8	9
6 B	0.000000			
7 B	1.747006	0.000000		
8 B	1.787198	1.701119	0.000000	
9 W	2.387946	3.316965	2.145217	0.000000



11. -909.8592834 +26.7 C_S

	1	2	3	4	5
1 B	0.000000				
2 W	2.192697	0.000000			
3 B	1.708819	3.193180	0.000000		
4 W	3.199174	3.151438	2.204119	0.000000	
5 B	1.741867	2.397716	1.738625	2.345108	0.000000
6 W	2.408192	2.522149	2.325758	2.449655	3.070916
7 B	3.634221	2.192017	3.615764	2.145093	3.169741
8 B	3.202991	2.226587	3.217516	2.196510	1.933241
9 H	3.316842	1.858679	3.922004	3.343686	2.432954

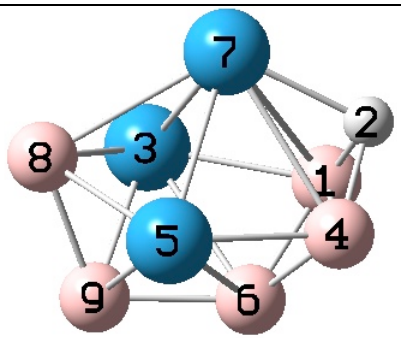
	6	7	8	9
6 W	0.000000			
7 B	2.532177	0.000000		
8 B	3.472793	1.992860	0.000000	
9 H	3.959959	2.526585	1.276532	0.000000



12. -909.8592105 +26.7 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	1.842812	0.000000			
3 W	3.375025	3.573561	0.000000		
4 W	2.163951	2.324395	2.628500	0.000000	
5 B	3.098227	1.749868	3.744132	2.084135	0.000000
6 W	2.218438	2.208414	2.568409	3.144167	3.494817
7 H	3.771594	3.604825	1.848265	3.829952	4.247538
8 B	1.860426	3.138665	2.153345	2.368794	3.980341
9 B	2.970812	1.763728	2.557076	2.383868	1.739777

	6	7	8	9
6 W	0.000000			
7 H	1.856808	0.000000		
8 B	2.256461	2.965868	0.000000	
9 B	2.218778	2.577650	3.289298	0.000000



13. -909.8560231 +28.7 C_S

		1	2	3	4	5
1	B	0.000000				
2	H	1.456282	0.000000			
3	W	2.180092	3.063292	0.000000		
4	B	1.812437	1.453049	3.244317	0.000000	
5	W	3.243316	3.057505	3.182957	2.180391	0.000000
6	B	1.741920	2.589170	2.352730	1.740712	2.354259
7	W	2.501807	1.904911	2.495444	2.510067	2.503228
8	B	3.614311	3.857711	2.155651	3.616255	2.157851
9	B	3.129996	3.850620	2.168658	3.128077	2.166696

		6	7	8	9
6	B	0.000000			
7	W	3.112987	0.000000		
8	B	3.074676	2.505692	0.000000	
9	B	1.839279	3.394505	1.873299	0.000000

Table S4C. Energy ranking for all of the $Cp_3W_3(H)B_5H_5$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	08v-06-Bipireex----W3----214	-909.6220988	0.00
2	08v-06-Bipireex----W3----212	-909.6220968	0.00
3	08v-02-Bisdisph----W3----104	-909.6174008	2.95
4	08v-01-DicapOh----W3----15	-909.6173133	3.00
5	08v-06-Bipireex----W3----211	-909.6169481	3.23
6	08v-06-Bipireex----W3----215	-909.6103829	7.35
7	08v-06-Bipireex----W3----213	-909.6102631	7.43
8	08v-07-Tdallcap----W3----264	-909.6099897	7.60
9	08v-06-Bipireex----W3----216	-909.6093215	8.02
10	08v-01-DicapOh----W3----13	-909.6028714	12.07
11	08v-03-Cube----W3----133	-909.6005785	13.50
12	08v-05-AntiprTrig----W3----198	-909.6004417	13.59
13	08v-02-Bisdisph----W3----85	-909.6003411	13.65
14	08v-05-AntiprTrig----W3----197	-909.6002626	13.70
15	08v-01-DicapOh----W3----3	-909.6002283	13.72
16	08v-06-Bipireex----W3----221	-909.5999527	13.90
17	08v-02-Bisdisph----W3----111	-909.5985221	14.79
18	08v-02-Bisdisph----W3----103	-909.5973858	15.51
19	08v-02-Bisdisph----W3----114	-909.5971017	15.69
20	08v-02-Bisdisph----W3----106	-909.5954999	16.69
21	08v-04-Antipr----W3----167	-909.5948203	17.12
22	08v-04-Antipr----W3----165	-909.5948064	17.13
23	08v-02-Bisdisph----W3----113	-909.5947194	17.18
24	08v-02-Bisdisph----W3----112	-909.5946970	17.20
25	08v-02-Bisdisph----W3----108	-909.5921880	18.77
26	08v-07-Tdallcap----W3----261	-909.5892332	20.62
27	08v-06-Bipireex----W3----233	-909.5891508	20.68
28	08v-04-Antipr----W3----147	-909.5877680	21.54
29	08v-01-DicapOh----W3----55	-909.5876802	21.60
30	08v-01-DicapOh----W3----30	-909.5869746	22.04
31	08v-01-DicapOh----W3----27	-909.5869456	22.06
32	08v-01-DicapOh----W3----26	-909.5859096	22.71
33	08v-06-Bipireex----W3----234	-909.5854990	22.97
34	08v-03-Cube----W3----127	-909.5848167	23.40
35	08v-01-DicapOh----W3----58	-909.5842705	23.74
36	08v-02-Bisdisph----W3----81	-909.5842535	23.75
37	08v-02-Bisdisph----W3----82	-909.5842505	23.75
38	08v-07-Tdallcap----W3----236_i-11	-909.5842451	23.75

39	08v-02-Bisdisph----W3----83	-909.5842371	23.76
40	08v-01-DicapOh----W3----56	-909.5842317	23.76
41	08v-02-Bisdisph----W3----79	-909.5842296	23.76
42	08v-07-Tdallcap----W3----236_r-11	-909.5841601	23.81
43	08v-07-Tdallcap----W3----242	-909.5838663	23.99
44	08v-07-Tdallcap----W3----243	-909.5838392	24.01
45	08v-07-Tdallcap----W3----246	-909.5836959	24.10
46	08v-07-Tdallcap----W3----255_r-11	-909.5836944	24.10
47	08v-07-Tdallcap----W3----241	-909.5834989	24.22
48	08v-07-Tdallcap----W3----255_i-11	-909.5833470	24.32
49	08v-02-Bisdisph----W3----80	-909.5818628	25.25
50	08v-04-Antipr----W3----146	-909.5818277	25.27
51	08v-03-Cube----W3----137	-909.5817767	25.30
52	08v-03-Cube----W3----135	-909.5817581	25.31
53	08v-05-AntiprTrig----W3----195	-909.5817541	25.32
54	08v-02-Bisdisph----W3----90	-909.5817024	25.35
55	08v-01-DicapOh----W3----38	-909.5815178	25.47
56	08v-07-Tdallcap----W3----245	-909.5813896	25.55
57	08v-07-Tdallcap----W3----244	-909.5813710	25.56
58	08v-07-Tdallcap----W3----254_i-22	-909.5813295	25.58
59	08v-07-Tdallcap----W3----254_r-22	-909.5812979	25.60
60	08v-07-Tdallcap----W3----258	-909.5811893	25.67
61	08v-02-Bisdisph----W3----87	-909.5807552	25.94
62	08v-03-Cube----W3----134	-909.5807486	25.95
63	08v-03-Cube----W3----138	-909.5806405	26.02
64	08v-06-Bipireex----W3----217	-909.5800396	26.39
65	08v-03-Cube----W3----124	-909.5796211	26.66
66	08v-03-Cube----W3----121	-909.5795317	26.71
67	08v-02-Bisdisph----W3----88	-909.5795088	26.73
68	08v-01-DicapOh----W3----37	-909.5794510	26.76
69	08v-07-Tdallcap----W3----257	-909.5793751	26.81
70	08v-01-DicapOh----W3----40_r-18	-909.5791920	26.92
71	08v-01-DicapOh----W3----40_i-18	-909.5791808	26.93
72	08v-03-Cube----W3----136	-909.5783859	27.43
73	08v-04-Antipr----W3----152	-909.5763219	28.73
74	08v-02-Bisdisph----W3----84	-909.5763088	28.73
75	08v-01-DicapOh----W3----10	-909.5760852	28.87
76	08v-04-Antipr----W3----166	-909.5760273	28.91
77	08v-03-Cube----W3----129	-909.5752829	29.38
78	08v-01-DicapOh----W3----8	-909.5750750	29.51
79	08v-02-Bisdisph----W3----74	-909.5743947	29.94

80	08v-02-Bisdisph----W3----78	-909.5742906	30.00
81	08v-02-Bisdisph----W3----73	-909.5742883	30.00
82	08v-02-Bisdisph----W3----75	-909.5742716	30.01
83	08v-02-Bisdisph----W3----76	-909.5742612	30.02
84	08v-07-Tdallcap----W3----267	-909.5732928	30.63
85	08v-07-Tdallcap----W3----268	-909.5732352	30.66
86	08v-07-Tdallcap----W3----266	-909.5732184	30.67
87	08v-07-Tdallcap----W3----269	-909.5732065	30.68
88	08v-05-AntiprTrig----W3----194	-909.5728696	30.89
89	08v-04-Antipr----W3----164	-909.5724299	31.17
90	08v-02-Bisdisph----W3----109	-909.5717412	31.60
91	08v-01-DicapOh----W3----11	-909.5716699	31.65
92	08v-01-DicapOh----W3----63	-909.5714894	31.76
93	08v-04-Antipr----W3----168	-909.5713288	31.86
94	08v-04-Antipr----W3----163_i-12	-909.5713260	31.86
95	08v-04-Antipr----W3----163_r-12	-909.5712757	31.89
96	08v-02-Bisdisph----W3----71	-909.5711760	31.96
97	08v-02-Bisdisph----W3----69	-909.5709592	32.09
98	08v-02-Bisdisph----W3----70	-909.5707492	32.22
99	08v-05-AntiprTrig----W3----196	-909.5698495	32.79
100	08v-07-Tdallcap----W3----253	-909.5694004	33.07
101	08v-01-DicapOh----W3----1	-909.5693822	33.08
102	08v-01-DicapOh----W3----39	-909.5692056	33.19
103	08v-02-Bisdisph----W3----107	-909.5690560	33.29
104	08v-05-AntiprTrig----W3----193	-909.5671132	34.50
105	08v-04-Antipr----W3----157	-909.5669128	34.63
106	08v-04-Antipr----W3----159	-909.5666749	34.78
107	08v-03-Cube----W3----141	-909.5659717	35.22
108	08v-06-Bipireex----W3----227	-909.5649354	35.87
109	08v-06-Bipireex----W3----225	-909.5649125	35.89
110	08v-06-Bipireex----W3----223	-909.5649040	35.89
111	08v-01-DicapOh----W3----18	-909.5647996	35.96
112	08v-05-AntiprTrig----W3----203	-909.5647497	35.99
113	08v-01-DicapOh----W3----14	-909.5647490	35.99
114	08v-01-DicapOh----W3----17	-909.5647309	36.00
115	08v-01-DicapOh----W3----16	-909.5647266	36.00
116	08v-05-AntiprTrig----W3----199	-909.5647016	36.02
117	08v-06-Bipireex----W3----226	-909.5645966	36.08
118	08v-01-DicapOh----W3----7	-909.5624927	37.40
119	08v-03-Cube----W3----143	-909.5617948	37.84
120	08v-01-DicapOh----W3----9	-909.5615869	37.97

121	08v-01-DicapOh----W3----47	-909.5615630	37.99
122	08v-06-Bipireex----W3----224	-909.5612846	38.16
123	08v-05-AntiprTrig----W3----201	-909.5611100	38.27
124	08v-05-AntiprTrig----W3----200	-909.5611038	38.28
125	08v-03-Cube----W3----144	-909.5610456	38.31
126	08v-06-Bipireex----W3----228	-909.5609865	38.35
127	08v-05-AntiprTrig----W3----202	-909.5608425	38.44
128	08v-02-Bisdisph----W3----77	-909.5606079	38.59
129	08v-05-AntiprTrig----W3----180	-909.5602624	38.80
130	08v-02-Bisdisph----W3----95	-909.5600570	38.93
131	08v-01-DicapOh----W3----60	-909.5600378	38.94
132	08v-02-Bisdisph----W3----68	-909.5585278	39.89
133	08v-02-Bisdisph----W3----67	-909.5584349	39.95
134	08v-02-Bisdisph----W3----105	-909.5582229	40.08
135	08v-05-AntiprTrig----W3----178	-909.5575444	40.51
136	08v-04-Antipr----W3----156	-909.5573791	40.61
137	08v-04-Antipr----W3----150	-909.5573243	40.65
138	08v-04-Antipr----W3----155	-909.5572837	40.67
139	08v-01-DicapOh----W3----6	-909.5570433	40.82
140	08v-07-Tdallcap----W3----259	-909.5569837	40.86
141	08v-03-Cube----W3----123	-909.5569683	40.87
142	08v-04-Antipr----W3----149	-909.5567796	40.99
143	08v-01-DicapOh----W3----41	-909.5567638	41.00
144	08v-01-DicapOh----W3----42	-909.5567402	41.01
145	08v-02-Bisdisph----W3----72	-909.5566984	41.04
146	08v-04-Antipr----W3----151	-909.5566450	41.07
147	08v-02-Bisdisph----W3----110	-909.5565565	41.13
148	08v-03-Cube----W3----122	-909.5565383	41.14
149	08v-03-Cube----W3----125	-909.5565108	41.16
150	08v-07-Tdallcap----W3----256	-909.5564704	41.18
151	08v-01-DicapOh----W3----28	-909.5545329	42.40
152	08v-04-Antipr----W3----158	-909.5543818	42.49
153	08v-07-Tdallcap----W3----260	-909.5529346	43.40
154	08v-04-Antipr----W3----162	-909.5527247	43.53
155	08v-06-Bipireex----W3----220	-909.5526775	43.56
156	08v-06-Bipireex----W3----222	-909.5526757	43.56
157	08v-06-Bipireex----W3----218	-909.5526041	43.61
158	08v-06-Bipireex----W3----219	-909.5525985	43.61
159	08v-04-Antipr----W3----154	-909.5525181	43.66
160	08v-04-Antipr----W3----153	-909.5521893	43.87
161	08v-01-DicapOh----W3----21	-909.5520535	43.95

162	08v-03-Cube----W3----128	-909.5519572	44.02
163	08v-04-Antipr----W3----148	-909.5519003	44.05
164	08v-05-AntiprTrig----W3----176	-909.5517846	44.12
165	08v-05-AntiprTrig----W3----175	-909.5517815	44.13
166	08v-05-AntiprTrig----W3----177	-909.5515990	44.24
167	08v-07-Tdallcap----W3----263	-909.5513868	44.37
168	08v-07-Tdallcap----W3----262	-909.5512488	44.46
169	08v-03-Cube----W3----126	-909.5511048	44.55
170	08v-02-Bisdisph----W3----93	-909.5509844	44.63
171	08v-01-DicapOh----W3----64_i-30	-909.5504895	44.94
172	08v-01-DicapOh----W3----64_r-30	-909.5503332	45.03
173	08v-01-DicapOh----W3----59	-909.5495356	45.53
174	08v-07-Tdallcap----W3----240	-909.5476286	46.73
175	08v-01-DicapOh----W3----46	-909.5474889	46.82
176	08v-01-DicapOh----W3----48	-909.5474847	46.82
177	08v-01-DicapOh----W3----44	-909.5474633	46.84
178	08v-01-DicapOh----W3----43	-909.5456903	47.95
179	08v-02-Bisdisph----W3----86	-909.5456275	47.99
180	08v-02-Bisdisph----W3----89	-909.5453908	48.14
181	08v-02-Bisdisph----W3----96	-909.5450997	48.32
182	08v-01-DicapOh----W3----12	-909.5446949	48.57
183	08v-04-Antipr----W3----160	-909.5439843	49.02
184	08v-01-DicapOh----W3----24	-909.5436483	49.23
185	08v-01-DicapOh----W3----29	-909.5433979	49.39
186	08v-05-AntiprTrig----W3----179	-909.5426631	49.85
187	08v-06-Bipireex----W3----229	-909.5420329	50.24
188	08v-02-Bisdisph----W3----91	-909.5414451	50.61
189	08v-02-Bisdisph----W3----92	-909.5413703	50.66
190	08v-07-Tdallcap----W3----265	-909.5412510	50.73
191	08v-07-Tdallcap----W3----270	-909.5406282	51.12
192	08v-01-DicapOh----W3----5	-909.5401000	51.46
193	08v-03-Cube----W3----131	-909.5396389	51.75
194	08v-07-Tdallcap----W3----249	-909.5394629	51.86
195	08v-07-Tdallcap----W3----250	-909.5394555	51.86
196	08v-03-Cube----W3----140	-909.5386393	52.37
197	08v-05-AntiprTrig----W3----204	-909.5381161	52.70
198	08v-06-Bipireex----W3----232	-909.5362438	53.88
199	08v-01-DicapOh----W3----25	-909.5356042	54.28
200	08v-05-AntiprTrig----W3----184	-909.5354103	54.40
201	08v-05-AntiprTrig----W3----186	-909.5353638	54.43
202	08v-05-AntiprTrig----W3----192	-909.5352103	54.52

203	08v-05-AntiprTrig----W3----183	-909.5351781	54.54
204	08v-05-AntiprTrig----W3----190	-909.5351318	54.57
205	08v-05-AntiprTrig----W3----189	-909.5351091	54.59
206	08v-05-AntiprTrig----W3----181	-909.5350803	54.61
207	08v-05-AntiprTrig----W3----185	-909.5347638	54.80
208	08v-01-DicapOh----W3----4	-909.5326375	56.14
209	08v-02-Bisdisph----W3----116	-909.5322131	56.41
210	08v-03-Cube----W3----139	-909.5318639	56.62
211	08v-02-Bisdisph----W3----97	-909.5307080	57.35
212	08v-02-Bisdisph----W3----100	-909.5307015	57.35
213	08v-02-Bisdisph----W3----98	-909.5306625	57.38
214	08v-02-Bisdisph----W3----102	-909.5306619	57.38
215	08v-07-Tdallcap----W3----235	-909.5306535	57.38
216	08v-07-Tdallcap----W3----237	-909.5306440	57.39
217	08v-01-DicapOh----W3----66	-909.5302498	57.64
218	08v-01-DicapOh----W3----23	-909.5281048	58.98
219	08v-03-Cube----W3----142	-909.5270441	59.65
220	08v-02-Bisdisph----W3----101	-909.5267820	59.81
221	08v-03-Cube----W3----132	-909.5267713	59.82
222	08v-05-AntiprTrig----W3----187	-909.5253803	60.69
223	08v-03-Cube----W3----130	-909.5250398	60.91
224	08v-04-Antipr----W3----161_r-15	-909.5248268	61.04
225	08v-04-Antipr----W3----161_i-15	-909.5248218	61.04
226	08v-05-AntiprTrig----W3----188	-909.5247947	61.06
227	08v-01-DicapOh----W3----52	-909.5247129	61.11
228	08v-01-DicapOh----W3----51	-909.5244150	61.30
229	08v-01-DicapOh----W3----22	-909.5230736	62.14
230	08v-01-DicapOh----W3----19	-909.5229073	62.24
231	08v-02-Bisdisph----W3----99	-909.5228452	62.28
232	08v-05-AntiprTrig----W3----191	-909.5226374	62.41
233	08v-07-Tdallcap----W3----239	-909.5222747	62.64
234	08v-07-Tdallcap----W3----238	-909.5182741	65.15
235	08v-01-DicapOh----W3----2	-909.5173502	65.73
236	08v-04-Antipr----W3----145	-909.5164704	66.28
237	08v-06-Bipireex----W3----231	-909.5155629	66.85
238	08v-02-Bisdisph----W3----117	-909.5148567	67.30
239	08v-01-DicapOh----W3----57	-909.5130137	68.45
240	08v-01-DicapOh----W3----50	-909.5099205	70.39
241	08v-01-DicapOh----W3----49	-909.5097597	70.50
242	08v-05-AntiprTrig----W3----207	-909.5096710	70.55
243	08v-01-DicapOh----W3----54_i-12	-909.5066054	72.47

244	08v-01-DicapOh----W3----53	-909.5065404	72.52
245	08v-01-DicapOh----W3----54_r-12	-909.5065143	72.53
246	08v-05-AntiprTrig----W3----174	-909.5051522	73.39
247	08v-05-AntiprTrig----W3----171	-909.5046979	73.67
248	08v-05-AntiprTrig----W3----170	-909.5046891	73.68
249	08v-05-AntiprTrig----W3----209	-909.5045913	73.74
250	08v-02-Bisdisph----W3----115	-909.5020894	75.31
251	08v-01-DicapOh----W3----36	-909.4992954	77.06
252	08v-01-DicapOh----W3----31	-909.4991638	77.14
253	08v-07-Tdallcap----W3----252	-909.4990246	77.23
254	08v-02-Bisdisph----W3----94	-909.4990217	77.23
255	08v-01-DicapOh----W3----35	-909.4990154	77.24
256	08v-01-DicapOh----W3----32_r-30	-909.4990043	77.24
257	08v-01-DicapOh----W3----62	-909.4988720	77.33
258	08v-05-AntiprTrig----W3----210	-909.4987778	77.39
259	08v-05-AntiprTrig----W3----205	-909.4984464	77.59
260	08v-01-DicapOh----W3----32_i-30	-909.4977037	78.06
261	08v-07-Tdallcap----W3----251	-909.4973317	78.29
262	08v-07-Tdallcap----W3----248	-909.4972931	78.32
263	08v-07-Tdallcap----W3----247	-909.4972430	78.35
264	08v-01-DicapOh----W3----20	-909.4962171	78.99
265	08v-06-Bipireex----W3----230	-909.4958871	79.20
266	08v-05-AntiprTrig----W3----169	-909.4955293	79.42
267	08v-02-Bisdisph----W3----119	-909.4949039	79.82
268	08v-02-Bisdisph----W3----118	-909.4947641	79.91
269	08v-02-Bisdisph----W3----120	-909.4946740	79.96
270	08v-01-DicapOh----W3----45	-909.4917445	81.80
271	08v-05-AntiprTrig----W3----172	-909.4889325	83.56
272	08v-01-DicapOh----W3----33	-909.4879351	84.19
273	08v-05-AntiprTrig----W3----208	-909.4873746	84.54
274	08v-05-AntiprTrig----W3----182	-909.4828796	87.36
275	08v-05-AntiprTrig----W3----173	-909.4820540	87.88
276	08v-01-DicapOh----W3----34	-909.4811845	88.43
277	08v-01-DicapOh----W3----61	-909.4765951	91.31
278	08v-01-DicapOh----W3----65	-909.4753145	92.11
279	08v-05-AntiprTrig----W3----206	-909.4623841	100.22

Table S5A. Initial $Cp_3W_3(H)B_6H_6$ structures, 325 structures.

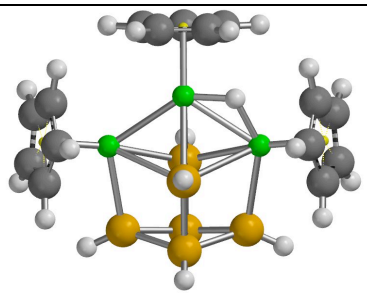
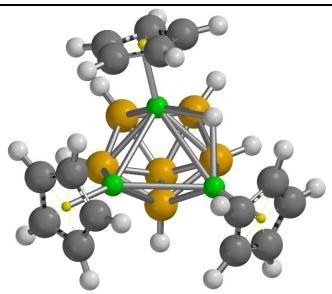
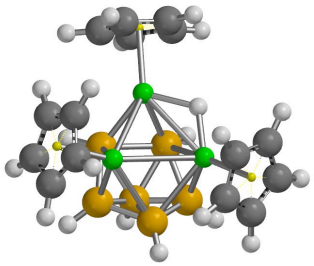
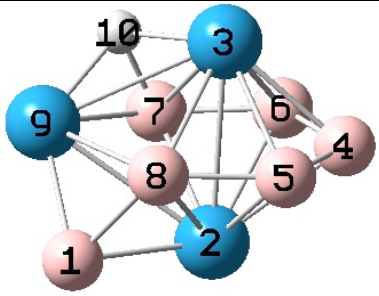
 Capped cube (128)	 Isocloso (119)	 Tricapped trigonal prism (78)

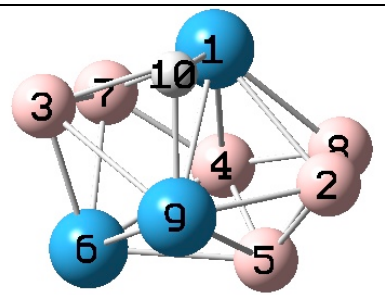
Table S5B. Distance table for the lowest-lying $Cp_3W_3(H)B_6H_6$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



1. -935.3663839 0.00 C_1

		1	2	3	4	5
1	B	0.000000				
2	W	2.255868	0.000000			
3	W	3.630160	2.849509	0.000000		
4	B	4.079025	2.246219	2.200265	0.000000	
5	B	3.142808	2.240284	2.237123	1.702730	0.000000
6	B	4.170468	2.299767	2.218534	1.713473	2.995611
7	B	3.366501	2.282139	2.446652	3.035029	3.609080
8	B	1.811355	2.318776	2.340926	3.034745	1.733024
9	W	2.040031	2.845787	2.713172	4.091374	3.603696
10	H	3.605858	3.153015	1.967641	3.523367	3.783032

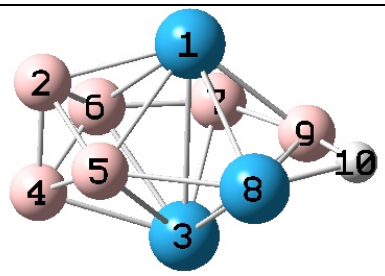
		6	7	8	9	10
6	B	0.000000				
7	B	1.713867	0.000000			
8	B	3.595433	3.345633	0.000000		
9	W	3.590823	2.315831	2.278209	0.000000	
10	H	2.485603	1.378932	3.228314	1.903964	0.000000



2. -935.3662725 +0.1 C_1

		1	2	3	4	5
1	W	0.000000				
2	B	2.361813	0.000000			
3	B	2.317410	3.843199	0.000000		
4	B	2.339924	2.837850	3.060670	0.000000	
5	B	2.838708	1.793990	3.529585	1.792862	0.000000
6	W	3.114024	3.496447	2.076150	2.285061	2.287878
7	B	2.181800	3.826214	1.832193	1.783466	3.123110
8	B	2.261236	1.678453	3.978406	1.753301	1.740711
9	W	2.652438	2.149050	2.635516	3.402238	2.437387
10	H	1.893981	2.673786	2.445286	3.832542	3.571200

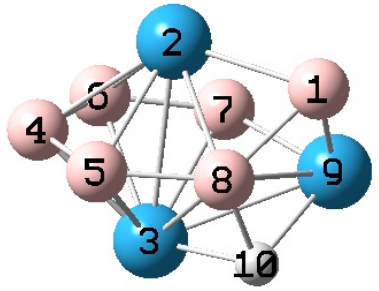
		6	7	8	9	10
6	W	0.000000				
7	B	2.167420	0.000000			
8	B	3.480074	3.165154	0.000000		
9	W	2.536444	3.564577	3.315094	0.000000	
10	H	3.558151	3.491443	3.592210	1.852535	0.000000



3. -935.3642706 +1.3 (C_S)

	1	2	3	4	5
1 W	0.000000				
2 B	2.200007	0.000000			
3 W	2.972334	3.149520	0.000000		
4 B	3.150157	1.696779	2.217378	0.000000	
5 B	2.366343	1.765157	2.382108	1.769086	0.000000
6 B	2.324039	1.740099	2.323545	1.749531	2.583137
7 B	2.220430	3.151817	2.204949	3.160218	3.394013
8 W	2.567893	3.660987	2.557623	3.659831	2.279691
9 B	2.278297	3.935517	2.314745	3.959840	3.414319
10 H	2.959854	4.688738	3.022925	4.720894	3.730548

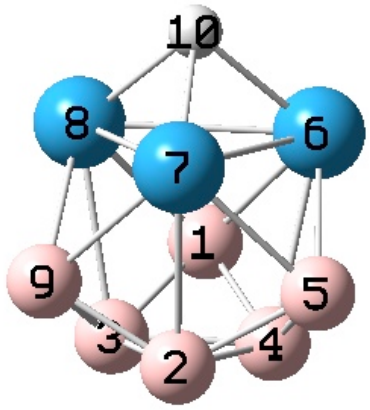
	6	7	8	9	10
6 B	0.000000				
7 B	1.779868	0.000000			
8 W	3.820783	3.467982	0.000000		
9 B	3.161960	1.806900	2.283210	0.000000	
10 H	4.294350	3.169423	1.765042	1.385767	0.000000



4. -935.3636234 +1.7 C_1

	1	2	3	4	5
1 B	0.000000				
2 W	2.257866	0.000000			
3 W	3.617069	2.879831	0.000000		
4 B	4.068949	2.230043	2.214089	0.000000	
5 B	3.203989	2.251074	2.288163	1.686666	0.000000
6 B	4.069896	2.239450	2.239165	1.731627	2.998987
7 B	3.285004	2.376926	2.297981	3.033324	3.594603
8 B	1.783630	2.281512	2.504625	3.037742	1.734178
9 W	2.048815	2.895474	2.663083	4.066732	3.652392
10 H	2.590911	3.204875	1.931366	3.534556	2.597046

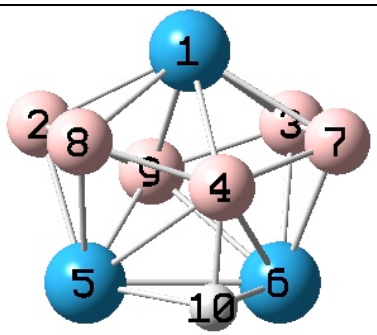
	6	7	8	9	10
6 B	0.000000				
7 B	1.705252	0.000000			
8 B	3.622912	3.363414	0.000000		
9 W	3.504742	2.152942	2.435855	0.000000	
10 H	3.752719	3.154608	1.514923	1.918604	0.000000



5. -935.3605999 +3.6 C_{3v}

		1	2	3	4	5
1	B	0.000000				
2	B	2.916150	0.000000			
3	B	1.747888	1.792727	0.000000		
4	B	1.752622	1.793211	1.790532	0.000000	
5	B	3.029338	1.753485	2.913305	1.746230	0.000000
6	W	2.210661	3.235193	3.229983	2.386953	2.214311
7	W	3.595790	2.388976	3.236150	3.230589	2.212561
8	W	2.219352	3.231265	2.390096	3.236470	3.596458
9	B	3.031364	1.751151	1.753814	2.916510	3.034919
10	H	3.217808	3.711069	3.710971	3.709194	3.218666

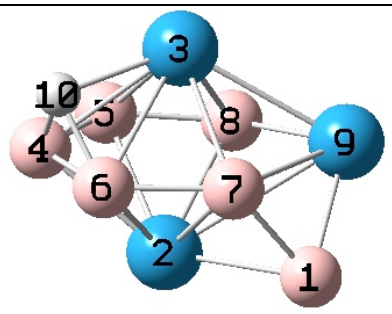
		6	7	8	9	10
6	W	0.000000				
7	W	2.648472	0.000000			
8	W	2.652177	2.647999	0.000000		
9	B	3.597871	2.220475	2.208577	0.000000	
10	H	1.959873	1.960774	1.961297	3.221421	0.000000



6. -935.3600419 +4.0 C_S

		1	2	3	4	5
1	W	0.000000				
2	B	2.148106	0.000000			
3	B	2.148712	3.274653	0.000000		
4	B	2.230592	3.093129	3.091370	0.000000	
5	W	3.165158	2.140795	3.589062	2.476099	0.000000
6	W	3.164592	3.584729	2.142896	2.472907	2.528001
7	B	2.186276	3.820586	1.907487	1.867221	3.614631
8	B	2.185383	1.910287	3.820562	1.867850	2.142775
9	B	2.279084	1.861689	1.863769	3.169025	2.338605
10	H	3.363025	3.520309	3.521643	1.537452	1.903347

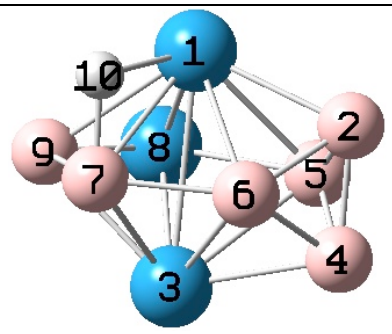
		6	7	8	9	10
6	W	0.000000				
7	B	2.144461	0.000000			
8	B	3.610508	3.344764	0.000000		
9	B	2.336775	3.077969	3.078201	0.000000	
10	H	1.901831	2.664595	2.661689	3.257706	0.000000



7. -935.3574118 +5.6 C_1

		1	2	3	4	5
1	B	0.000000				
2	W	2.284967	0.000000			
3	W	3.546514	2.852548	0.000000		
4	B	4.087160	2.200459	2.343260	0.000000	
5	B	4.131173	2.282368	2.235869	1.710886	0.000000
6	B	3.112336	2.205100	2.390194	1.800392	3.057945
7	B	1.786601	2.340302	2.345837	3.099823	3.607950
8	B	3.297950	2.314700	2.288796	3.013489	1.695448
9	W	2.030632	2.871417	2.582223	4.095467	3.521625
10	H	4.199653	3.003521	1.927244	1.447506	2.706125

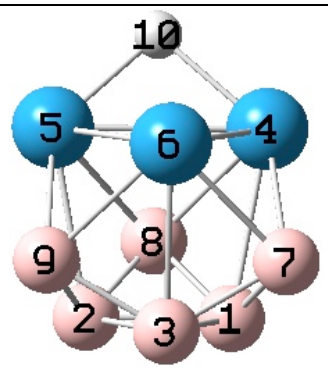
		6	7	8	9	10
6	B	0.000000				
7	B	1.744091	0.000000			
8	B	3.605329	3.291340	0.000000		
9	W	3.634083	2.309183	2.184219	0.000000	
10	H	1.411707	2.692430	3.631466	4.096216	0.000000



8. -935.3572741 +5.7 $C_1(C_S)$

		1	2	3	4	5
1	W	0.000000				
2	B	2.216179	0.000000			
3	W	2.949835	3.131985	0.000000		
4	B	3.150037	1.673925	2.224442	0.000000	
5	B	2.360459	1.788497	2.367172	1.775562	0.000000
6	B	2.355767	1.737718	2.304758	1.740666	2.597661
7	B	2.295677	3.254385	2.193720	3.247902	3.463269
8	W	2.576527	3.714951	2.559284	3.701288	2.313397
9	B	2.344995	4.010234	2.306416	4.013364	3.388726
10	H	1.838734	3.243162	3.256413	3.852830	3.788695

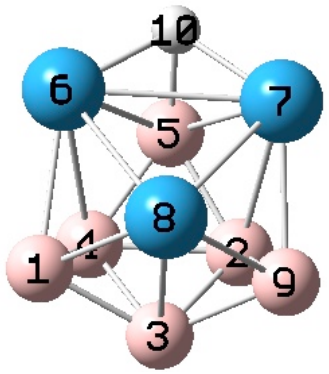
		6	7	8	9	10
6	B	0.000000				
7	B	1.893102	0.000000			
8	W	3.858499	3.475711	0.000000		
9	B	3.297884	1.930824	2.121135	0.000000	
10	H	2.324867	1.308511	3.805087	2.369864	0.000000



9. -935.3572683 +5.7 C_S

		1	2	3	4	5
1	B	0.000000				
2	B	1.807883	0.000000			
3	B	1.804842	1.804844	0.000000		
4	W	2.383504	3.239645	3.257937	0.000000	
5	W	3.239647	2.383506	3.257944	2.662900	0.000000
6	W	3.207430	3.207429	2.408858	2.609742	2.609746
7	B	1.748580	2.905680	1.726775	2.247203	3.603106
8	B	1.753003	1.753000	2.937376	2.232560	2.232554
9	B	2.905681	1.748583	1.726777	3.603102	2.247210
10	H	3.663576	3.663576	4.248945	1.848152	1.848149

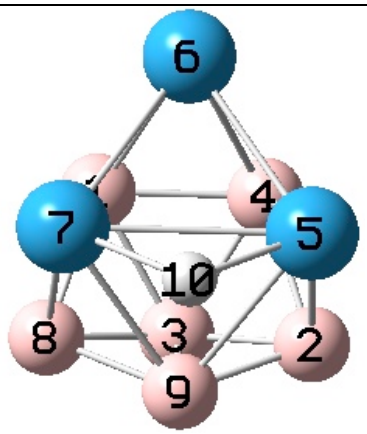
		6	7	8	9	10
6	W	0.000000				
7	B	2.195826	0.000000			
8	B	3.570779	3.052488	0.000000		
9	B	2.195820	2.978865	3.052488	0.000000	
10	H	3.097998	3.790813	2.614165	3.790814	0.000000



10. -935.3391276 +17.1 C_S

		1	2	3	4	5
1	B	0.000000				
2	B	2.929405	0.000000			
3	B	1.735620	1.820624	0.000000		
4	B	1.740785	1.839813	1.820617	0.000000	
5	B	3.057309	1.731121	2.924958	1.731128	0.000000
6	W	2.209236	3.265068	3.232470	2.396033	2.328382
7	W	3.598440	2.396062	3.232486	3.265087	2.328402
8	W	2.215645	3.221836	2.390379	3.221821	3.621228
9	B	3.017181	1.740784	1.735620	2.929394	3.057296
10	H	3.567098	2.844862	3.805464	2.844864	1.485319

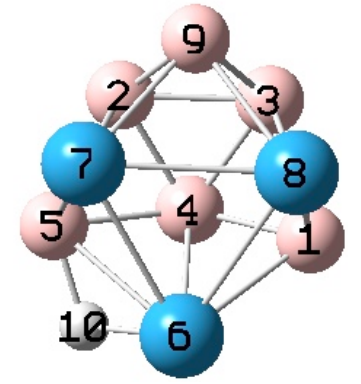
		6	7	8	9	10
6	W	0.000000				
7	W	2.674015	0.000000			
8	W	2.574772	2.574779	0.000000		
9	B	3.598426	2.209240	2.215666	0.000000	
10	H	1.881441	1.881449	3.520348	3.567088	0.000000



11. -935.3377672 +18.0 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	2.891193	0.000000			
3 B	1.838102	1.723726	0.000000		
4 B	1.823080	1.760173	1.838101	0.000000	
5 W	3.259930	2.175631	3.269648	2.385333	0.000000
6 W	2.219482	3.522026	3.524938	2.219482	2.508471
7 W	2.385315	3.542360	3.269633	3.259911	2.708224
8 B	1.760172	2.885658	1.723727	2.891191	3.542372
9 B	2.658357	1.724892	1.818212	2.658356	2.446568
10 H	3.730519	3.391039	3.981320	3.730534	1.877443

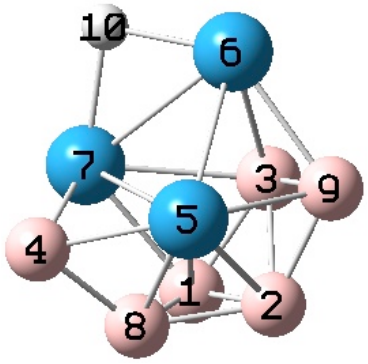
	6	7	8	9	10
6 W	0.000000				
7 W	2.508454	0.000000			
8 B	3.522024	2.175621	0.000000		
9 B	3.643202	2.446561	1.724892	0.000000	
10 H	3.225976	1.877400	3.391009	2.536094	0.000000



12. -935.3347324 +20.0 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	2.874128	0.000000			
3 B	1.744117	1.802724	0.000000		
4 B	1.725874	1.765912	1.795650	0.000000	
5 B	3.098711	1.771775	3.014365	1.882375	0.000000
6 W	2.244981	3.241013	3.271511	2.497593	2.297816
7 W	3.579841	2.437406	3.258896	3.285960	2.223814
8 W	2.222797	3.196344	2.371875	3.225546	3.607359
9 B	3.029680	1.752635	1.758171	2.913253	3.048572
10 H	2.935308	2.819451	3.526651	1.976988	1.311739

	6	7	8	9	10
6 W	0.000000				
7 W	2.584741	0.000000			
8 W	2.577659	2.572479	0.000000		
9 B	3.577248	2.216350	2.196176	0.000000	
10 H	1.836496	3.099316	3.933898	3.998102	0.000000



13. -935.3317186 +21.8 C_1

		1	2	3	4	5
1	B	0.000000				
2	B	1.729383	0.000000			
3	B	1.760740	1.950245	0.000000		
4	B	3.163271	3.265599	3.756086	0.000000	
5	W	3.323986	2.387500	3.140181	2.110318	0.000000
6	W	3.614046	3.305044	2.308456	3.592549	2.586967
7	W	2.193949	3.076115	2.363340	2.179052	2.964200
8	B	1.730396	1.769125	2.813881	1.837925	2.256781
9	B	2.898312	1.729900	1.800021	3.860129	2.277670
10	H	3.728672	4.154491	2.971930	3.237955	3.380547

		6	7	8	9	10
6	W	0.000000				
7	W	2.670968	0.000000			
8	B	3.725017	2.334110	0.000000		
9	B	2.146394	3.382272	3.054168	0.000000	
10	H	1.813580	1.854116	3.862918	3.622500	0.000000

Table S5C. Energy ranking for all of the $Cp_3W_3(H)B_6H_6$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	09v-02-Tl99----------142	-935.0806153	0.00
2	09v-02-Tl99----------137_i-33	-935.0804723	0.09
3	09v-02-Tl99----------137_r-33	-935.0802431	0.23
4	09v-03-TricTrPrism----------279	-935.0795623	0.66
5	09v-01-PressCapCube----------20	-935.0794047	0.76
6	09v-02-Tl99----------188	-935.0794026	0.76
7	09v-03-TricTrPrism----------262	-935.0766310	2.50
8	09v-01-PressCapCube----------18	-935.0732718	4.61
9	09v-01-PressCapCube----------21	-935.0732713	4.61
10	09v-01-PressCapCube----------100	-935.0684246	7.65
11	09v-03-TricTrPrism----------287	-935.0680203	7.90
12	09v-03-TricTrPrism----------291_r-13	-935.0679890	7.92
13	09v-01-PressCapCube----------41	-935.0679639	7.94
14	09v-03-TricTrPrism----------291_i-13	-935.0679562	7.94
15	09v-03-TricTrPrism----------307	-935.0679402	7.95
16	09v-03-TricTrPrism----------273	-935.0679357	7.96
17	09v-03-TricTrPrism----------274	-935.0679346	7.96
18	09v-01-PressCapCube----------101	-935.0654862	9.49
19	09v-01-PressCapCube----------16	-935.0645804	10.06
20	09v-03-TricTrPrism----------308_r-25	-935.0623843	11.44
21	09v-02-Tl99----------125	-935.0615822	11.94
22	09v-03-TricTrPrism----------240	-935.0615765	11.95
23	09v-01-PressCapCube----------68	-935.0615755	11.95
24	09v-02-Tl99----------190	-935.0615670	11.95
25	09v-03-TricTrPrism----------308_i-25	-935.0614479	12.03
26	09v-02-Tl99----------139	-935.0596788	13.14
27	09v-03-TricTrPrism----------280	-935.0596695	13.14
28	09v-01-PressCapCube----------102	-935.0589015	13.63
29	09v-01-PressCapCube----------99	-935.0588979	13.63
30	09v-01-PressCapCube----------19	-935.0586002	13.81
31	09v-02-Tl99----------140	-935.0574986	14.51
32	09v-02-Tl99----------230	-935.0574336	14.55
33	09v-02-Tl99----------228	-935.0574326	14.55
34	09v-03-TricTrPrism----------282	-935.0574299	14.55
35	09v-02-Tl99----------138	-935.0574144	14.56
36	09v-03-TricTrPrism----------278	-935.0572913	14.64
37	09v-03-TricTrPrism----------239	-935.0572318	14.67
38	09v-02-Tl99----------129	-935.0572298	14.67

39	09v-01-PressCapCube----------72	-935.0572287	14.68
40	09v-02-Tl99----------194	-935.0572282	14.68
41	09v-01-PressCapCube----------60	-935.0572281	14.68
42	09v-03-TricTrPrism----------286	-935.0555900	15.70
43	09v-03-TricTrPrism----------267	-935.0555868	15.71
44	09v-03-TricTrPrism----------254	-935.0554838	15.77
45	09v-03-TricTrPrism----------272	-935.0554762	15.78
46	09v-03-TricTrPrism----------268	-935.0554748	15.78
47	09v-01-PressCapCube----------103	-935.0545494	16.36
48	09v-01-PressCapCube----------104	-935.0533779	17.09
49	09v-01-PressCapCube----------17	-935.0532804	17.15
50	09v-01-PressCapCube----------37	-935.0514447	18.31
51	09v-01-PressCapCube----------36	-935.0509278	18.63
52	09v-03-TricTrPrism----------306	-935.0499685	19.23
53	09v-02-Tl99----------219	-935.0499468	19.25
54	09v-01-PressCapCube----------95	-935.0492374	19.69
55	09v-03-TricTrPrism----------289	-935.0464961	21.41
56	09v-01-PressCapCube----------35	-935.0464797	21.42
57	09v-03-TricTrPrism----------288	-935.0464784	21.42
58	09v-01-PressCapCube----------39	-935.0464503	21.44
59	09v-03-TricTrPrism----------304	-935.0447221	22.52
60	09v-03-TricTrPrism----------305	-935.0447211	22.52
61	09v-03-TricTrPrism----------303	-935.0447198	22.53
62	09v-01-PressCapCube----------13	-935.0447196	22.53
63	09v-02-Tl99----------185	-935.0437746	23.12
64	09v-03-TricTrPrism----------251	-935.0436655	23.19
65	09v-03-TricTrPrism----------277	-935.0430761	23.56
66	09v-02-Tl99----------143	-935.0419857	24.24
67	09v-02-Tl99----------144	-935.0419756	24.25
68	09v-01-PressCapCube----------119	-935.0419538	24.26
69	09v-03-TricTrPrism----------271	-935.0410653	24.82
70	09v-01-PressCapCube----------84	-935.0405850	25.12
71	09v-01-PressCapCube----------89	-935.0399858	25.50
72	09v-01-PressCapCube----------3	-935.0378340	26.85
73	09v-01-PressCapCube----------86	-935.0371980	27.25
74	09v-02-Tl99----------131	-935.0369425	27.41
75	09v-01-PressCapCube----------88	-935.0365120	27.68
76	09v-01-PressCapCube----------38	-935.0360855	27.94
77	09v-02-Tl99----------132	-935.0359205	28.05
78	09v-01-PressCapCube----------69	-935.0347965	28.75
79	09v-01-PressCapCube----------81	-935.0347907	28.76

80	09v-02-Tl99----------192	-935.0347906	28.76
81	09v-01-PressCapCube----------67	-935.0347870	28.76
82	09v-03-TricTrPrism----------241_r-40	-935.0345297	28.92
83	09v-03-TricTrPrism----------241_i-40	-935.0339211	29.30
84	09v-02-Tl99----------151	-935.0332927	29.70
85	09v-02-Tl99----------141_i-14	-935.0322880	30.33
86	09v-02-Tl99----------233	-935.0322183	30.37
87	09v-02-Tl99----------231	-935.0321680	30.40
88	09v-03-TricTrPrism----------281_i-16	-935.0320464	30.48
89	09v-02-Tl99----------141_r-14	-935.0320257	30.49
90	09v-03-TricTrPrism----------281_r-16	-935.0319302	30.55
91	09v-02-Tl99----------186	-935.0291372	32.30
92	09v-03-TricTrPrism----------276	-935.0288454	32.49
93	09v-03-TricTrPrism----------284	-935.0287514	32.55
94	09v-03-TricTrPrism----------248	-935.0274465	33.36
95	09v-01-PressCapCube----------87	-935.0274464	33.36
96	09v-01-PressCapCube----------85	-935.0274434	33.37
97	09v-02-Tl99----------156	-935.0274414	33.37
98	09v-03-TricTrPrism----------275	-935.0271688	33.54
99	09v-02-Tl99----------150	-935.0257872	34.41
100	09v-03-TricTrPrism----------285	-935.0257813	34.41
101	09v-01-PressCapCube----------122	-935.0250436	34.87
102	09v-03-TricTrPrism----------270	-935.0246063	35.15
103	09v-01-PressCapCube----------78	-935.0226035	36.40
104	09v-01-PressCapCube----------80	-935.0226013	36.40
105	09v-01-PressCapCube----------115	-935.0219161	36.83
106	09v-01-PressCapCube----------111	-935.0219147	36.84
107	09v-02-Tl99----------189	-935.0199102	38.09
108	09v-01-PressCapCube----------58_r-29	-935.0197835	38.17
109	09v-01-PressCapCube----------83	-935.0196050	38.29
110	09v-02-Tl99----------130	-935.0196023	38.29
111	09v-01-PressCapCube----------71	-935.0195979	38.29
112	09v-02-Tl99----------229	-935.0194819	38.36
113	09v-02-Tl99----------193_r-30	-935.0194764	38.37
114	09v-03-TricTrPrism----------243	-935.0194361	38.39
115	09v-01-PressCapCube----------58_i-29	-935.0190719	38.62
116	09v-02-Tl99----------205	-935.0189572	38.69
117	09v-02-Tl99----------153	-935.0186797	38.87
118	09v-02-Tl99----------193_i-30	-935.0186760	38.87
119	09v-03-TricTrPrism----------266	-935.0182204	39.15
120	09v-03-TricTrPrism----------269	-935.0182165	39.16

121	09v-01-PressCapCube----------46	-935.0181563	39.19
122	09v-01-PressCapCube----------109	-935.0176987	39.48
123	09v-01-PressCapCube----------108	-935.0176973	39.48
124	09v-02-Tl99----------163	-935.0169204	39.97
125	09v-01-PressCapCube----------40	-935.0168486	40.01
126	09v-02-Tl99----------191	-935.0160757	40.50
127	09v-03-TricTrPrism----------255	-935.0156909	40.74
128	09v-01-PressCapCube----------5	-935.0154708	40.88
129	09v-02-Tl99----------200	-935.0154180	40.91
130	09v-02-Tl99----------154	-935.0136304	42.03
131	09v-02-Tl99----------203	-935.0133630	42.20
132	09v-02-Tl99----------202	-935.0133325	42.22
133	09v-02-Tl99----------201	-935.0133315	42.22
134	09v-02-Tl99----------126	-935.0127234	42.60
135	09v-02-Tl99----------159	-935.0121858	42.94
136	09v-02-Tl99----------162	-935.0121852	42.94
137	09v-03-TricTrPrism----------264	-935.0108306	43.79
138	09v-03-TricTrPrism----------309	-935.0101034	44.25
139	09v-01-PressCapCube----------15	-935.0099459	44.35
140	09v-03-TricTrPrism----------300	-935.0098716	44.39
141	09v-03-TricTrPrism----------242	-935.0091043	44.87
142	09v-01-PressCapCube----------76	-935.0090449	44.91
143	09v-01-PressCapCube----------82_r-40	-935.0090138	44.93
144	09v-01-PressCapCube----------121	-935.0088768	45.02
145	09v-01-PressCapCube----------120	-935.0088739	45.02
146	09v-02-Tl99----------148	-935.0081954	45.44
147	09v-02-Tl99----------168	-935.0077552	45.72
148	09v-01-PressCapCube----------62	-935.0074657	45.90
149	09v-02-Tl99----------214	-935.0073074	46.00
150	09v-03-TricTrPrism----------244	-935.0068386	46.30
151	09v-03-TricTrPrism----------245	-935.0068233	46.31
152	09v-01-PressCapCube----------34	-935.0064801	46.52
153	09v-01-PressCapCube----------64	-935.0061352	46.74
154	09v-02-Tl99----------170	-935.0059900	46.83
155	09v-01-PressCapCube----------98	-935.0057390	46.99
156	09v-01-PressCapCube----------96_i-15	-935.0055026	47.13
157	09v-01-PressCapCube----------96_r-15	-935.0053299	47.24
158	09v-02-Tl99----------149	-935.0049548	47.48
159	09v-02-Tl99----------160	-935.0047347	47.62
160	09v-02-Tl99----------238	-935.0040676	48.04
161	09v-02-Tl99----------235	-935.0040666	48.04

162	09v-02-Tl99----------234	-935.0040645	48.04
163	09v-02-Tl99----------237	-935.0039033	48.14
164	09v-02-Tl99----------135	-935.0036766	48.28
165	09v-01-PressCapCube----------48	-935.0036247	48.31
166	09v-02-Tl99----------218	-935.0036241	48.31
167	09v-02-Tl99----------177	-935.0036225	48.31
168	09v-02-Tl99----------224	-935.0036174	48.32
169	09v-02-Tl99----------134	-935.0036154	48.32
170	09v-02-Tl99----------133	-935.0033345	48.50
171	09v-02-Tl99----------152	-935.0030358	48.68
172	09v-01-PressCapCube----------29	-935.0025195	49.01
173	09v-01-PressCapCube----------26	-935.0021124	49.26
174	09v-01-PressCapCube----------27	-935.0021059	49.27
175	09v-01-PressCapCube----------6	-935.0020220	49.32
176	09v-02-Tl99----------146	-935.0014848	49.66
177	09v-02-Tl99----------232	-935.0002467	50.43
178	09v-01-PressCapCube----------112	-934.9999539	50.62
179	09v-01-PressCapCube----------28	-934.9991661	51.11
180	09v-01-PressCapCube----------32	-934.9983430	51.63
181	09v-02-Tl99----------155	-934.9982946	51.66
182	09v-02-Tl99----------161	-934.9980701	51.80
183	09v-02-Tl99----------136	-934.9972980	52.28
184	09v-01-PressCapCube----------52	-934.9964590	52.81
185	09v-02-Tl99----------220	-934.9964525	52.81
186	09v-02-Tl99----------227	-934.9964506	52.82
187	09v-03-TricTrPrism----------301	-934.9964469	52.82
188	09v-02-Tl99----------145	-934.9961788	52.99
189	09v-02-Tl99----------157	-934.9957678	53.24
190	09v-02-Tl99----------173	-934.9955980	53.35
191	09v-01-PressCapCube----------23	-934.9952351	53.58
192	09v-03-TricTrPrism----------265	-934.9937959	54.48
193	09v-02-Tl99----------179	-934.9937876	54.49
194	09v-02-Tl99----------158	-934.9937240	54.53
195	09v-01-PressCapCube----------113	-934.9934217	54.72
196	09v-03-TricTrPrism----------292	-934.9925031	55.29
197	09v-01-PressCapCube----------11	-934.9922563	55.45
198	09v-03-TricTrPrism----------302	-934.9922504	55.45
199	09v-01-PressCapCube----------7	-934.9915190	55.91
200	09v-01-PressCapCube----------25	-934.9912441	56.08
201	09v-01-PressCapCube----------33	-934.9909061	56.29
202	09v-01-PressCapCube----------118	-934.9900922	56.81

203	09v-01-PressCapCube----------70	-934.9900444	56.84
204	09v-03-TricTrPrism----------250	-934.9898608	56.95
205	09v-01-PressCapCube----------79	-934.9896582	57.08
206	09v-02-Tl99----------225	-934.9893147	57.29
207	09v-03-TricTrPrism----------249	-934.9891300	57.41
208	09v-03-TricTrPrism----------253	-934.9891238	57.41
209	09v-02-Tl99----------165	-934.9888227	57.60
210	09v-01-PressCapCube----------73	-934.9884346	57.85
211	09v-03-TricTrPrism----------293_i-16	-934.9878528	58.21
212	09v-03-TricTrPrism----------295	-934.9878363	58.22
213	09v-03-TricTrPrism----------293_r-16	-934.9878237	58.23
214	09v-02-Tl99----------127	-934.9877912	58.25
215	09v-02-Tl99----------128	-934.9877804	58.26
216	09v-01-PressCapCube----------90	-934.9877157	58.30
217	09v-02-Tl99----------236_i-20	-934.9872324	58.60
218	09v-02-Tl99----------236_r-20	-934.9871216	58.67
219	09v-01-PressCapCube----------63	-934.9866683	58.95
220	09v-01-PressCapCube----------117	-934.9856949	59.56
221	09v-01-PressCapCube----------49	-934.9856788	59.57
222	09v-03-TricTrPrism----------283	-934.9852744	59.83
223	09v-01-PressCapCube----------61	-934.9852362	59.85
224	09v-01-PressCapCube----------77	-934.9852323	59.85
225	09v-02-Tl99----------223	-934.9847111	60.18
226	09v-01-PressCapCube----------14	-934.9847081	60.18
227	09v-03-TricTrPrism----------246	-934.9834103	61.00
228	09v-03-TricTrPrism----------296	-934.9830209	61.24
229	09v-01-PressCapCube----------55	-934.9829945	61.26
230	09v-03-TricTrPrism----------294_r-186	-934.9827741	61.40
231	09v-03-TricTrPrism----------252	-934.9827354	61.42
232	09v-01-PressCapCube----------57	-934.9827286	61.43
233	09v-01-PressCapCube----------56	-934.9827284	61.43
234	09v-02-Tl99----------174	-934.9827282	61.43
235	09v-02-Tl99----------204	-934.9826129	61.50
236	09v-01-PressCapCube----------22	-934.9819306	61.93
237	09v-01-PressCapCube----------65	-934.9818339	61.99
238	09v-01-PressCapCube----------59	-934.9818324	61.99
239	09v-01-PressCapCube----------97	-934.9797657	63.29
240	09v-01-PressCapCube----------54	-934.9795506	63.42
241	09v-03-TricTrPrism----------290	-934.9794671	63.47
242	09v-02-Tl99----------226	-934.9792038	63.64
243	09v-02-Tl99----------182	-934.9792003	63.64

244	09v-02-Tl99----------164	-934.9789559	63.79
245	09v-03-TricTrPrism----------299	-934.9786068	64.01
246	09v-02-Tl99----------187	-934.9785677	64.04
247	09v-03-TricTrPrism----------247	-934.9783897	64.15
248	09v-03-TricTrPrism----------260	-934.9778528	64.49
249	09v-03-TricTrPrism----------263	-934.9778451	64.49
250	09v-03-TricTrPrism----------297	-934.9768908	65.09
251	09v-01-PressCapCube----------114	-934.9756895	65.84
252	09v-01-PressCapCube----------31	-934.9748218	66.39
253	09v-03-TricTrPrism----------259	-934.9737479	67.06
254	09v-03-TricTrPrism----------311	-934.9731473	67.44
255	09v-01-PressCapCube----------116	-934.9730866	67.48
256	09v-02-Tl99----------212	-934.9724197	67.89
257	09v-02-Tl99----------213	-934.9724178	67.90
258	09v-01-PressCapCube----------92	-934.9709206	68.84
259	09v-01-PressCapCube----------91	-934.9709182	68.84
260	09v-01-PressCapCube----------110	-934.9700763	69.37
261	09v-01-PressCapCube----------74	-934.9699650	69.44
262	09v-02-Tl99----------167	-934.9693012	69.85
263	09v-01-PressCapCube----------47	-934.9690857	69.99
264	09v-02-Tl99----------169	-934.9681456	70.58
265	09v-03-TricTrPrism----------258	-934.9679603	70.69
266	09v-03-TricTrPrism----------256	-934.9679136	70.72
267	09v-03-TricTrPrism----------261	-934.9678701	70.75
268	09v-02-Tl99----------166	-934.9677898	70.80
269	09v-02-Tl99----------211	-934.9676895	70.86
270	09v-02-Tl99----------216	-934.9667617	71.45
271	09v-01-PressCapCube----------24	-934.9664029	71.67
272	09v-01-PressCapCube----------4	-934.9657470	72.08
273	09v-01-PressCapCube----------45	-934.9656750	72.13
274	09v-01-PressCapCube----------94	-934.9655185	72.23
275	09v-02-Tl99----------196	-934.9651885	72.43
276	09v-03-TricTrPrism----------310	-934.9651522	72.46
277	09v-02-Tl99----------175	-934.9642098	73.05
278	09v-01-PressCapCube----------93	-934.9617738	74.58
279	09v-01-PressCapCube----------12	-934.9607761	75.20
280	09v-02-Tl99----------176	-934.9607314	75.23
281	09v-02-Tl99----------171	-934.9607294	75.23
282	09v-02-Tl99----------221	-934.9604242	75.42
283	09v-02-Tl99----------199	-934.9588154	76.43
284	09v-02-Tl99----------181	-934.9586020	76.57

285	09v-03-TricTrPrism----------294_i-186	-934.9573221	77.37
286	09v-02-Tl99----------198	-934.9563466	77.98
287	09v-01-PressCapCube----------2	-934.9547780	78.97
288	09v-02-Tl99----------184	-934.9542447	79.30
289	09v-01-PressCapCube----------82_i-40	-934.9532141	79.95
290	09v-01-PressCapCube----------30	-934.9523221	80.51
291	09v-02-Tl99----------217	-934.9518763	80.79
292	09v-02-Tl99----------147	-934.9516052	80.96
293	09v-01-PressCapCube----------42	-934.9508096	81.46
294	09v-02-Tl99----------222	-934.9505325	81.63
295	09v-03-TricTrPrism----------257	-934.9501719	81.86
296	09v-01-PressCapCube----------44	-934.9500585	81.93
297	09v-01-PressCapCube----------53	-934.9493099	82.40
298	09v-01-PressCapCube----------51	-934.9459858	84.48
299	09v-01-PressCapCube----------107	-934.9458014	84.60
300	09v-02-Tl99----------183	-934.9450512	85.07
301	09v-01-PressCapCube----------1	-934.9420335	86.96
302	09v-01-PressCapCube----------75	-934.9406773	87.81
303	09v-01-PressCapCube----------50	-934.9406314	87.84
304	09v-02-Tl99----------208_i-15	-934.9401184	88.16
305	09v-02-Tl99----------208_r-15	-934.9401148	88.17
306	09v-02-Tl99----------206	-934.9401069	88.17
307	09v-01-PressCapCube----------124	-934.9395945	88.49
308	09v-02-Tl99----------209	-934.9368133	90.24
309	09v-02-Tl99----------210	-934.9368101	90.24
310	09v-03-TricTrPrism----------298	-934.9356694	90.96
311	09v-01-PressCapCube----------123	-934.9351742	91.27
312	09v-02-Tl99----------215	-934.9336028	92.25
313	09v-02-Tl99----------172	-934.9333113	92.44
314	09v-01-PressCapCube----------43	-934.9318686	93.34
315	09v-01-PressCapCube----------105	-934.9291230	95.06
316	09v-02-Tl99----------195	-934.9286959	95.33
317	09v-02-Tl99----------197	-934.9279799	95.78
318	09v-01-PressCapCube----------66	-934.9251679	97.55
319	09v-01-PressCapCube----------8	-934.9236397	98.51
320	09v-02-Tl99----------180	-934.9150982	103.87
321	09v-01-PressCapCube----------9	-934.9068969	109.01
322	09v-02-Tl99----------178	-934.9045281	110.50
323	09v-02-Tl99----------207	-934.8998868	113.41
324	09v-01-PressCapCube----------106	-934.8988753	114.05
325	09v-01-PressCapCube----------10	-934.8918173	118.47

Table S6A. Initial $Cp_3W_3(H)B_7H_7$ structures, 349 structures.

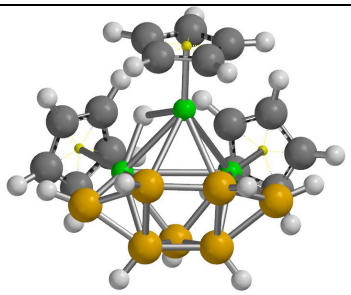
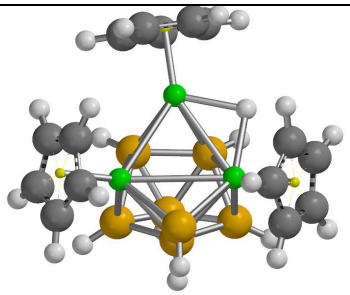
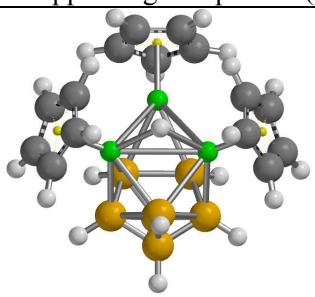
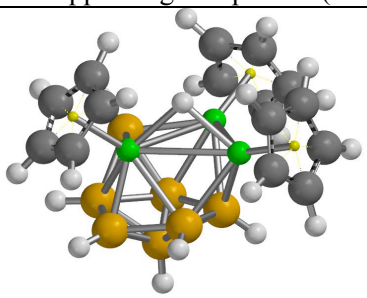
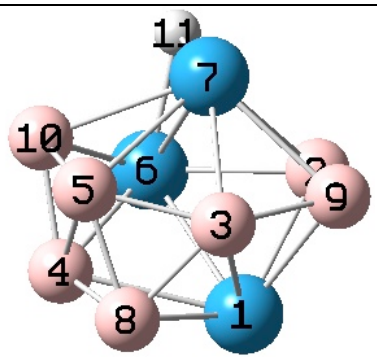
 Tetracapped trigonal prism1 (38)	 Tetracapped trigonal prism1 (165)
 Closo (113)	 Isocloso (33)

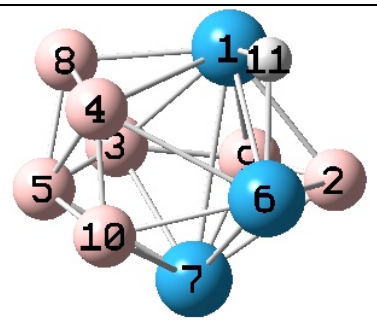
Table S6B. Distance table for the lowest-lying $Cp_3W_3(H)B_7H_7$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



1. -960.84885800 0.0 C_1

		1	2	3	4	5
1	W	0.000000				
2	B	2.216265	0.000000			
3	B	2.255779	3.076525	0.000000		
4	B	2.405668	3.657721	2.774988	0.000000	
5	B	3.046705	3.856220	1.838224	1.814509	0.000000
6	W	2.691435	2.271454	3.663388	2.428760	3.288404
7	W	3.118305	2.305939	2.323992	3.148862	2.386819
8	B	2.146513	3.887336	1.760242	1.731624	1.745925
9	B	2.129472	1.783159	1.818609	3.737678	3.307850
10	B	3.429842	3.677613	3.137849	1.718551	1.737178
11	H	3.865219	2.533089	3.966534	3.636457	3.618087

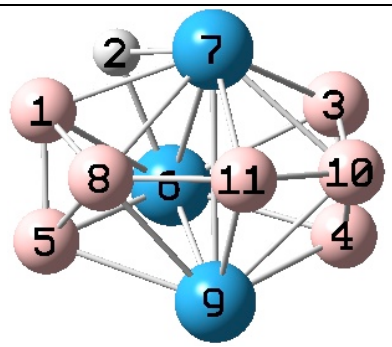
		6	7	8	9	10
6	W	0.000000				
7	W	2.553934	0.000000			
8	B	3.648075	3.412614	0.000000		
9	B	3.461329	2.270946	3.176076	0.000000	
10	B	2.202538	2.328965	2.936359	3.942262	0.000000
11	H	1.835708	1.854266	4.590117	3.577499	2.538003



2. -960.84663970 +1.4 C_1

		1	2	3	4	5
1	W	0.000000				
2	B	2.248087	0.000000			
3	B	2.296383	3.072547	0.000000		
4	B	2.500507	3.754476	2.799011	0.000000	
5	B	3.100194	3.887471	1.831672	1.810382	0.000000
6	W	2.751089	2.259061	3.659372	2.555433	3.328521
7	W	3.105809	2.282532	2.255046	3.150859	2.368935
8	B	2.167348	3.901133	1.780257	1.717722	1.746909
9	B	2.163716	1.778878	1.812617	3.799694	3.316601
10	B	3.453676	3.694292	3.126847	1.694472	1.757203
11	H	1.858249	2.705543	3.746996	2.386420	3.749680

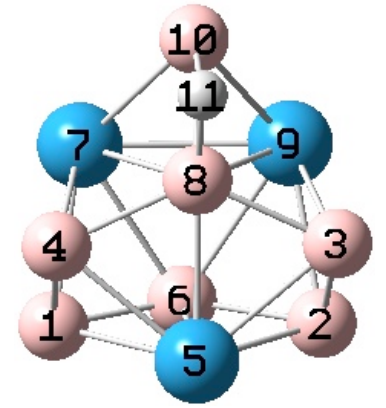
		6	7	8	9	10
6	W	0.000000				
7	W	2.491940	0.000000			
8	B	3.685121	3.363238	0.000000		
9	B	3.446374	2.222552	3.186319	0.000000	
10	B	2.205922	2.331310	2.917361	3.943398	0.000000
11	H	1.846110	3.661569	3.198061	3.604279	3.202791



3. -960.83862080 +6.4 C_1

	1	2	3	4	5
1 B	0.000000				
2 H	1.538350	0.000000			
3 B	3.798457	2.810994	0.000000		
4 B	4.201303	3.647695	1.641903	0.000000	
5 B	1.637615	2.684595	4.112113	3.842302	0.000000
6 W	2.493904	1.920202	2.378217	2.335254	2.336419
7 W	2.290561	1.852651	2.221828	3.197556	3.212020
8 B	1.749021	2.833791	3.896476	3.938398	1.768788
9 W	3.235996	3.606916	3.195979	2.266318	2.277460
10 B	3.956152	3.615532	1.770014	1.741042	3.946552
11 B	3.197125	3.578609	3.192885	3.175078	3.183983

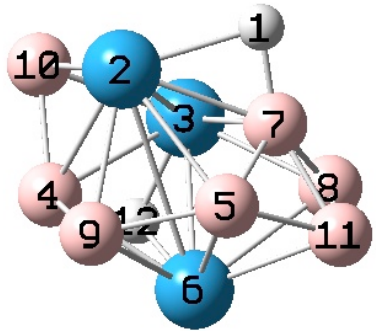
	6	7	8	9	10
6 W	0.000000				
7 W	2.741659	0.000000			
8 B	3.151707	2.329456	0.000000		
9 W	2.529066	3.162384	2.354099	0.000000	
10 B	3.134274	2.313004	3.243862	2.357541	0.000000
11 B	3.577570	2.165354	1.839153	2.152662	1.860679



4. -960.83824150 +6.7 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	3.205031	0.000000			
3 B	3.759989	1.841477	0.000000		
4 B	1.839692	3.758236	3.351973	0.000000	
5 W	2.146857	2.145566	2.183359	2.183272	0.000000
6 B	1.834981	1.830724	3.012133	3.012829	2.317003
7 W	2.184648	3.575765	3.610305	2.155521	3.249950
8 B	2.940308	2.940786	1.855752	1.854498	2.192699
9 W	3.581605	2.182005	2.153056	3.614554	3.250808
10 B	4.029805	4.029409	2.972240	2.972761	3.835476
11 H	4.116083	4.114276	2.661977	2.665371	3.410005

	6	7	8	9	10
6 B	0.000000				
7 W	2.340222	0.000000			
8 B	2.971525	2.338113	0.000000		
9 W	2.341546	2.508582	2.341559	0.000000	
10 B	3.861451	2.395002	1.708620	2.398443	0.000000
11 H	4.239699	3.114047	1.328480	3.114387	1.352956

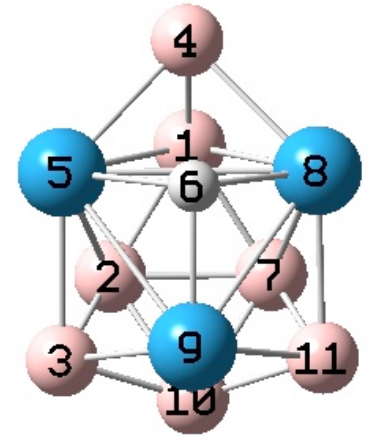


5. -960.83757240 +7.1 C_1

	1	2	3	4	5
1 H	0.000000				
2 W	1.912397	0.000000			
3 W	2.807541	2.933530	0.000000		
4 B	3.605682	2.308093	2.436243	0.000000	
5 B	2.585772	2.329146	3.681294	3.088573	0.000000
6 W	3.570442	3.208035	2.711119	2.233633	2.217907
7 B	1.285200	2.196930	2.391779	3.124082	1.838070
8 B	2.707994	3.622626	2.226579	3.649033	2.951752
9 B	3.518328	2.180282	3.657963	1.882024	1.811095
10 B	3.233263	2.106111	2.211230	1.738010	3.942997
11 B	2.856393	3.535717	3.499695	3.920811	1.809716
12 H	4.405673	4.141254	1.720517	2.565268	4.519627

	6	7	8	9	10
6 W	0.000000				
7 B	2.428141	0.000000			
8 B	2.305563	1.652099	0.000000		
9 B	2.160530	2.938221	3.869165	0.000000	
10 B	3.574486	3.343895	4.064711	3.153358	0.000000
11 B	2.189968	1.689996	1.734877	3.266258	4.703308
12 H	2.726851	3.701068	3.066386	4.062452	2.996453

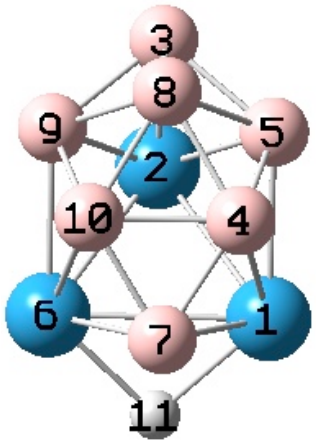
	11	12
11 B	0.000000	
12 H	4.260460	0.000000



6. -960.83586950 +8.2 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	1.762227	0.000000			
3 B	3.070161	1.737061	0.000000		
4 B	1.742950	3.202586	3.938978	0.000000	
5 W	2.297411	2.362443	2.243138	2.142786	0.000000
6 H	3.171837	3.637050	3.213610	2.515783	2.058362
7 B	1.765351	1.844130	2.918718	3.215136	3.320596
8 W	2.294304	3.306606	3.698898	2.163716	2.929232
9 W	3.554883	3.178272	2.188367	3.795910	2.672356
10 B	2.920525	1.787248	1.731576	4.200050	3.296857
11 B	3.075386	2.923789	2.986605	3.954563	3.720602

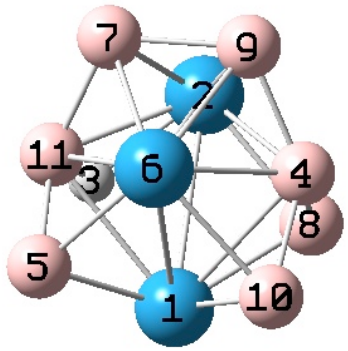
	6	7	8	9	10
6 H	0.000000				
7 B	3.625122	0.000000			
8 W	2.000405	2.361183	0.000000		
9 W	1.884908	3.181710	2.657024	0.000000	
10 B	3.688173	1.782323	3.280291	2.419604	0.000000
11 B	3.187773	1.742048	2.235227	2.193779	1.729625



7. -960.83204060 +10.6 C_S

	1	2	3	4	5
1 W	0.000000				
2 W	2.568944	0.000000			
3 B	3.569518	2.122428	0.000000		
4 B	2.357930	3.471146	2.948647	0.000000	
5 B	2.320092	2.371916	1.763944	1.788853	0.000000
6 W	2.632741	2.569786	3.569072	3.211782	3.515106
7 B	2.249017	3.715603	3.928018	1.712545	3.065896
8 B	3.483408	3.194823	1.701857	1.784253	1.810602
9 B	3.514455	2.369444	1.762705	2.828179	2.649263
10 B	3.215223	3.474512	2.948370	1.806498	2.826404
11 H	1.859875	3.048241	4.556592	3.614145	3.855239

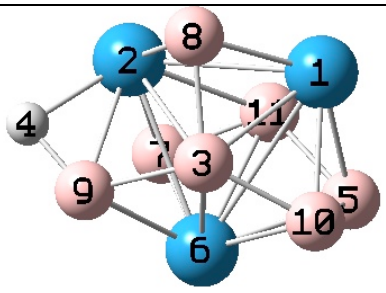
	6	7	8	9	10
6 W	0.000000				
7 B	2.247848	0.000000			
8 B	3.483976	2.962499	0.000000		
9 B	2.318386	3.066628	1.815157	0.000000	
10 B	2.362481	1.714511	1.782990	1.793173	0.000000
11 H	1.864546	2.560682	4.536216	3.855851	3.620377



8. -960.83179550 +10.7 C1

	1	2	3	4	5
1 W	0.000000				
2 W	2.868589	0.000000			
3 H	2.210092	1.829504	0.000000		
4 B	2.550179	2.317853	3.317456	0.000000	
5 B	2.171614	3.635134	2.564910	3.599164	0.000000
6 W	2.822260	3.147472	3.282189	2.289793	2.170180
7 B	3.696750	2.214809	2.679113	3.033113	3.097671
8 B	2.192211	2.147966	2.885747	1.778368	4.032287
9 B	3.698601	2.155411	3.461438	1.798325	3.905154
10 B	2.082420	3.663399	3.846353	1.815259	3.038230
11 B	2.531061	2.328876	1.390706	3.289457	1.735758

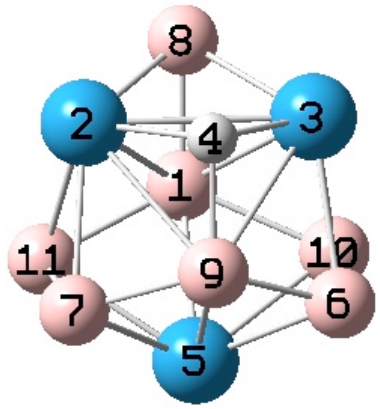
	6	7	8	9	10
6 W	0.000000				
7 B	2.169588	0.000000			
8 B	3.616860	3.907257	0.000000		
9 B	2.199511	1.814222	3.116838	0.000000	
10 B	2.289360	4.002649	2.649268	3.267074	0.000000
11 B	2.333059	1.814778	3.580027	3.041842	3.645820



9. -960.83070940 +11.4 C_1

	1	2	3	4	5
1	W	0.000000			
2	W	2.808842	0.000000		
3	B	2.294455	2.572400	0.000000	
4	H	4.141038	1.858119	2.716440	0.000000
5	B	2.168883	3.638119	3.047502	4.740063	0.000000
6	W	3.128550	2.818001	2.337692	3.126602	2.184392
7	B	3.591793	2.196427	3.644332	3.167126	3.032991
8	B	2.141395	2.186598	1.758880	2.850443	3.885560
9	B	3.687348	2.265555	1.819309	1.279308	3.998420
10	B	2.134795	3.692805	1.808292	4.254611	1.837598
11	B	2.194639	2.361540	3.219821	3.884211	1.829930

	6	7	8	9	10
6	W	0.000000			
7	B	2.150263	0.000000		
8	B	3.623740	4.051770	0.000000	
9	B	2.260299	3.158517	2.725509	0.000000
10	B	2.235765	3.903687	3.113704	3.232877	0.000000
11	B	2.349659	1.712872	3.433396	3.639076	3.023912



10. -960.83047440 +11.5 C_S

	1	2	3	4	5
1	B	0.000000			
2	W	2.395613	0.000000		
3	W	2.395507	2.710983	0.000000	
4	H	3.190792	1.905609	1.905454	0.000000
5	W	2.241314	3.260176	3.260056	3.436812	0.000000
6	B	3.072317	3.676909	2.235845	2.685506	2.149004
7	B	3.072320	2.235790	3.676711	2.685450	2.149102
8	B	1.753689	2.159829	2.159800	2.952235	3.784459
9	B	3.126274	2.515192	2.515113	1.587411	2.296558
10	B	1.962755	3.721558	2.126234	3.472868	2.158758
11	B	1.962779	2.126188	3.721390	3.472844	2.158797

	6	7	8	9	10
6	B	0.000000			
7	B	3.142791	0.000000		
8	B	3.933501	3.933422	0.000000	
9	B	1.777823	1.777720	3.719219	0.000000
10	B	1.869292	3.782695	3.057677	3.037135	0.000000
11	B	3.782663	1.869260	3.057628	3.037050	3.441038

Table S6C. Energy ranking for all of the $Cp_3W_3(H)B_7H_7$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	10v-01-TetrcTriPri1----------23	-960.54036470	0.00
2	10v-03-Isocloso----------222	-960.53981200	0.35
3	10v-03-Isocloso----------221	-960.53976430	0.38
4	10v-01-TetrcTriPri1----------4	-960.53972350	0.40
5	10v-03-Isocloso----------251	-960.53964670	0.45
6	10v-03-Isocloso----------211	-960.53957910	0.49
7	10v-01-TetrcTriPri1----------24	-960.53836290	1.26
8	10v-03-Isocloso----------250	-960.53492580	3.41
9	10v-02-TetrcTriPri2----------38	-960.53049990	6.19
10	10v-02-TetrcTriPri2----------198	-960.53034830	6.29
11	10v-02-TetrcTriPri2----------199	-960.53034510	6.29
12	10v-03-Isocloso----------209	-960.53034190	6.29
13	10v-03-Isocloso----------205	-960.53033770	6.29
14	10v-02-TetrcTriPri2----------195	-960.53025660	6.34
15	10v-03-Isocloso----------210	-960.53025660	6.34
16	10v-02-TetrcTriPri2----------47	-960.53004110	6.48
17	10v-01-TetrcTriPri1----------18	-960.52998820	6.51
18	10v-02-TetrcTriPri2----------200	-960.52985720	6.59
19	10v-02-TetrcTriPri2----------88	-960.52787370	7.84
20	10v-03-Isocloso----------289	-960.52785920	7.85
21	10v-03-Isocloso----------287	-960.52552600	9.31
22	10v-03-Isocloso----------261	-960.52415900	10.17
23	10v-02-TetrcTriPri2----------131	-960.52342760	10.63
24	10v-02-TetrcTriPri2----------63	-960.52329850	10.71
25	10v-01-TetrcTriPri1----------25	-960.52200640	11.52
26	10v-02-TetrcTriPri2----------141	-960.52041070	12.52
27	10v-02-TetrcTriPri2----------124	-960.52040350	12.53
28	10v-03-Isocloso----------259	-960.52038790	12.54
29	10v-02-TetrcTriPri2----------65	-960.52038620	12.54
30	10v-04-closo----------326	-960.52031160	12.58
31	10v-01-TetrcTriPri1----------20	-960.51909190	13.35
32	10v-02-TetrcTriPri2----------129	-960.51872710	13.58
33	10v-03-Isocloso----------275	-960.51535720	15.69
34	10v-03-Isocloso----------271	-960.51535640	15.69
35	10v-01-TetrcTriPri1----------26	-960.51388990	16.61
36	10v-02-TetrcTriPri2----------158	-960.51296570	17.19
37	10v-02-TetrcTriPri2----------179	-960.51286770	17.25
38	10v-04-closo----------325	-960.51191170	17.85
39	10v-03-Isocloso----------247	-960.51161490	18.04

40	10v-03-Isocloso----------241	-960.51159740	18.05
41	10v-03-Isocloso----------269	-960.51159410	18.05
42	10v-02-TetrcTriPri2----------142	-960.51127340	18.26
43	10v-03-Isocloso----------227	-960.51055320	18.71
44	10v-03-Isocloso----------231	-960.51032760	18.85
45	10v-01-TetrcTriPri1----------30	-960.50943610	19.41
46	10v-02-TetrcTriPri2----------144	-960.50904630	19.65
47	10v-03-Isocloso----------311	-960.50894990	19.71
48	10v-03-Isocloso----------290	-960.50893780	19.72
49	10v-02-TetrcTriPri2----------132	-960.50885870	19.77
50	10v-02-TetrcTriPri2----------120	-960.50876390	19.83
51	10v-03-Isocloso----------246	-960.50875940	19.83
52	10v-04-closo----------316	-960.50775650	20.46
53	10v-01-TetrcTriPri1----------27	-960.50774900	20.47
54	10v-01-TetrcTriPri1----------5	-960.50746960	20.64
55	10v-03-Isocloso----------225	-960.50684220	21.04
56	10v-03-Isocloso----------208	-960.50672010	21.11
57	10v-02-TetrcTriPri2----------185	-960.50668530	21.13
58	10v-02-TetrcTriPri2----------68	-960.50668370	21.14
59	10v-03-Isocloso----------279	-960.50660900	21.18
60	10v-02-TetrcTriPri2----------126	-960.50619850	21.44
61	10v-02-TetrcTriPri2----------52	-960.50524680	22.04
62	10v-03-Isocloso----------288	-960.50500280	22.19
63	10v-03-Isocloso----------207	-960.50341400	23.19
64	10v-02-TetrcTriPri2----------45	-960.50301530	23.44
65	10v-02-TetrcTriPri2----------152	-960.50289320	23.51
66	10v-03-Isocloso----------204	-960.50239660	23.83
67	10v-03-Isocloso----------234	-960.50186760	24.16
68	10v-03-Isocloso----------270	-960.50148300	24.40
69	10v-03-Isocloso----------273	-960.50147900	24.40
70	10v-03-Isocloso----------230	-960.50094660	24.74
71	10v-03-Isocloso----------272	-960.50081060	24.82
72	10v-03-Isocloso----------274	-960.50076670	24.85
73	10v-03-Isocloso----------238	-960.50076590	24.85
74	10v-02-TetrcTriPri2----------190	-960.50063180	24.93
75	10v-03-Isocloso----------228	-960.50037390	25.10
76	10v-04-closo----------317	-960.49983250	25.43
77	10v-03-Isocloso----------256	-960.49980800	25.45
78	10v-04-closo----------315	-960.49971490	25.51
79	10v-01-TetrcTriPri1----------32	-960.49865800	26.17
80	10v-01-TetrcTriPri1----------28	-960.49863240	26.19
81	10v-01-TetrcTriPri1----------1	-960.49852810	26.25
82	10v-01-TetrcTriPri1----------10	-960.49851600	26.26

83	10v-01-TetrcTriPri1----------34_i-14	-960.49845190	26.30
84	10v-01-TetrcTriPri1----------34_r-14	-960.49842410	26.32
85	10v-02-TetrcTriPri2----------130	-960.49796870	26.60
86	10v-02-TetrcTriPri2----------53	-960.49724760	27.06
87	10v-03-Isocloso----------296	-960.49724360	27.06
88	10v-02-TetrcTriPri2----------194	-960.49724040	27.06
89	10v-02-TetrcTriPri2----------186	-960.49560830	28.09
90	10v-02-TetrcTriPri2----------166	-960.49513680	28.38
91	10v-02-TetrcTriPri2----------50	-960.49484580	28.56
92	10v-02-TetrcTriPri2----------180	-960.49445500	28.81
93	10v-02-TetrcTriPri2----------54	-960.49429780	28.91
94	10v-02-TetrcTriPri2----------39	-960.49429150	28.91
95	10v-02-TetrcTriPri2----------183	-960.49428550	28.92
96	10v-03-Isocloso----------260	-960.49427460	28.92
97	10v-03-Isocloso----------224	-960.49423160	28.95
98	10v-03-Isocloso----------257	-960.49420330	28.97
99	10v-01-TetrcTriPri1----------6	-960.49261070	29.97
100	10v-04-closo----------329	-960.49260470	29.97
101	10v-02-TetrcTriPri2----------56	-960.49248590	30.04
102	10v-01-TetrcTriPri1----------36	-960.49223400	30.20
103	10v-02-TetrcTriPri2----------155	-960.49193180	30.39
104	10v-02-TetrcTriPri2----------108	-960.49184470	30.45
105	10v-02-TetrcTriPri2----------107	-960.49184140	30.45
106	10v-03-Isocloso----------264	-960.49081900	31.09
107	10v-01-TetrcTriPri1----------3	-960.49055680	31.26
108	10v-02-TetrcTriPri2----------40	-960.49040510	31.35
109	10v-01-TetrcTriPri1----------35	-960.49030850	31.41
110	10v-02-TetrcTriPri2----------191	-960.48989110	31.67
111	10v-02-TetrcTriPri2----------59	-960.48975190	31.76
112	10v-02-TetrcTriPri2----------69	-960.48912070	32.16
113	10v-03-Isocloso----------295	-960.48911220	32.16
114	10v-02-TetrcTriPri2----------72	-960.48848260	32.56
115	10v-02-TetrcTriPri2----------98	-960.48847390	32.56
116	10v-04-closo----------331_r-21	-960.48795350	32.89
117	10v-03-Isocloso----------202	-960.48777410	33.00
118	10v-03-Isocloso----------201	-960.48775260	33.02
119	10v-01-TetrcTriPri1----------31	-960.48765820	33.07
120	10v-04-closo----------331_i-21	-960.48712620	33.41
121	10v-03-Isocloso----------212	-960.48525200	34.58
122	10v-02-TetrcTriPri2----------46	-960.48487840	34.82
123	10v-03-Isocloso----------206	-960.48420240	35.24
124	10v-03-Isocloso----------223	-960.48419290	35.25

125	10v-03-Isocloso----------217	-960.48374710	35.53
126	10v-03-Isocloso----------248	-960.48361620	35.61
127	10v-04-closo----------327	-960.48343750	35.72
128	10v-02-TetrcTriPri2----------178	-960.48278500	36.13
129	10v-02-TetrcTriPri2----------148	-960.48244250	36.35
130	10v-02-TetrcTriPri2----------136	-960.48200580	36.62
131	10v-02-TetrcTriPri2----------135	-960.48199540	36.63
132	10v-02-TetrcTriPri2----------128	-960.48199410	36.63
133	10v-02-TetrcTriPri2----------71	-960.48175610	36.78
134	10v-02-TetrcTriPri2----------77	-960.48072870	37.42
135	10v-03-Isocloso----------258	-960.48067790	37.45
136	10v-01-TetrcTriPri1----------21	-960.48027550	37.71
137	10v-01-TetrcTriPri1----------19	-960.48027430	37.71
138	10v-03-Isocloso----------297	-960.47990080	37.94
139	10v-01-TetrcTriPri1----------12	-960.47972240	38.05
140	10v-01-TetrcTriPri1----------13	-960.47971900	38.06
141	10v-04-closo----------330	-960.47962480	38.12
142	10v-03-Isocloso----------243	-960.47936250	38.28
143	10v-02-TetrcTriPri2----------80	-960.47916990	38.40
144	10v-03-Isocloso----------255	-960.47910860	38.44
145	10v-02-TetrcTriPri2----------43	-960.47862620	38.74
146	10v-02-TetrcTriPri2----------76	-960.47759930	39.39
147	10v-02-TetrcTriPri2----------139	-960.47756160	39.41
148	10v-02-TetrcTriPri2----------48	-960.47737440	39.53
149	10v-02-TetrcTriPri2----------42	-960.47705650	39.73
150	10v-02-TetrcTriPri2----------189	-960.47610000	40.33
151	10v-03-Isocloso----------254	-960.47602090	40.38
152	10v-01-TetrcTriPri1----------9	-960.47548790	40.71
153	10v-02-TetrcTriPri2----------153	-960.47515580	40.92
154	10v-02-TetrcTriPri2----------67	-960.47344470	41.99
155	10v-02-TetrcTriPri2----------99	-960.47333990	42.06
156	10v-02-TetrcTriPri2----------115	-960.47303550	42.25
157	10v-04-closo----------339	-960.47251500	42.58
158	10v-03-Isocloso----------245	-960.47250550	42.58
159	10v-02-TetrcTriPri2----------157	-960.47244730	42.62
160	10v-03-Isocloso----------240	-960.47230850	42.71
161	10v-02-TetrcTriPri2----------118	-960.47141510	43.27
162	10v-03-Isocloso----------293	-960.47114530	43.44
163	10v-02-TetrcTriPri2----------97	-960.47100860	43.52
164	10v-01-TetrcTriPri1----------16	-960.47062290	43.76
165	10v-03-Isocloso----------291	-960.46994660	44.19
166	10v-03-Isocloso----------263	-960.46894950	44.81
167	10v-02-TetrcTriPri2----------167	-960.46889000	44.85

168	10v-02-TetrcTriPri2----------169	-960.46887960	44.86
169	10v-03-Isocloso----------220	-960.46882390	44.89
170	10v-02-TetrcTriPri2----------171	-960.46878760	44.92
171	10v-03-Isocloso----------239	-960.46878140	44.92
172	10v-03-Isocloso----------203	-960.46862470	45.02
173	10v-02-TetrcTriPri2----------170	-960.46836980	45.18
174	10v-01-TetrcTriPri1----------22	-960.46817850	45.30
175	10v-02-TetrcTriPri2----------168_r-16	-960.46813110	45.33
176	10v-02-TetrcTriPri2----------156	-960.46812590	45.33
177	10v-04-closo----------318	-960.46807590	45.36
178	10v-02-TetrcTriPri2----------74	-960.46801620	45.40
179	10v-02-TetrcTriPri2----------122	-960.46796130	45.43
180	10v-02-TetrcTriPri2----------168_i-16	-960.46789100	45.48
181	10v-02-TetrcTriPri2----------94	-960.46779150	45.54
182	10v-02-TetrcTriPri2----------91	-960.46777690	45.55
183	10v-02-TetrcTriPri2----------112	-960.46769710	45.60
184	10v-02-TetrcTriPri2----------70	-960.46728290	45.86
185	10v-02-TetrcTriPri2----------160	-960.46728040	45.86
186	10v-02-TetrcTriPri2----------84	-960.46690450	46.10
187	10v-01-TetrcTriPri1----------11	-960.46671030	46.22
188	10v-02-TetrcTriPri2----------182	-960.46623990	46.51
189	10v-03-Isocloso----------282	-960.46620180	46.54
190	10v-03-Isocloso----------309	-960.46599970	46.67
191	10v-01-TetrcTriPri1----------37	-960.46590410	46.73
192	10v-02-TetrcTriPri2----------57	-960.46535390	47.07
193	10v-02-TetrcTriPri2----------172	-960.46497080	47.31
194	10v-04-closo----------314	-960.46490900	47.35
195	10v-02-TetrcTriPri2----------82	-960.46463890	47.52
196	10v-03-Isocloso----------310	-960.46434750	47.70
197	10v-02-TetrcTriPri2----------64	-960.46356280	48.19
198	10v-02-TetrcTriPri2----------66	-960.46355820	48.20
199	10v-02-TetrcTriPri2----------192	-960.46287620	48.63
200	10v-02-TetrcTriPri2----------196	-960.46278800	48.68
201	10v-02-TetrcTriPri2----------41	-960.46249070	48.87
202	10v-02-TetrcTriPri2----------123	-960.46227590	49.00
203	10v-03-Isocloso----------213	-960.46211450	49.10
204	10v-02-TetrcTriPri2----------116	-960.46200760	49.17
205	10v-03-Isocloso----------252	-960.46195040	49.21
206	10v-03-Isocloso----------235	-960.46131230	49.61
207	10v-02-TetrcTriPri2----------197	-960.46096740	49.82
208	10v-01-TetrcTriPri1----------29	-960.46096030	49.83
209	10v-02-TetrcTriPri2----------44	-960.46059570	50.06

210	10v-03-Isocloso----------308	-960.45898680	51.07
211	10v-03-Isocloso----------216	-960.45872140	51.23
212	10v-02-TetrcTriPri2----------177	-960.45854940	51.34
213	10v-04-closo----------332	-960.45851220	51.36
214	10v-04-closo----------333	-960.45848510	51.38
215	10v-01-TetrcTriPri1----------8	-960.45832220	51.48
216	10v-03-Isocloso----------292	-960.45815630	51.59
217	10v-02-TetrcTriPri2----------143	-960.45804310	51.66
218	10v-03-Isocloso----------300	-960.45791840	51.74
219	10v-03-Isocloso----------306	-960.45791820	51.74
220	10v-02-TetrcTriPri2----------61	-960.45743450	52.04
221	10v-02-TetrcTriPri2----------137	-960.45735170	52.09
222	10v-02-TetrcTriPri2----------62	-960.45735100	52.09
223	10v-03-Isocloso----------262	-960.45734850	52.09
224	10v-03-Isocloso----------299	-960.45716360	52.21
225	10v-02-TetrcTriPri2----------111	-960.45697130	52.33
226	10v-01-TetrcTriPri1----------33	-960.45686520	52.40
227	10v-02-TetrcTriPri2----------55	-960.45665480	52.53
228	10v-03-Isocloso----------268	-960.45663550	52.54
229	10v-03-Isocloso----------294	-960.45642570	52.67
230	10v-03-Isocloso----------253	-960.45621910	52.80
231	10v-02-TetrcTriPri2----------138	-960.45561520	53.18
232	10v-02-TetrcTriPri2----------151	-960.45551950	53.24
233	10v-03-Isocloso----------219	-960.45549950	53.25
234	10v-02-TetrcTriPri2----------78	-960.45498950	53.57
235	10v-02-TetrcTriPri2----------79	-960.45498740	53.58
236	10v-02-TetrcTriPri2----------187	-960.45473690	53.73
237	10v-02-TetrcTriPri2----------188	-960.45473070	53.74
238	10v-03-Isocloso----------276	-960.45472710	53.74
239	10v-01-TetrcTriPri1----------14	-960.45353020	54.49
240	10v-01-TetrcTriPri1----------7	-960.45299750	54.82
241	10v-02-TetrcTriPri2----------106	-960.45255960	55.10
242	10v-02-TetrcTriPri2----------134	-960.45250110	55.14
243	10v-02-TetrcTriPri2----------127	-960.45246300	55.16
244	10v-03-Isocloso----------267	-960.45224270	55.30
245	10v-03-Isocloso----------242	-960.45147210	55.78
246	10v-03-Isocloso----------312	-960.45145700	55.79
247	10v-02-TetrcTriPri2----------173	-960.45128280	55.90
248	10v-04-closo----------335	-960.45124980	55.92
249	10v-03-Isocloso----------305	-960.45059260	56.33
250	10v-02-TetrcTriPri2----------90	-960.45024510	56.55
251	10v-02-TetrcTriPri2----------83	-960.44989380	56.77
252	10v-03-Isocloso----------249	-960.44989110	56.77

253	10v-01-TetrcTriPri1----------17	-960.44909500	57.27
254	10v-04-closo----------345	-960.44867370	57.54
255	10v-03-Isocloso----------237	-960.44849600	57.65
256	10v-04-closo----------343	-960.44843640	57.69
257	10v-03-Isocloso----------232	-960.44744100	58.31
258	10v-03-Isocloso----------265	-960.44686110	58.68
259	10v-02-TetrcTriPri2----------93	-960.44600880	59.21
260	10v-03-Isocloso----------283	-960.44575060	59.37
261	10v-02-TetrcTriPri2----------162	-960.44548660	59.54
262	10v-02-TetrcTriPri2----------133	-960.44471280	60.02
263	10v-02-TetrcTriPri2----------145	-960.44434530	60.25
264	10v-02-TetrcTriPri2----------92	-960.44434420	60.25
265	10v-02-TetrcTriPri2----------81	-960.44433050	60.26
266	10v-02-TetrcTriPri2----------154	-960.44425070	60.31
267	10v-04-closo----------338	-960.44385390	60.56
268	10v-02-TetrcTriPri2----------140	-960.44277750	61.24
269	10v-03-Isocloso----------304	-960.44227350	61.55
270	10v-02-TetrcTriPri2----------146	-960.44178950	61.86
271	10v-02-TetrcTriPri2----------147	-960.44143690	62.08
272	10v-03-Isocloso----------266	-960.44093820	62.39
273	10v-03-Isocloso----------214	-960.44058980	62.61
274	10v-02-TetrcTriPri2----------51	-960.44045580	62.69
275	10v-03-Isocloso----------301	-960.43845560	63.95
276	10v-03-Isocloso----------244	-960.43829120	64.05
277	10v-03-Isocloso----------236	-960.43804810	64.21
278	10v-03-Isocloso----------286	-960.43731130	64.67
279	10v-02-TetrcTriPri2----------184	-960.43717120	64.76
280	10v-02-TetrcTriPri2----------85	-960.43706050	64.83
281	10v-02-TetrcTriPri2----------181	-960.43616570	65.39
282	10v-03-Isocloso----------303	-960.43586610	65.57
283	10v-02-TetrcTriPri2----------149	-960.43563260	65.72
284	10v-02-TetrcTriPri2----------58	-960.43499380	66.12
285	10v-04-closo----------321	-960.43483540	66.22
286	10v-04-closo----------319	-960.43471210	66.30
287	10v-03-Isocloso----------229	-960.43445390	66.46
288	10v-04-closo----------328	-960.43440670	66.49
289	10v-03-Isocloso----------285	-960.43431600	66.55
290	10v-01-TetrcTriPri1----------15	-960.43312210	67.30
291	10v-02-TetrcTriPri2----------73	-960.43180250	68.12
292	10v-02-TetrcTriPri2----------119	-960.43148150	68.33
293	10v-03-Isocloso----------215	-960.43134030	68.41
294	10v-02-TetrcTriPri2----------89	-960.43126370	68.46
295	10v-03-Isocloso----------218	-960.42960500	69.50

296	10v-02-TetrcTriPri2----------163	-960.42862110	70.12
297	10v-04-closo----------340	-960.42858390	70.14
298	10v-03-Isocloso----------284	-960.42825600	70.35
299	10v-02-TetrcTriPri2----------110	-960.42820440	70.38
300	10v-02-TetrcTriPri2----------103	-960.42703270	71.12
301	10v-03-Isocloso----------226	-960.42683280	71.24
302	10v-01-TetrcTriPri1----------2	-960.42611050	71.70
303	10v-02-TetrcTriPri2----------101	-960.42593550	71.81
304	10v-02-TetrcTriPri2----------114	-960.42576720	71.91
305	10v-02-TetrcTriPri2----------121	-960.42575940	71.92
306	10v-02-TetrcTriPri2----------164	-960.42512450	72.32
307	10v-03-Isocloso----------298	-960.42499480	72.40
308	10v-03-Isocloso----------233	-960.42463110	72.63
309	10v-02-TetrcTriPri2----------75	-960.42188800	74.35
310	10v-04-closo----------344	-960.42118700	74.79
311	10v-02-TetrcTriPri2----------96	-960.42107220	74.86
312	10v-02-TetrcTriPri2----------117	-960.42073550	75.07
313	10v-02-TetrcTriPri2----------104	-960.41961490	75.77
314	10v-02-TetrcTriPri2----------159	-960.41802170	76.77
315	10v-03-Isocloso----------307	-960.41739680	77.16
316	10v-02-TetrcTriPri2----------109_i-14	-960.41686160	77.50
317	10v-02-TetrcTriPri2----------109_r-14	-960.41677740	77.55
318	10v-02-TetrcTriPri2----------193	-960.41673840	77.58
319	10v-02-TetrcTriPri2----------102	-960.41611450	77.97
320	10v-02-TetrcTriPri2----------176	-960.41605680	78.01
321	10v-04-closo----------337	-960.41598570	78.05
322	10v-03-Isocloso----------302	-960.41595090	78.07
323	10v-02-TetrcTriPri2----------175	-960.41559710	78.29
324	10v-04-closo----------336	-960.41426580	79.13
325	10v-02-TetrcTriPri2----------113	-960.41365650	79.51
326	10v-03-Isocloso----------281	-960.41358910	79.55
327	10v-04-closo----------322	-960.40979900	81.93
328	10v-04-closo----------320	-960.40976680	81.95
329	10v-04-closo----------323	-960.40950750	82.12
330	10v-02-TetrcTriPri2----------125	-960.40908620	82.38
331	10v-02-TetrcTriPri2----------86	-960.40902320	82.42
332	10v-03-Isocloso----------277	-960.40702870	83.67
333	10v-03-Isocloso----------278	-960.40702570	83.67
334	10v-04-closo----------324	-960.40299590	86.20
335	10v-02-TetrcTriPri2----------95	-960.40243630	86.55
336	10v-02-TetrcTriPri2----------161	-960.40098940	87.46
337	10v-02-TetrcTriPri2----------87	-960.39959620	88.34

338	10v-03-Isocloso----------313	-960.39849300	89.03
339	10v-04-closo----------334	-960.39668520	90.16
340	10v-02-TetrcTriPri2----------150	-960.39242590	92.83
341	10v-02-TetrcTriPri2----------165	-960.39176710	93.25
342	10v-02-TetrcTriPri2----------174	-960.39130130	93.54
343	10v-02-TetrcTriPri2----------100	-960.38932480	94.78
344	10v-04-closo----------342	-960.38745230	95.96
345	10v-04-closo----------341	-960.38742830	95.97
346	10v-03-Isocloso----------280	-960.38717400	96.13
347	10v-02-TetrcTriPri2----------49	-960.38517430	97.39
348	10v-02-TetrcTriPri2----------60	-960.38377140	98.27
349	10v-02-TetrcTriPri2----------105	-960.35802870	114.42

Table S7A. Initial $Cp_3W_3(H)B_8H_8$ structures, 618 structures.

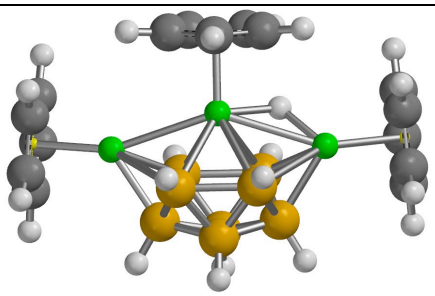
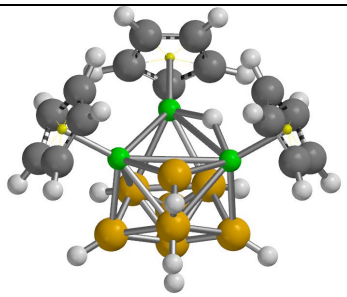
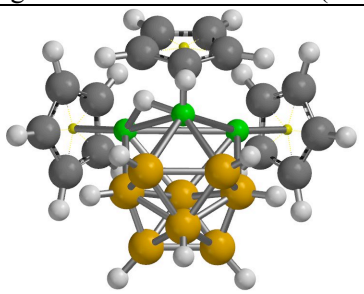
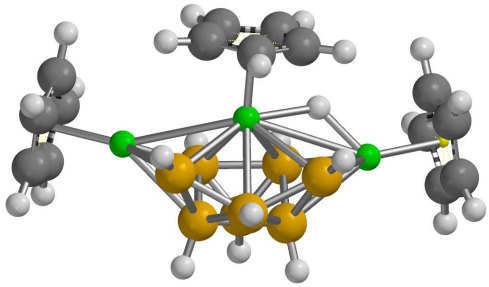
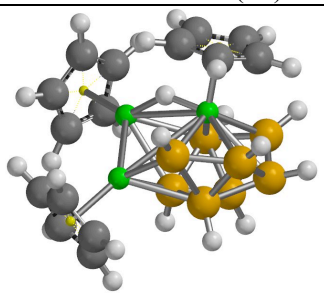
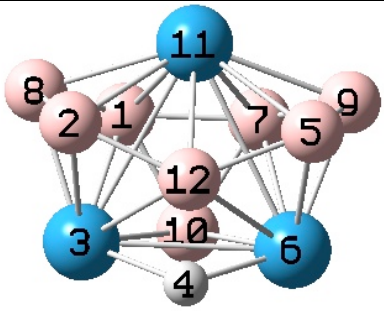
Initial structures	 Edge-coalesced icosahedron (108)
 Pentacapped trigonal prism (58)	 Oblate structure (69)
 Dg 6 vx structure (148)	 Oblatocloso (235)

Table S7B. Distance table for the lowest-lying $Cp_3W_3(H)B_8H_8$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

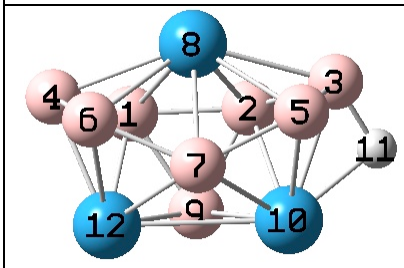


1. -986.3671014 0.0 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	3.091895	0.000000			
3 W	2.317031	2.186020	0.000000		
4 H	3.596481	2.628714	1.913985	0.000000	
5 B	3.905870	3.196465	3.699271	2.623990	0.000000
6 W	3.219365	3.704821	2.791618	1.912052	2.187467
7 B	1.782949	3.907331	3.217413	3.597476	3.092734
8 B	1.788528	1.803724	2.093314	3.512494	4.061986
9 B	3.254928	4.064164	3.992075	3.508145	1.804483
10 B	1.765198	3.864790	2.228544	3.017200	3.862973
11 W	2.320284	2.230551	3.037902	3.262152	2.228756
12 B	3.548071	1.770557	2.469449	1.512179	1.770312

	6	7	8	9	10
7 B	2.322248	0.000000			
8 B	3.996782	3.254216	0.000000		
9 B	2.092532	1.788877	4.146391	0.000000	
10 B	2.228977	1.766093	3.140135	3.137346	0.000000
11 W	3.041260	2.319134	2.266205	2.266829	3.272525
12 B	2.473549	3.549883	3.093914	3.095010	3.632357

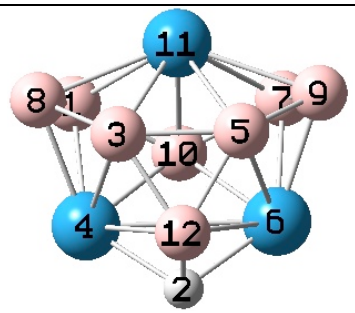
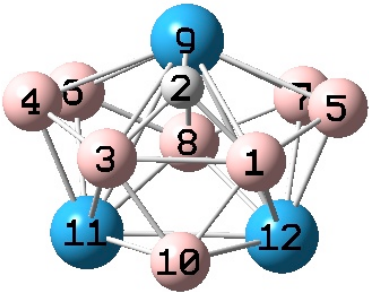
	11	12
12 B	2.287210	0.000000

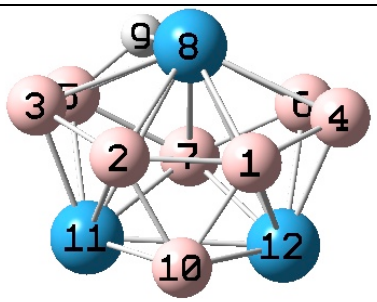
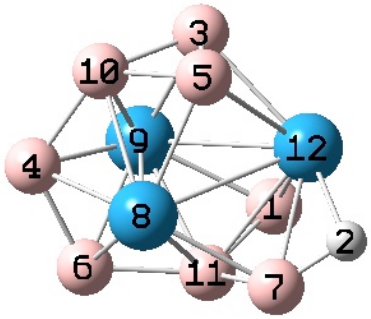


2. -986.3609759 +3.8 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	1.768902	0.000000			
3 B	3.353405	1.904417	0.000000		
4 B	1.787743	3.231498	4.202258	0.000000	
5 B	3.955549	3.166512	1.845331	4.062046	0.000000
6 B	3.100365	3.888728	4.077256	1.810257	3.146704
7 B	3.517441	3.514615	3.101644	3.067261	1.752463
8 W	2.338998	2.301435	2.267135	2.281947	2.228689
9 B	1.767594	1.742353	3.216296	3.138458	3.888905
10 W	3.246752	2.397364	2.191861	3.961553	2.179114
11 H	3.785659	2.162865	1.275487	4.900526	2.546837
12 W	2.314182	3.182905	4.024235	2.085164	3.653412

	6	7	8	9	10
7 B	1.760041	0.000000			
8 W	2.226120	2.292192	0.000000		
9 B	3.861322	3.555712	3.254716	0.000000	
10 W	3.624266	2.326228	3.005003	2.255241	0.000000
11 H	4.831856	3.641184	3.326388	3.018893	1.851932
12 W	2.168734	2.356685	3.005136	2.227273	2.706235

	11 12 12 W 4.240286 0.000000
 3. -986.3493994 +11.1 C_S	1 2 3 4 5 1 B 0.000000 2 H 3.754981 0.000000 3 B 3.099605 2.678774 0.000000 4 W 2.165305 1.898126 2.321211 0.000000 5 B 3.907274 2.679541 1.828873 3.249565 0.000000 6 W 3.675029 1.897329 3.249928 2.832759 2.317808 7 B 3.111623 3.756974 3.912951 3.675997 3.096600 8 B 1.838968 3.535659 1.785294 2.082978 3.286126 9 B 4.047004 3.539042 3.293556 4.022678 1.786177 10 B 1.774200 3.094547 3.493864 2.337517 3.488473 11 W 2.208946 3.699129 2.332145 3.029063 2.326300 12 B 3.950943 1.347406 1.748033 2.364637 1.747683 6 7 8 9 10 7 B 2.168248 0.000000 8 B 4.018527 4.045240 0.000000 9 B 2.083801 1.839238 4.174285 0.000000 10 B 2.336003 1.770892 3.091669 3.090093 0.000000 11 W 3.027981 2.208362 2.275163 2.276613 2.333625 12 B 2.359730 3.950792 3.184904 3.185603 3.621214 11 12 11 W 0.000000 12 B 3.312626 0.000000
 4. -986.3492387 +11.2 C_S	1 2 3 4 5 1 B 0.000000 2 H 1.458741 0.000000 3 B 2.061338 1.452652 0.000000 4 B 3.460796 2.559969 1.802859 0.000000 5 B 1.801703 2.559321 3.454242 4.223589 0.000000 6 B 4.034135 3.514054 3.118252 1.795414 4.073539 7 B 3.121904 3.511544 4.026301 4.066951 1.800505 8 B 3.551877 3.671050 3.547529 3.067162 3.070352 9 W 2.492448 1.870393 2.486889 2.313837 2.313664 10 B 1.754092 2.450465 1.759455 3.182511 3.175830 11 W 3.264341 3.279433 2.260690 2.096740 3.967464 12 W 2.265876 3.285847 3.268669 3.973365 2.097244 6 7 8 9 10 7 B 3.157096 0.000000 8 B 1.772875 1.771552 0.000000 9 W 2.226938 2.219689 2.310446 0.000000 10 B 3.882494 3.880621 3.548411 3.320329 0.000000 11 W 2.169004 3.631679 2.321062 3.029212 2.233851 12 W 3.636591 2.171663 2.322576 3.032375 2.236425 11 12

	11 W 0.000000 12 W 2.691281 0.000000
 5. -986.3444136 +14.2 C_1	1 2 3 4 5 1 B 0.000000 2 B 1.823211 0.000000 3 B 3.288771 1.782336 0.000000 4 B 1.792789 3.294938 4.190930 0.000000 5 B 3.966330 3.109922 1.810688 4.143055 0.000000 6 B 3.081685 3.907411 4.069958 1.804280 3.244728 7 B 3.512502 3.521733 3.140392 3.108176 1.906474 8 W 2.344779 2.332714 2.289420 2.315315 2.307342 9 H 3.949022 3.614170 2.672720 3.592752 1.331091 10 B 1.748553 1.755917 3.141393 3.138678 3.897575 11 W 3.187417 2.300194 2.102161 3.950222 2.174075 12 W 2.299308 3.209139 3.982504 2.081842 3.722032 6 7 8 9 10 7 B 1.819715 0.000000 8 W 2.255561 2.443418 0.000000 9 H 2.448423 1.786616 1.847893 0.000000 10 B 3.859621 3.517182 3.290752 4.386394 0.000000 11 W 3.631174 2.293815 3.032632 3.124103 2.221242 12 W 2.174518 2.301319 3.061516 3.694313 2.229378 11 12 11 W 0.000000 12 W 2.709655 0.000000
 6. -986.3369197 +18.9 C_1	1 2 3 4 5 1 B 0.000000 2 H 3.207789 0.000000 3 B 3.219609 3.950943 0.000000 4 B 4.014351 4.860434 3.143662 0.000000 5 B 3.893097 3.189111 1.716944 3.158969 0.000000 6 B 3.162302 4.220973 3.850408 1.759810 3.839477 7 B 2.915959 1.267307 4.005637 4.060891 3.290333 8 W 3.664260 3.002923 3.167272 2.195109 2.215768 9 W 2.208257 4.270824 2.236984 2.188856 3.183658 10 B 3.998427 4.412532 1.724808 1.797032 1.741354 11 B 1.793281 2.771137 3.549864 3.069714 3.541350 12 W 2.102651 1.860708 2.310994 4.037175 2.308384 6 7 8 9 10 7 B 3.150328 0.000000 8 W 2.191204 2.250211 0.000000 9 W 2.214742 3.730710 2.986486 0.000000 10 B 3.091409 4.073102 2.325378 2.344234 0.000000 11 B 1.801440 1.824862 2.334322 2.317659 3.553917 12 W 3.753716 2.239713 2.903430 2.884102 3.275322 11 12

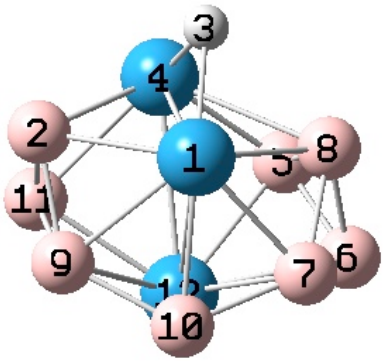
	11 B 0.000000 12 W 2.446638 0.000000
 7. -986.3308747 +22.7 C_1	1 2 3 4 5 1 W 0.000000 2 B 2.242024 0.000000 3 H 1.858264 2.568132 0.000000 4 W 2.629579 2.300703 1.833652 0.000000 5 B 3.507260 4.050533 3.258744 2.172435 0.000000 6 B 3.500247 4.680868 3.965185 3.408527 1.684169 7 B 2.281009 3.937593 3.466190 3.499127 2.813535 8 B 2.398748 3.869201 2.419792 2.492578 1.767139 9 B 2.354186 1.729244 3.587520 3.148761 4.049399 10 B 2.258937 3.165273 3.913951 3.765261 3.795128 11 B 3.144857 1.680453 3.498191 2.267138 3.427147 12 W 3.126539 3.272894 3.920523 2.832758 2.311455 6 7 8 9 10 6 B 0.000000 7 B 1.745209 0.000000 8 B 1.709673 1.814199 0.000000 9 B 4.128316 3.175783 3.873496 0.000000 10 B 3.141710 1.807141 3.227412 1.793232 0.000000 11 B 4.157503 3.896017 3.926978 1.742091 3.107787 12 W 2.251544 2.337524 2.859655 2.372051 2.134335 11 12 11 B 0.000000 12 W 2.257260 0.000000

Table S7C. Energy ranking for all of the $Cp_3W_3(H)B_8H_8$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	11v-02-PentaCapTriPri----------130	-986.0275845	0.00
2	11v-04-ThatStructure----------359	-986.0161074	7.20
3	11v-04-ThatStructure----------357	-986.0100616	11.00
4	11v-02-PentaCapTriPri----------129	-986.0079308	12.33
5	11v-02-PentaCapTriPri----------131	-986.0077252	12.46
6	11v-03-TriFlatPentaCapTrigPrism----------209	-986.0053525	13.95
7	11v-04-ThatStructure----------358	-986.0023843	15.81
8	11v-05-Oblatocloso----------560	-985.9991276	17.86
9	11v-05-Oblatocloso----------561	-985.9991172	17.86
10	11v-03-TriFlatPentaCapTrigPrism----------181	-985.9966520	19.41
11	11v-03-TriFlatPentaCapTrigPrism----------180	-985.9965905	19.45
12	11v-05-Oblatocloso----------528	-985.9963979	19.57
13	11v-04-ThatStructure----------296	-985.9925372	21.99
14	11v-02-PentaCapTriPri----------159	-985.9925159	22.01
15	11v-02-PentaCapTriPri----------105	-985.9925141	22.01
16	11v-04-ThatStructure----------325	-985.9917877	22.46
17	11v-04-ThatStructure----------324	-985.9917473	22.49
18	11v-04-ThatStructure----------342	-985.9917174	22.51
19	11v-05-Oblatocloso----------557	-985.9904815	23.28
20	11v-05-Oblatocloso----------559	-985.9902788	23.41
21	11v-05-Oblatocloso----------568	-985.9902457	23.43
22	11v-02-PentaCapTriPri----------144	-985.9898660	23.67
23	11v-04-ThatStructure----------282	-985.9893276	24.01
24	11v-05-Oblatocloso----------588_i-20	-985.9875475	25.12
25	11v-05-Oblatocloso----------588_r-20	-985.9873755	25.23
26	11v-05-Oblatocloso----------587	-985.9873574	25.24
27	11v-05-Oblatocloso----------591	-985.9871472	25.38
28	11v-05-Oblatocloso----------404	-985.9860155	26.09
29	11v-03-TriFlatPentaCapTrigPrism----------190	-985.9852422	26.57
30	11v-04-ThatStructure----------292	-985.9849671	26.74
31	11v-05-Oblatocloso----------414	-985.9849634	26.75
32	11v-05-Oblatocloso----------415	-985.9849473	26.76
33	11v-01-Icos-1vx----------50	-985.9849437	26.76
34	11v-03-TriFlatPentaCapTrigPrism----------175	-985.9848955	26.79
35	11v-04-ThatStructure----------264	-985.9844649	27.06
36	11v-05-Oblatocloso----------406	-985.9839158	27.40
37	11v-02-PentaCapTriPri----------127	-985.9838552	27.44
38	11v-02-PentaCapTriPri----------126	-985.9838160	27.47

39	11v-05-Oblatocloso----------452	-985.9831735	27.87
40	11v-05-Oblatocloso----------521	-985.9831384	27.89
41	11v-05-Oblatocloso----------520	-985.9831225	27.90
42	11v-01-Icos-1vx----------77	-985.9830861	27.92
43	11v-05-Oblatocloso----------589_r-15	-985.9819825	28.62
44	11v-05-Oblatocloso----------589_i-15	-985.9817122	28.79
45	11v-04-ThatStructure----------356	-985.9815382	28.89
46	11v-04-ThatStructure----------341	-985.9814108	28.97
47	11v-03-TriFlatPentaCapTrigPrism----------185	-985.9799476	29.89
48	11v-05-Oblatocloso----------432	-985.9797343	30.03
49	11v-05-Oblatocloso----------582	-985.9796670	30.07
50	11v-05-Oblatocloso----------443	-985.9794102	30.23
51	11v-05-Oblatocloso----------444	-985.9793877	30.24
52	11v-05-Oblatocloso----------497	-985.9793017	30.30
53	11v-05-Oblatocloso----------447	-985.9792960	30.30
54	11v-05-Oblatocloso----------428	-985.9792960	30.30
55	11v-01-Icos-1vx----------36	-985.9792922	30.30
56	11v-01-Icos-1vx----------41	-985.9791585	30.39
57	11v-04-ThatStructure----------311	-985.9791025	30.42
58	11v-03-TriFlatPentaCapTrigPrism----------199	-985.9785667	30.76
59	11v-04-ThatStructure----------318	-985.9783552	30.89
60	11v-04-ThatStructure----------304_i-22	-985.9783496	30.90
61	11v-04-ThatStructure----------305	-985.9783466	30.90
62	11v-04-ThatStructure----------343	-985.9782723	30.94
63	11v-04-ThatStructure----------304_r-22	-985.9782434	30.96
64	11v-05-Oblatocloso----------592	-985.9780117	31.11
65	11v-03-TriFlatPentaCapTrigPrism----------186	-985.9777227	31.29
66	11v-04-ThatStructure----------295_i-14	-985.9769356	31.78
67	11v-04-ThatStructure----------295_r-14	-985.9769304	31.79
68	11v-05-Oblatocloso----------586	-985.9765736	32.01
69	11v-04-ThatStructure----------286	-985.9757903	32.50
70	11v-02-PentaCapTriPri----------113	-985.9756677	32.58
71	11v-04-ThatStructure----------254	-985.9755911	32.63
72	11v-04-ThatStructure----------355	-985.9750836	32.95
73	11v-03-TriFlatPentaCapTrigPrism----------179	-985.9749148	33.05
74	11v-03-TriFlatPentaCapTrigPrism----------206	-985.9743213	33.42
75	11v-03-TriFlatPentaCapTrigPrism----------207	-985.9741680	33.52
76	11v-02-PentaCapTriPri----------161	-985.9736135	33.87
77	11v-05-Oblatocloso----------462	-985.9735502	33.91
78	11v-03-TriFlatPentaCapTrigPrism----------215	-985.9732069	34.12
79	11v-05-Oblatocloso----------512	-985.9728786	34.33

80	11v-05-Oblatocloso----------513	-985.9727956	34.38
81	11v-03-TriFlatPentaCapTrigPrism----------221	-985.9719164	34.93
82	11v-05-Oblatocloso----------438	-985.9715878	35.14
83	11v-05-Oblatocloso----------437	-985.9715855	35.14
84	11v-05-Oblatocloso----------455	-985.9715348	35.17
85	11v-04-ThatStructure----------297	-985.9715319	35.17
86	11v-03-TriFlatPentaCapTrigPrism----------191	-985.9696027	36.38
87	11v-04-ThatStructure----------320	-985.9693867	36.52
88	11v-01-Icos-1vx----------76	-985.9693583	36.54
89	11v-05-Oblatocloso----------454	-985.9690677	36.72
90	11v-05-Oblatocloso----------542	-985.9686597	36.98
91	11v-02-PentaCapTriPri----------128	-985.9665390	38.31
92	11v-04-ThatStructure----------332	-985.9662261	38.50
93	11v-05-Oblatocloso----------511	-985.9649326	39.32
94	11v-04-ThatStructure----------301	-985.9637299	40.07
95	11v-05-Oblatocloso----------379	-985.9634004	40.28
96	11v-05-Oblatocloso----------551	-985.9633177	40.33
97	11v-05-Oblatocloso----------430	-985.9633051	40.34
98	11v-04-ThatStructure----------302	-985.9632027	40.40
99	11v-03-TriFlatPentaCapTrigPrism----------169	-985.9630036	40.53
100	11v-05-Oblatocloso----------524	-985.9629997	40.53
101	11v-04-ThatStructure----------310	-985.9629361	40.57
102	11v-05-Oblatocloso----------525	-985.9628915	40.60
103	11v-05-Oblatocloso----------424	-985.9628365	40.63
104	11v-03-TriFlatPentaCapTrigPrism----------162	-985.9628235	40.64
105	11v-01-Icos-1vx----------90	-985.9626317	40.76
106	11v-01-Icos-1vx----------89_r-46	-985.9626138	40.77
107	11v-05-Oblatocloso----------515	-985.9626028	40.78
108	11v-01-Icos-1vx----------37	-985.9625825	40.79
109	11v-05-Oblatocloso----------500	-985.9625245	40.83
110	11v-05-Oblatocloso----------517	-985.9625164	40.83
111	11v-05-Oblatocloso----------518	-985.9624971	40.84
112	11v-05-Oblatocloso----------516	-985.9624843	40.85
113	11v-04-ThatStructure----------337	-985.9622718	40.99
114	11v-04-ThatStructure----------336	-985.9622489	41.00
115	11v-05-Oblatocloso----------461	-985.9618280	41.26
116	11v-04-ThatStructure----------280	-985.9617401	41.32
117	11v-05-Oblatocloso----------423	-985.9613213	41.58
118	11v-05-Oblatocloso----------581	-985.9603728	42.18
119	11v-01-Icos-1vx----------49	-985.9599982	42.41
120	11v-05-Oblatocloso----------531	-985.9596116	42.65

121	11v-05-Oblatocloso----------534	-985.9594980	42.73
122	11v-03-TriFlatPentaCapTrigPrism----------167	-985.9591546	42.94
123	11v-01-Icos-1vx----------39	-985.9586382	43.27
124	11v-03-TriFlatPentaCapTrigPrism----------220	-985.9582346	43.52
125	11v-03-TriFlatPentaCapTrigPrism----------216	-985.9581867	43.55
126	11v-05-Oblatocloso----------509	-985.9580905	43.61
127	11v-02-PentaCapTriPri----------160	-985.9577491	43.82
128	11v-05-Oblatocloso----------488	-985.9562593	44.76
129	11v-05-Oblatocloso----------543	-985.9561601	44.82
130	11v-05-Oblatocloso----------578	-985.9561436	44.83
131	11v-05-Oblatocloso----------580	-985.9560068	44.92
132	11v-01-Icos-1vx----------89_i-46	-985.9556279	45.15
133	11v-05-Oblatocloso----------549	-985.9555138	45.23
134	11v-05-Oblatocloso----------483	-985.9553257	45.34
135	11v-05-Oblatocloso----------530	-985.9551969	45.42
136	11v-01-Icos-1vx----------13	-985.9551537	45.45
137	11v-04-ThatStructure----------365	-985.9551441	45.46
138	11v-05-Oblatocloso----------523	-985.9551172	45.47
139	11v-04-ThatStructure----------333	-985.9550884	45.49
140	11v-05-Oblatocloso----------445	-985.9549323	45.59
141	11v-05-Oblatocloso----------498	-985.9548191	45.66
142	11v-04-ThatStructure----------307	-985.9545672	45.82
143	11v-05-Oblatocloso----------393	-985.9543972	45.93
144	11v-02-PentaCapTriPri----------132	-985.9541705	46.07
145	11v-04-ThatStructure----------340	-985.9539530	46.21
146	11v-04-ThatStructure----------339	-985.9539204	46.23
147	11v-01-Icos-1vx----------47	-985.9533297	46.60
148	11v-01-Icos-1vx----------45	-985.9532354	46.66
149	11v-01-Icos-1vx----------46	-985.9532179	46.67
150	11v-05-Oblatocloso----------527	-985.9531755	46.69
151	11v-05-Oblatocloso----------526	-985.9531687	46.70
152	11v-02-PentaCapTriPri----------111	-985.9530791	46.75
153	11v-02-PentaCapTriPri----------107	-985.9528758	46.88
154	11v-01-Icos-1vx----------91	-985.9528001	46.93
155	11v-02-PentaCapTriPri----------143	-985.9527684	46.95
156	11v-01-Icos-1vx----------75	-985.9526891	47.00
157	11v-02-PentaCapTriPri----------145	-985.9526578	47.02
158	11v-04-ThatStructure----------290	-985.9525236	47.10
159	11v-04-ThatStructure----------272	-985.9524211	47.17
160	11v-03-TriFlatPentaCapTrigPrism----------164	-985.9522905	47.25
161	11v-04-ThatStructure----------300	-985.9520102	47.42

162	11v-03-TriFlatPentaCapTrigPrism----------201	-985.9516913	47.62
163	11v-05-Oblatocloso----------522	-985.9515374	47.72
164	11v-05-Oblatocloso----------392	-985.9513664	47.83
165	11v-04-ThatStructure----------361	-985.9513655	47.83
166	11v-02-PentaCapTriPri----------117	-985.9512868	47.88
167	11v-02-PentaCapTriPri----------121	-985.9512708	47.89
168	11v-03-TriFlatPentaCapTrigPrism----------218	-985.9512328	47.91
169	11v-04-ThatStructure----------283	-985.9511648	47.95
170	11v-03-TriFlatPentaCapTrigPrism----------170	-985.9509708	48.08
171	11v-05-Oblatocloso----------457	-985.9508171	48.17
172	11v-02-PentaCapTriPri----------152	-985.9504960	48.37
173	11v-05-Oblatocloso----------413	-985.9501654	48.58
174	11v-04-ThatStructure----------303	-985.9492108	49.18
175	11v-01-Icos-1vx----------58	-985.9487588	49.46
176	11v-04-ThatStructure----------360	-985.9486990	49.50
177	11v-04-ThatStructure----------350	-985.9485302	49.61
178	11v-01-Icos-1vx----------42	-985.9484117	49.68
179	11v-03-TriFlatPentaCapTrigPrism----------198	-985.9481349	49.86
180	11v-05-Oblatocloso----------380	-985.9479849	49.95
181	11v-05-Oblatocloso----------577	-985.9478811	50.02
182	11v-01-Icos-1vx----------43	-985.9478526	50.03
183	11v-01-Icos-1vx----------103	-985.9478105	50.06
184	11v-05-Oblatocloso----------397	-985.9477399	50.10
185	11v-05-Oblatocloso----------439	-985.9476631	50.15
186	11v-05-Oblatocloso----------552	-985.9469152	50.62
187	11v-01-Icos-1vx----------8	-985.9454188	51.56
188	11v-05-Oblatocloso----------570	-985.9453752	51.59
189	11v-05-Oblatocloso----------565	-985.9453408	51.61
190	11v-05-Oblatocloso----------564	-985.9453294	51.62
191	11v-01-Icos-1vx----------63	-985.9452224	51.68
192	11v-01-Icos-1vx----------32	-985.9451537	51.73
193	11v-05-Oblatocloso----------487	-985.9448682	51.91
194	11v-03-TriFlatPentaCapTrigPrism----------205	-985.9444088	52.19
195	11v-05-Oblatocloso----------496	-985.9444062	52.20
196	11v-05-Oblatocloso----------433	-985.9443758	52.22
197	11v-04-ThatStructure----------331	-985.9439514	52.48
198	11v-04-ThatStructure----------330	-985.9435712	52.72
199	11v-05-Oblatocloso----------441	-985.9435429	52.74
200	11v-03-TriFlatPentaCapTrigPrism----------204	-985.9434608	52.79
201	11v-03-TriFlatPentaCapTrigPrism----------226	-985.9432752	52.91
202	11v-03-TriFlatPentaCapTrigPrism----------217	-985.9430220	53.06

203	11v-05-Oblatocloso----------584	-985.9429685	53.10
204	11v-05-Oblatocloso----------456	-985.9427554	53.23
205	11v-04-ThatStructure----------353	-985.9419242	53.75
206	11v-02-PentaCapTriPri----------116	-985.9415910	53.96
207	11v-04-ThatStructure----------334	-985.9412082	54.20
208	11v-02-PentaCapTriPri----------139	-985.9411034	54.27
209	11v-02-PentaCapTriPri----------114	-985.9410575	54.30
210	11v-03-TriFlatPentaCapTrigPrism----------208	-985.9409128	54.39
211	11v-05-Oblatocloso----------535_i-12	-985.9408518	54.43
212	11v-04-ThatStructure----------327_i-15	-985.9407345	54.50
213	11v-05-Oblatocloso----------535_r-12	-985.9407013	54.52
214	11v-04-ThatStructure----------327_r-15	-985.9406598	54.55
215	11v-02-PentaCapTriPri----------148	-985.9405984	54.59
216	11v-02-PentaCapTriPri----------106	-985.9405458	54.62
217	11v-01-Icos-1vx----------95	-985.9404620	54.67
218	11v-05-Oblatocloso----------422	-985.9400353	54.94
219	11v-04-ThatStructure----------241	-985.9390847	55.54
220	11v-01-Icos-1vx----------38	-985.9377947	56.34
221	11v-04-ThatStructure----------351	-985.9375484	56.50
222	11v-05-Oblatocloso----------468	-985.9374753	56.55
223	11v-05-Oblatocloso----------467	-985.9374354	56.57
224	11v-05-Oblatocloso----------374	-985.9373464	56.63
225	11v-01-Icos-1vx----------35	-985.9373095	56.65
226	11v-04-ThatStructure----------347	-985.9365954	57.10
227	11v-04-ThatStructure----------348	-985.9365047	57.15
228	11v-03-TriFlatPentaCapTrigPrism----------228	-985.9360922	57.41
229	11v-02-PentaCapTriPri----------155	-985.9359625	57.49
230	11v-02-PentaCapTriPri----------154	-985.9358739	57.55
231	11v-01-Icos-1vx----------54	-985.9357570	57.62
232	11v-03-TriFlatPentaCapTrigPrism----------229	-985.9357174	57.65
233	11v-01-Icos-1vx----------2	-985.9357152	57.65
234	11v-03-TriFlatPentaCapTrigPrism----------174	-985.9356595	57.68
235	11v-03-TriFlatPentaCapTrigPrism----------189	-985.9355915	57.73
236	11v-02-PentaCapTriPri----------157_r-11	-985.9353960	57.85
237	11v-03-TriFlatPentaCapTrigPrism----------188	-985.9352520	57.94
238	11v-01-Icos-1vx----------6	-985.9351989	57.97
239	11v-01-Icos-1vx----------62	-985.9350508	58.07
240	11v-01-Icos-1vx----------19	-985.9349917	58.10
241	11v-02-PentaCapTriPri----------157_i-11	-985.9344738	58.43
242	11v-05-Oblatocloso----------482	-985.9340338	58.70
243	11v-05-Oblatocloso----------481	-985.9339794	58.74

244	11v-02-PentaCapTriPri----------109	-985.9337395	58.89
245	11v-05-Oblatocloso----------484	-985.9333215	59.15
246	11v-05-Oblatocloso----------573	-985.9328537	59.45
247	11v-05-Oblatocloso----------572	-985.9327950	59.48
248	11v-02-PentaCapTriPri----------118	-985.9325727	59.62
249	11v-01-Icos-1vx----------56	-985.9318432	60.08
250	11v-01-Icos-1vx----------57	-985.9317241	60.15
251	11v-05-Oblatocloso----------532	-985.9316731	60.19
252	11v-04-ThatStructure----------314	-985.9314690	60.31
253	11v-03-TriFlatPentaCapTrigPrism----------176	-985.9311633	60.51
254	11v-04-ThatStructure----------230	-985.9304412	60.96
255	11v-01-Icos-1vx----------101	-985.9300353	61.21
256	11v-01-Icos-1vx----------78_r-11	-985.9298409	61.34
257	11v-05-Oblatocloso----------463	-985.9297911	61.37
258	11v-01-Icos-1vx----------48	-985.9297691	61.38
259	11v-01-Icos-1vx----------78_i-11	-985.9297439	61.40
260	11v-02-PentaCapTriPri----------158	-985.9297085	61.42
261	11v-01-Icos-1vx----------22	-985.9296202	61.47
262	11v-04-ThatStructure----------267	-985.9292255	61.72
263	11v-05-Oblatocloso----------473	-985.9291950	61.74
264	11v-02-PentaCapTriPri----------142	-985.9291185	61.79
265	11v-05-Oblatocloso----------590	-985.9290749	61.82
266	11v-02-PentaCapTriPri----------140	-985.9290653	61.82
267	11v-01-Icos-1vx----------14	-985.9287492	62.02
268	11v-05-Oblatocloso----------453	-985.9286348	62.09
269	11v-01-Icos-1vx----------86	-985.9285345	62.16
270	11v-02-PentaCapTriPri----------147	-985.9283043	62.30
271	11v-03-TriFlatPentaCapTrigPrism----------222	-985.9283005	62.30
272	11v-05-Oblatocloso----------514	-985.9282545	62.33
273	11v-05-Oblatocloso----------574	-985.9278499	62.59
274	11v-04-ThatStructure----------242	-985.9275927	62.75
275	11v-05-Oblatocloso----------449	-985.9272485	62.96
276	11v-01-Icos-1vx----------55	-985.9272076	62.99
277	11v-02-PentaCapTriPri----------141	-985.9271325	63.04
278	11v-04-ThatStructure----------335	-985.9270530	63.09
279	11v-04-ThatStructure----------250	-985.9269708	63.14
280	11v-05-Oblatocloso----------501	-985.9268684	63.20
281	11v-01-Icos-1vx----------59	-985.9266146	63.36
282	11v-01-Icos-1vx----------102	-985.9263714	63.51
283	11v-01-Icos-1vx----------80	-985.9261087	63.68
284	11v-02-PentaCapTriPri----------112	-985.9259906	63.75

285	11v-05-Oblatocloso----------493	-985.9257231	63.92
286	11v-02-PentaCapTriPri----------136	-985.9253770	64.14
287	11v-01-Icos-1vx----------53	-985.9251355	64.29
288	11v-03-TriFlatPentaCapTrigPrism----------166	-985.9248991	64.44
289	11v-01-Icos-1vx----------52	-985.9248248	64.48
290	11v-05-Oblatocloso----------477	-985.9245331	64.67
291	11v-01-Icos-1vx----------64	-985.9242906	64.82
292	11v-05-Oblatocloso----------382	-985.9242597	64.84
293	11v-05-Oblatocloso----------519	-985.9240477	64.97
294	11v-03-TriFlatPentaCapTrigPrism----------195	-985.9239256	65.05
295	11v-05-Oblatocloso----------593	-985.9237030	65.19
296	11v-03-TriFlatPentaCapTrigPrism----------173	-985.9234238	65.36
297	11v-05-Oblatocloso----------545	-985.9234004	65.38
298	11v-05-Oblatocloso----------446	-985.9226999	65.82
299	11v-05-Oblatocloso----------489	-985.9224399	65.98
300	11v-04-ThatStructure----------253	-985.9224175	65.99
301	11v-05-Oblatocloso----------563	-985.9224069	66.00
302	11v-01-Icos-1vx----------87	-985.9213468	66.67
303	11v-04-ThatStructure----------362_i-18	-985.9212146	66.75
304	11v-02-PentaCapTriPri----------115	-985.9210990	66.82
305	11v-04-ThatStructure----------362_r-18	-985.9210630	66.84
306	11v-05-Oblatocloso----------492	-985.9210013	66.88
307	11v-04-ThatStructure----------345	-985.9204905	67.20
308	11v-04-ThatStructure----------312_r-14	-985.9204040	67.26
309	11v-05-Oblatocloso----------396	-985.9203385	67.30
310	11v-05-Oblatocloso----------554	-985.9202841	67.33
311	11v-05-Oblatocloso----------555	-985.9202831	67.33
312	11v-04-ThatStructure----------312_i-14	-985.9202711	67.34
313	11v-05-Oblatocloso----------536	-985.9199730	67.53
314	11v-03-TriFlatPentaCapTrigPrism----------225	-985.9198006	67.64
315	11v-01-Icos-1vx----------73	-985.9195578	67.79
316	11v-05-Oblatocloso----------585	-985.9192214	68.00
317	11v-05-Oblatocloso----------569	-985.9189725	68.16
318	11v-05-Oblatocloso----------533	-985.9189657	68.16
319	11v-03-TriFlatPentaCapTrigPrism----------224	-985.9187016	68.33
320	11v-03-TriFlatPentaCapTrigPrism----------165	-985.9185912	68.40
321	11v-03-TriFlatPentaCapTrigPrism----------183	-985.9184384	68.49
322	11v-01-Icos-1vx----------68	-985.9180751	68.72
323	11v-01-Icos-1vx----------69	-985.9180606	68.73
324	11v-04-ThatStructure----------306	-985.9179968	68.77
325	11v-05-Oblatocloso----------375	-985.9179918	68.77

326	11v-05-Oblatocloso----------435_r-20	-985.9179097	68.82
327	11v-04-ThatStructure----------366	-985.9177256	68.94
328	11v-05-Oblatocloso----------575	-985.9176697	68.97
329	11v-01-Icos-1vx----------83	-985.9175473	69.05
330	11v-05-Oblatocloso----------435_i-20	-985.9175383	69.06
331	11v-03-TriFlatPentaCapTrigPrism----------178	-985.9172022	69.27
332	11v-01-Icos-1vx----------84	-985.9171664	69.29
333	11v-03-TriFlatPentaCapTrigPrism----------177	-985.9171562	69.30
334	11v-05-Oblatocloso----------540	-985.9169675	69.41
335	11v-02-PentaCapTriPri----------151	-985.9168557	69.48
336	11v-03-TriFlatPentaCapTrigPrism----------168	-985.9167973	69.52
337	11v-03-TriFlatPentaCapTrigPrism----------171	-985.9164990	69.71
338	11v-03-TriFlatPentaCapTrigPrism----------203	-985.9159909	70.03
339	11v-04-ThatStructure----------352	-985.9158580	70.11
340	11v-01-Icos-1vx----------61	-985.9149834	70.66
341	11v-05-Oblatocloso----------474	-985.9145719	70.92
342	11v-04-ThatStructure----------289	-985.9145327	70.94
343	11v-04-ThatStructure----------285	-985.9144035	71.02
344	11v-01-Icos-1vx----------23	-985.9142581	71.11
345	11v-02-PentaCapTriPri----------120	-985.9141832	71.16
346	11v-01-Icos-1vx----------92	-985.9140995	71.21
347	11v-04-ThatStructure----------281	-985.9140874	71.22
348	11v-05-Oblatocloso----------494	-985.9140753	71.23
349	11v-04-ThatStructure----------364	-985.9140303	71.26
350	11v-04-ThatStructure----------239	-985.9139688	71.30
351	11v-01-Icos-1vx----------10	-985.9139465	71.31
352	11v-04-ThatStructure----------243	-985.9139424	71.31
353	11v-01-Icos-1vx----------67	-985.9139141	71.33
354	11v-01-Icos-1vx----------94	-985.9137508	71.43
355	11v-05-Oblatocloso----------576	-985.9134520	71.62
356	11v-01-Icos-1vx----------20	-985.9134423	71.63
357	11v-01-Icos-1vx----------16	-985.9131488	71.81
358	11v-04-ThatStructure----------287	-985.9129253	71.95
359	11v-01-Icos-1vx----------79	-985.9127076	72.09
360	11v-05-Oblatocloso----------503	-985.9125319	72.20
361	11v-02-PentaCapTriPri----------156	-985.9124421	72.25
362	11v-05-Oblatocloso----------440	-985.9120661	72.49
363	11v-01-Icos-1vx----------40	-985.9119512	72.56
364	11v-05-Oblatocloso----------464	-985.9118451	72.63
365	11v-04-ThatStructure----------256	-985.9116715	72.74
366	11v-04-ThatStructure----------363	-985.9107748	73.30

367	11v-05-Oblatocloso----------548	-985.9105173	73.46
368	11v-01-Icos-1vx----------66_i-26	-985.9105155	73.46
369	11v-01-Icos-1vx----------66_r-26	-985.9103918	73.54
370	11v-04-ThatStructure----------261	-985.9102990	73.60
371	11v-04-ThatStructure----------349	-985.9102001	73.66
372	11v-01-Icos-1vx----------29	-985.9100395	73.76
373	11v-05-Oblatocloso----------594	-985.9099688	73.81
374	11v-05-Oblatocloso----------595	-985.9099205	73.84
375	11v-02-PentaCapTriPri----------137	-985.9096870	73.98
376	11v-04-ThatStructure----------266	-985.9096739	73.99
377	11v-01-Icos-1vx----------12	-985.9095176	74.09
378	11v-05-Oblatocloso----------384	-985.9083970	74.79
379	11v-04-ThatStructure----------319	-985.9079501	75.07
380	11v-04-ThatStructure----------258	-985.9074658	75.38
381	11v-01-Icos-1vx----------100	-985.9073345	75.46
382	11v-05-Oblatocloso----------508	-985.9072791	75.49
383	11v-04-ThatStructure----------273	-985.9072204	75.53
384	11v-01-Icos-1vx----------71	-985.9070701	75.63
385	11v-01-Icos-1vx----------7	-985.9069095	75.73
386	11v-04-ThatStructure----------288	-985.9068799	75.74
387	11v-02-PentaCapTriPri----------110	-985.9067765	75.81
388	11v-01-Icos-1vx----------30	-985.9066279	75.90
389	11v-05-Oblatocloso----------391	-985.9065719	75.94
390	11v-05-Oblatocloso----------459	-985.9065255	75.97
391	11v-03-TriFlatPentaCapTrigPrism----------227	-985.9064883	75.99
392	11v-05-Oblatocloso----------389	-985.9063950	76.05
393	11v-05-Oblatocloso----------371	-985.9058554	76.39
394	11v-05-Oblatocloso----------372	-985.9058449	76.39
395	11v-05-Oblatocloso----------499	-985.9053518	76.70
396	11v-04-ThatStructure----------313	-985.9052633	76.76
397	11v-01-Icos-1vx----------72	-985.9047704	77.07
398	11v-05-Oblatocloso----------395	-985.9043498	77.33
399	11v-04-ThatStructure----------370	-985.9042077	77.42
400	11v-05-Oblatocloso----------472	-985.9041837	77.44
401	11v-05-Oblatocloso----------381	-985.9040722	77.51
402	11v-01-Icos-1vx----------82	-985.9039757	77.57
403	11v-05-Oblatocloso----------466	-985.9038701	77.63
404	11v-03-TriFlatPentaCapTrigPrism----------214	-985.9036375	77.78
405	11v-05-Oblatocloso----------598	-985.9036177	77.79
406	11v-04-ThatStructure----------236	-985.9033504	77.96
407	11v-04-ThatStructure----------291	-985.9029805	78.19

408	11v-05-Oblatocloso----------417	-985.9026669	78.39
409	11v-05-Oblatocloso----------416	-985.9026498	78.40
410	11v-05-Oblatocloso----------418	-985.9026419	78.40
411	11v-04-ThatStructure----------315	-985.9026236	78.42
412	11v-02-PentaCapTriPri----------108	-985.9024977	78.49
413	11v-01-Icos-1vx----------5	-985.9023341	78.60
414	11v-01-Icos-1vx----------4	-985.9022919	78.62
415	11v-05-Oblatocloso----------599	-985.9022042	78.68
416	11v-05-Oblatocloso----------486	-985.9017846	78.94
417	11v-05-Oblatocloso----------504	-985.9017513	78.96
418	11v-01-Icos-1vx----------81_r-11	-985.9015526	79.09
419	11v-05-Oblatocloso----------431	-985.9015241	79.11
420	11v-01-Icos-1vx----------81_i-11	-985.9015227	79.11
421	11v-04-ThatStructure----------308	-985.9015039	79.12
422	11v-05-Oblatocloso----------450	-985.9012039	79.31
423	11v-05-Oblatocloso----------429	-985.9005101	79.74
424	11v-05-Oblatocloso----------579	-985.9002068	79.93
425	11v-01-Icos-1vx----------34	-985.8998401	80.16
426	11v-04-ThatStructure----------344	-985.8997642	80.21
427	11v-03-TriFlatPentaCapTrigPrism----------194	-985.8997483	80.22
428	11v-04-ThatStructure----------277	-985.8997214	80.24
429	11v-05-Oblatocloso----------550	-985.8995099	80.37
430	11v-04-ThatStructure----------326	-985.8988318	80.79
431	11v-05-Oblatocloso----------485	-985.8986991	80.88
432	11v-04-ThatStructure----------240	-985.8986905	80.88
433	11v-03-TriFlatPentaCapTrigPrism----------219_i-13	-985.8984381	81.04
434	11v-03-TriFlatPentaCapTrigPrism----------219_r-13	-985.8982515	81.16
435	11v-02-PentaCapTriPri----------149	-985.8980821	81.27
436	11v-04-ThatStructure----------265	-985.8971714	81.84
437	11v-05-Oblatocloso----------378	-985.8968144	82.06
438	11v-04-ThatStructure----------328	-985.8968105	82.06
439	11v-05-Oblatocloso----------386	-985.8967206	82.12
440	11v-04-ThatStructure----------255	-985.8950285	83.18
441	11v-01-Icos-1vx----------27	-985.8948706	83.28
442	11v-05-Oblatocloso----------539	-985.8948701	83.28
443	11v-01-Icos-1vx----------3	-985.8946819	83.40
444	11v-03-TriFlatPentaCapTrigPrism----------184	-985.8942409	83.68
445	11v-01-Icos-1vx----------15	-985.8942401	83.68
446	11v-05-Oblatocloso----------401	-985.8942285	83.68
447	11v-01-Icos-1vx----------51	-985.8938615	83.91

448	11v-04-ThatStructure----------369	-985.8933937	84.21
449	11v-05-Oblatocloso----------478	-985.8931809	84.34
450	11v-05-Oblatocloso----------479	-985.8931123	84.38
451	11v-01-Icos-1vx----------96	-985.8929343	84.50
452	11v-01-Icos-1vx----------85	-985.8928091	84.57
453	11v-04-ThatStructure----------367	-985.8926970	84.64
454	11v-02-PentaCapTriPri----------150	-985.8926309	84.69
455	11v-04-ThatStructure----------269	-985.8926047	84.70
456	11v-05-Oblatocloso----------567	-985.8925698	84.72
457	11v-05-Oblatocloso----------566	-985.8925662	84.73
458	11v-01-Icos-1vx----------74	-985.8924824	84.78
459	11v-02-PentaCapTriPri----------122	-985.8924512	84.80
460	11v-05-Oblatocloso----------596	-985.8921914	84.96
461	11v-02-PentaCapTriPri----------153	-985.8920350	85.06
462	11v-05-Oblatocloso----------541	-985.8918400	85.18
463	11v-04-ThatStructure----------278	-985.8917926	85.21
464	11v-04-ThatStructure----------309_i-20	-985.8916255	85.32
465	11v-04-ThatStructure----------321	-985.8915157	85.39
466	11v-05-Oblatocloso----------470	-985.8914400	85.43
467	11v-04-ThatStructure----------293	-985.8914345	85.44
468	11v-04-ThatStructure----------309_r-20	-985.8914182	85.45
469	11v-05-Oblatocloso----------471	-985.8914035	85.46
470	11v-05-Oblatocloso----------460	-985.8910238	85.69
471	11v-03-TriFlatPentaCapTrigPrism----------197	-985.8909952	85.71
472	11v-05-Oblatocloso----------388	-985.8909678	85.73
473	11v-05-Oblatocloso----------495	-985.8906072	85.96
474	11v-05-Oblatocloso----------458	-985.8901004	86.27
475	11v-05-Oblatocloso----------426	-985.8898059	86.46
476	11v-05-Oblatocloso----------451	-985.8897058	86.52
477	11v-04-ThatStructure----------249	-985.8896762	86.54
478	11v-02-PentaCapTriPri----------119	-985.8896027	86.59
479	11v-04-ThatStructure----------275	-985.8889404	87.00
480	11v-05-Oblatocloso----------434	-985.8888755	87.04
481	11v-03-TriFlatPentaCapTrigPrism----------182	-985.8886303	87.20
482	11v-03-TriFlatPentaCapTrigPrism----------187	-985.8884089	87.34
483	11v-05-Oblatocloso----------398	-985.8884003	87.34
484	11v-05-Oblatocloso----------538	-985.8882372	87.44
485	11v-02-PentaCapTriPri----------138	-985.8879823	87.60
486	11v-04-ThatStructure----------231	-985.8878604	87.68
487	11v-02-PentaCapTriPri----------134	-985.8870359	88.20
488	11v-05-Oblatocloso----------465	-985.8869938	88.22

489	11v-04-ThatStructure----------338	-985.8866036	88.47
490	11v-04-ThatStructure----------276	-985.8865233	88.52
491	11v-02-PentaCapTriPri----------146	-985.8864335	88.58
492	11v-01-Icos-1vx----------1	-985.8861003	88.78
493	11v-05-Oblatocloso----------476	-985.8860578	88.81
494	11v-01-Icos-1vx----------65	-985.8854806	89.17
495	11v-05-Oblatocloso----------583	-985.8850852	89.42
496	11v-01-Icos-1vx----------44	-985.8849894	89.48
497	11v-04-ThatStructure----------262_r-51	-985.8849233	89.52
498	11v-04-ThatStructure----------322	-985.8847702	89.62
499	11v-05-Oblatocloso----------405	-985.8846541	89.69
500	11v-01-Icos-1vx----------104	-985.8842805	89.93
501	11v-01-Icos-1vx----------24	-985.8841564	90.00
502	11v-05-Oblatocloso----------597	-985.8832711	90.56
503	11v-04-ThatStructure----------251	-985.8832261	90.59
504	11v-04-ThatStructure----------252	-985.8831851	90.61
505	11v-04-ThatStructure----------263	-985.8830796	90.68
506	11v-01-Icos-1vx----------70	-985.8830619	90.69
507	11v-04-ThatStructure----------354	-985.8828027	90.85
508	11v-05-Oblatocloso----------442	-985.8824713	91.06
509	11v-05-Oblatocloso----------502	-985.8824522	91.07
510	11v-04-ThatStructure----------299	-985.8823947	91.11
511	11v-04-ThatStructure----------298	-985.8822257	91.22
512	11v-03-TriFlatPentaCapTrigPrism----------200	-985.8821302	91.28
513	11v-05-Oblatocloso----------420	-985.8816217	91.59
514	11v-05-Oblatocloso----------553	-985.8815734	91.62
515	11v-01-Icos-1vx----------21	-985.8812610	91.82
516	11v-05-Oblatocloso----------373	-985.8808526	92.08
517	11v-01-Icos-1vx----------31	-985.8805730	92.25
518	11v-03-TriFlatPentaCapTrigPrism----------210	-985.8801513	92.52
519	11v-04-ThatStructure----------245	-985.8801061	92.55
520	11v-02-PentaCapTriPri----------133	-985.8798674	92.70
521	11v-04-ThatStructure----------368	-985.8797791	92.75
522	11v-05-Oblatocloso----------407	-985.8792413	93.09
523	11v-04-ThatStructure----------262_i-51	-985.8792153	93.10
524	11v-05-Oblatocloso----------408	-985.8790682	93.20
525	11v-04-ThatStructure----------279	-985.8788085	93.36
526	11v-04-ThatStructure----------271	-985.8786273	93.47
527	11v-05-Oblatocloso----------537	-985.8785082	93.55
528	11v-03-TriFlatPentaCapTrigPrism----------202	-985.8780609	93.83
529	11v-05-Oblatocloso----------387	-985.8779629	93.89

530	11v-04-ThatStructure----------268	-985.8778364	93.97
531	11v-05-Oblatocloso----------506	-985.8776655	94.08
532	11v-01-Icos-1vx----------11	-985.8775795	94.13
533	11v-05-Oblatocloso----------571	-985.8772940	94.31
534	11v-04-ThatStructure----------323	-985.8767696	94.64
535	11v-04-ThatStructure----------316	-985.8763146	94.92
536	11v-04-ThatStructure----------270	-985.8762666	94.96
537	11v-04-ThatStructure----------274	-985.8758113	95.24
538	11v-04-ThatStructure----------259	-985.8755277	95.42
539	11v-04-ThatStructure----------244	-985.8753674	95.52
540	11v-01-Icos-1vx----------25	-985.8752391	95.60
541	11v-05-Oblatocloso----------448	-985.8750789	95.70
542	11v-05-Oblatocloso----------547	-985.8749698	95.77
543	11v-04-ThatStructure----------294	-985.8740745	96.33
544	11v-05-Oblatocloso----------410_r-16	-985.8737429	96.54
545	11v-01-Icos-1vx----------99	-985.8734534	96.72
546	11v-01-Icos-1vx----------60	-985.8733706	96.77
547	11v-01-Icos-1vx----------98	-985.8731477	96.91
548	11v-05-Oblatocloso----------410_i-16	-985.8731225	96.93
549	11v-02-PentaCapTriPri----------125	-985.8731005	96.94
550	11v-05-Oblatocloso----------558	-985.8729456	97.04
551	11v-05-Oblatocloso----------385	-985.8728060	97.13
552	11v-01-Icos-1vx----------26	-985.8726586	97.22
553	11v-01-Icos-1vx----------28	-985.8726427	97.23
554	11v-01-Icos-1vx----------93	-985.8725784	97.27
555	11v-05-Oblatocloso----------402	-985.8717430	97.79
556	11v-04-ThatStructure----------247	-985.8714029	98.01
557	11v-05-Oblatocloso----------469	-985.8713523	98.04
558	11v-05-Oblatocloso----------427	-985.8712412	98.11
559	11v-05-Oblatocloso----------529	-985.8706820	98.46
560	11v-01-Icos-1vx----------17	-985.8697585	99.04
561	11v-05-Oblatocloso----------510	-985.8681447	100.05
562	11v-03-TriFlatPentaCapTrigPrism----------212	-985.8675363	100.43
563	11v-03-TriFlatPentaCapTrigPrism----------213	-985.8665304	101.06
564	11v-02-PentaCapTriPri----------123	-985.8663031	101.21
565	11v-02-PentaCapTriPri----------135	-985.8662428	101.25
566	11v-02-PentaCapTriPri----------124	-985.8662293	101.25
567	11v-04-ThatStructure----------284	-985.8648355	102.13
568	11v-05-Oblatocloso----------490	-985.8647613	102.17
569	11v-05-Oblatocloso----------480	-985.8646091	102.27
570	11v-01-Icos-1vx----------9	-985.8639371	102.69

571	11v-05-Oblatocloso----------544_i-35	-985.8636606	102.87
572	11v-05-Oblatocloso----------544_r-35	-985.8635727	102.92
573	11v-04-ThatStructure----------257	-985.8630477	103.25
574	11v-04-ThatStructure----------237	-985.8616129	104.15
575	11v-04-ThatStructure----------232	-985.8613304	104.33
576	11v-05-Oblatocloso----------546	-985.8606298	104.77
577	11v-01-Icos-1vx----------33	-985.8604276	104.89
578	11v-04-ThatStructure----------233	-985.8602400	105.01
579	11v-05-Oblatocloso----------390	-985.8583577	106.19
580	11v-05-Oblatocloso----------491	-985.8578802	106.49
581	11v-05-Oblatocloso----------425	-985.8573086	106.85
582	11v-04-ThatStructure----------329	-985.8569183	107.10
583	11v-04-ThatStructure----------246	-985.8561863	107.56
584	11v-05-Oblatocloso----------383	-985.8555942	107.93
585	11v-05-Oblatocloso----------399	-985.8552766	108.13
586	11v-04-ThatStructure----------238	-985.8550700	108.26
587	11v-03-TriFlatPentaCapTrigPrism----------196	-985.8545424	108.59
588	11v-03-TriFlatPentaCapTrigPrism----------193	-985.8535208	109.23
589	11v-01-Icos-1vx----------88	-985.8534517	109.27
590	11v-05-Oblatocloso----------419	-985.8534430	109.28
591	11v-05-Oblatocloso----------562	-985.8521337	110.10
592	11v-03-TriFlatPentaCapTrigPrism----------192	-985.8518486	110.28
593	11v-05-Oblatocloso----------505	-985.8517845	110.32
594	11v-04-ThatStructure----------260	-985.8514350	110.54
595	11v-05-Oblatocloso----------475	-985.8498911	111.51
596	11v-05-Oblatocloso----------556	-985.8462830	113.77
597	11v-04-ThatStructure----------234	-985.8460832	113.90
598	11v-03-TriFlatPentaCapTrigPrism----------172	-985.8459932	113.95
599	11v-05-Oblatocloso----------421	-985.8458768	114.03
600	11v-05-Oblatocloso----------436	-985.8448595	114.66
601	11v-05-Oblatocloso----------403	-985.8417047	116.64
602	11v-05-Oblatocloso----------507	-985.8385084	118.65
603	11v-04-ThatStructure----------248	-985.8378980	119.03
604	11v-05-Oblatocloso----------409	-985.8359799	120.24
605	11v-05-Oblatocloso----------377	-985.8350441	120.82
606	11v-05-Oblatocloso----------411	-985.8278397	125.34
607	11v-03-TriFlatPentaCapTrigPrism----------211	-985.8277667	125.39
608	11v-04-ThatStructure----------346	-985.8263776	126.26
609	11v-01-Icos-1vx----------97	-985.8241254	127.67
610	11v-05-Oblatocloso----------394	-985.8226840	128.58
611	11v-01-Icos-1vx----------18	-985.8214137	129.38

612	11v-05-Oblatocloso----------412	-985.8211345	129.55
613	11v-05-Oblatocloso----------400	-985.8136806	134.23
614	11v-04-ThatStructure----------235	-985.8122957	135.10
615	11v-03-TriFlatPentaCapTrigPrism----------163	-985.8105877	136.17
616	11v-04-ThatStructure----------317	-985.8005219	142.49
617	11v-03-TriFlatPentaCapTrigPrism----------223	-985.7917665	147.98
618	11v-05-Oblatocloso----------376	-985.7633611	165.81

Table S8A. Initial $Cp_3W_3(H)B_9H_9$ structures, 223 structures.

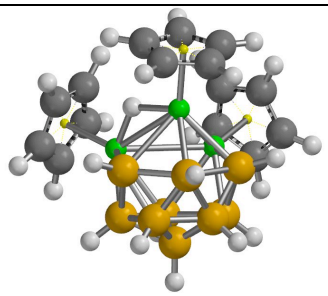
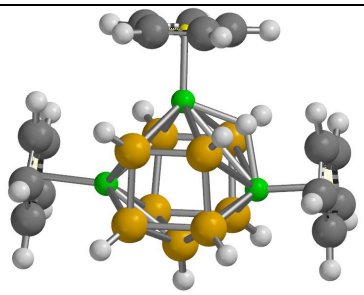
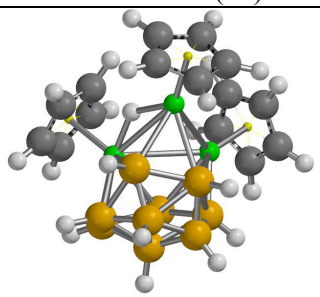
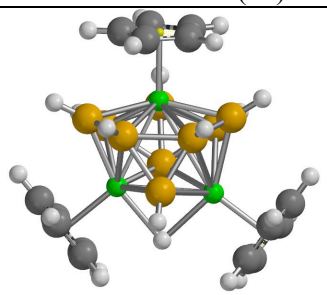
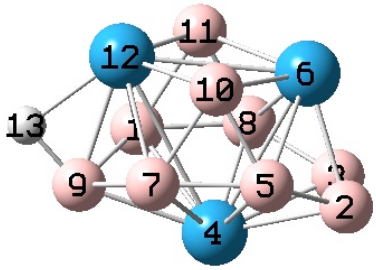
 Icosahedron (17)	 Cubeoctahedron (76)
 Anticubeoctahedron (102)	 Oblatocloso (28)

Table S8B. Distance table for the lowest-lying $Cp_3W_3(H)B_9H_9$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

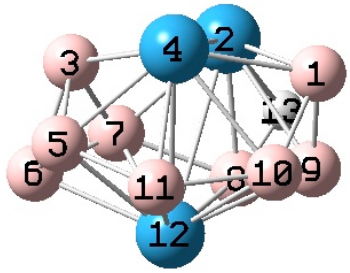


1. -1011.8213562 0.0 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	4.007052	0.000000			
3 B	3.207945	1.771325	0.000000		
4 W	2.314474	2.250904	2.254395	0.000000	
5 B	3.881612	1.729255	3.079971	2.313915	0.000000
6 W	3.266025	2.166290	2.166444	2.902486	2.360068
7 B	3.263508	3.215615	4.016944	2.326458	1.769821
8 B	1.769920	3.078647	1.726322	2.317502	3.667821
9 B	1.989018	4.174728	4.186202	2.255883	3.342050
10 B	3.797477	3.103040	3.957871	3.251905	1.715862
11 B	1.811574	3.953639	3.092657	3.246688	3.930471
12 W	2.320755	4.179769	4.177863	3.196369	3.230294
13 H	2.513994	5.102819	5.105193	3.412735	4.061691

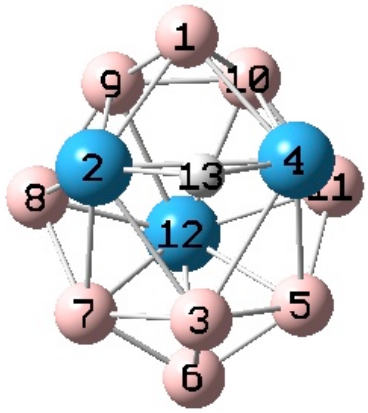
	6	7	8	9	10
6 W	0.000000				
7 B	3.262916	0.000000			
8 B	2.364691	3.890714	0.000000		
9 B	3.932902	1.955106	3.371513	0.000000	
10 B	2.311476	1.807151	3.933030	3.262672	0.000000
11 B	2.315463	3.798026	1.706598	3.286245	3.416303
12 W	2.899431	2.317922	3.229722	2.144621	2.171563
13 H	4.417187	2.504920	4.069689	1.257920	3.431650

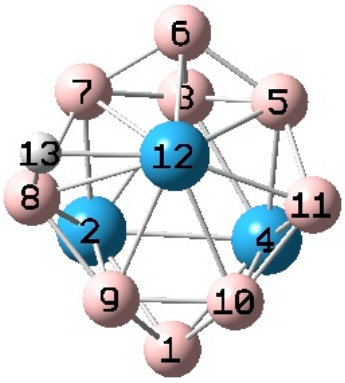
	11	12	13
11 B	0.000000		
12 W	2.172928	0.000000	
13 H	3.439079	1.825692	0.000000



2. -1011.8199560 0.9 C_1

	1	2	3	4	5
1 B	0.000000				
2 W	2.267909	0.000000			
3 B	3.796376	2.371204	0.000000		
4 W	2.251793	2.579516	2.401434	0.000000	
5 B	3.930862	3.500214	1.831393	2.229457	0.000000
6 B	4.612649	3.436446	1.718544	3.450418	1.728550
7 B	3.959920	2.240673	1.817032	3.531314	2.855315
8 B	3.243735	2.216972	3.309210	3.931020	3.896068
9 B	1.713682	2.405883	3.867775	3.179937	3.929614
10 B	1.731923	3.214397	3.851700	2.325690	3.206028
11 B	3.154696	3.844830	3.260738	2.107491	1.855441
12 W	3.288299	3.100745	2.906093	3.101149	2.339093
13 H	3.133211	1.860000	3.701343	4.175064	4.659674

	6 7 8 9 10 6 B 0.000000 7 B 1.719737 0.000000 8 B 3.211836 1.901751 0.000000 9 B 4.093157 3.283063 1.953516 0.000000 10 B 4.085646 3.981374 3.352589 1.793512 0.000000 11 B 3.201016 3.872058 4.048424 3.230483 1.827935 12 W 2.246932 2.356943 2.196393 2.299889 2.327828 13 H 4.092802 2.523768 1.267877 2.257655 3.855295 11 12 13 11 B 0.000000 12 W 2.195566 0.000000 13 H 4.816125 3.300270 0.000000
 3. -1011.8162830 3.2 C_S	1 2 3 4 5 1 B 0.000000 2 W 2.248142 0.000000 3 B 3.784788 2.461442 0.000000 4 W 2.250308 2.682300 2.453150 0.000000 5 B 3.910787 3.576990 1.815736 2.253711 0.000000 6 B 4.596074 3.506379 1.702139 3.503671 1.744154 7 B 3.911733 2.255130 1.818894 3.573444 2.870597 8 B 3.150361 2.154285 3.244531 3.890187 3.823985 9 B 1.737943 2.339838 3.814901 3.212290 3.904028 10 B 1.736014 3.212942 3.812257 2.335012 3.170687 11 B 3.150626 3.892035 3.241244 2.157202 1.843058 12 W 3.346923 3.203967 2.915947 3.203598 2.353877 13 H 2.627863 1.818700 2.298736 1.820756 3.307148 6 7 8 9 10 6 B 0.000000 7 B 1.743626 0.000000 8 B 3.163104 1.845226 0.000000 9 B 4.036607 3.175731 1.804655 0.000000 10 B 4.039118 3.910709 3.218834 1.810901 0.000000 11 B 3.164248 3.826122 3.912141 3.210166 1.800120 12 W 2.222937 2.357338 2.158890 2.328896 2.335847 13 H 3.874059 3.301968 3.799111 3.589543 3.586901 11 12 13 11 B 0.000000 12 W 2.158587 0.000000 13 H 3.803890 4.052155 0.000000

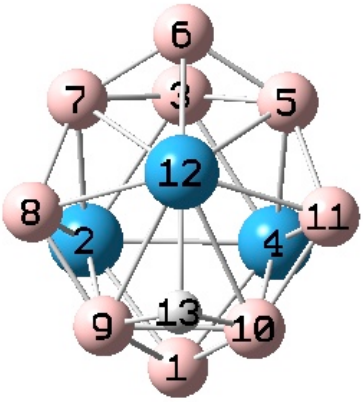


4. -1011.8039500 10.9 (C_S)

	1	2	3	4	5
1 B	0.000000				
2 W	2.241249	0.000000			
3 B	3.802053	2.378983	0.000000		
4 W	2.245260	2.537468	2.387648	0.000000	
5 B	3.918046	3.465564	1.829291	2.260479	0.000000
6 B	4.618187	3.405257	1.716581	3.475098	1.740711
7 B	3.958055	2.211005	1.825066	3.524155	2.847173
8 B	3.189443	2.146858	3.374508	3.933999	3.934875
9 B	1.717647	2.345409	3.869610	3.188918	3.906322
10 B	1.736017	3.155328	3.830664	2.344643	3.161880
11 B	3.127018	3.768325	3.215889	2.107986	1.809796
12 W	3.342941	3.100823	2.948134	3.185718	2.336200
13 H	4.034048	3.246896	3.853807	4.571490	4.015534

	6	7	8	9	10
6 B	0.000000				
7 B	1.709724	0.000000			
8 B	3.292937	1.983636	0.000000		
9 B	4.089466	3.274264	1.882541	0.000000	
10 B	4.071883	3.961299	3.319897	1.799417	0.000000
11 B	3.203779	3.852845	4.065142	3.227204	1.806483
12 W	2.259000	2.385399	2.273246	2.336446	2.346901
13 H	3.178318	2.332563	1.236196	2.501384	3.641841

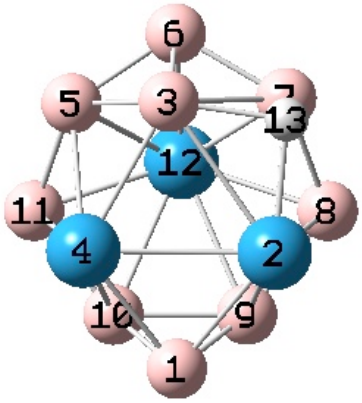
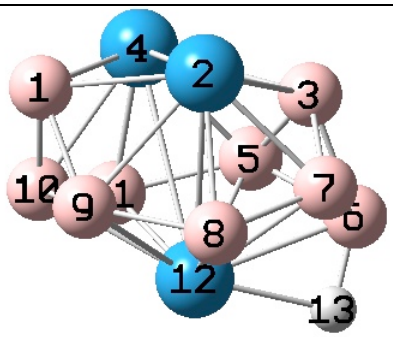
	11	12	13
11 B	0.000000		
12 W	2.230865	0.000000	
13 H	4.131351	1.963386	0.000000

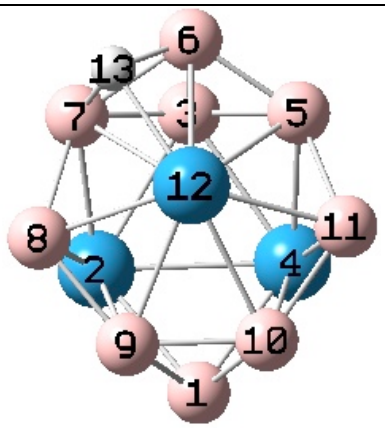


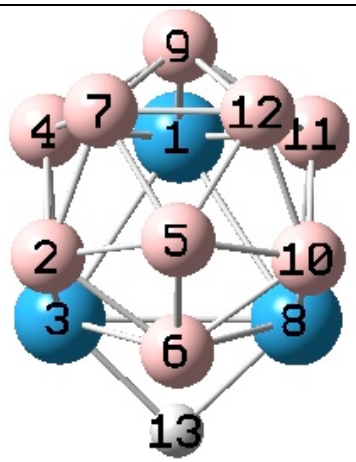
5. -1011.7991680 13.9 C_S

	1	2	3	4	5
1 B	0.000000				
2 W	2.234930	0.000000			
3 B	3.773186	2.374413	0.000000		
4 W	2.248509	2.581645	2.378166	0.000000	
5 B	3.940316	3.514164	1.844795	2.223317	0.000000
6 B	4.618601	3.435321	1.715397	3.435667	1.734308
7 B	3.936004	2.225570	1.840345	3.517935	2.871993
8 B	3.190360	2.115990	3.263304	3.868668	3.881077
9 B	1.750517	2.282905	3.870127	3.249979	4.035454
10 B	1.746985	3.238635	3.873258	2.284965	3.226105
11 B	3.191781	3.858648	3.268179	2.115274	1.853334
12 W	3.358941	3.124570	2.916243	3.128621	2.339205
13 H	2.365976	3.297668	4.153096	3.303676	3.670618

	6	7	8	9	10
6 B	0.000000				
7 B	1.734716	0.000000			
8 B	3.217107	1.848819	0.000000		
9 B	4.151669	3.219934	1.836261	0.000000	

	10 B 4.157469 4.037758 3.424536 2.056555 0.000000 11 B 3.217972 3.878820 4.048593 3.416282 1.836981 12 W 2.242209 2.338173 2.230967 2.462783 2.471180 13 H 4.044547 3.669820 2.601491 1.404594 1.409765 11 12 13 11 B 0.000000 12 W 2.227378 0.000000 13 H 2.594200 1.917737 0.000000
 6. -1011.7960870 15.9 C_1	1 2 3 4 5 1 B 0.000000 2 W 2.258154 0.000000 3 B 3.829100 2.539436 0.000000 4 W 2.229941 2.617805 2.368223 0.000000 5 B 3.910281 3.587389 1.801924 2.234636 0.000000 6 B 4.605781 3.512646 1.724524 3.440875 1.731325 7 B 4.000784 2.341231 2.014280 3.600642 2.935739 8 B 3.162792 2.126436 3.402090 3.872058 3.909259 9 B 1.740097 2.322124 3.903286 3.187672 3.926721 10 B 1.718094 3.206351 3.854715 2.343663 3.177745 11 B 3.107854 3.873328 3.230114 2.111815 1.836150 12 W 3.306357 3.140157 2.944344 3.129825 2.339670 13 H 3.918486 1.859896 1.633794 3.329157 3.222694 6 7 8 9 10 6 B 0.000000 7 B 1.767208 0.000000 8 B 3.272539 1.891713 0.000000 9 B 4.075503 3.224635 1.810764 0.000000 10 B 4.058093 3.973736 3.264569 1.825569 0.000000 11 B 3.193338 3.902097 4.013912 3.244541 1.803070 12 W 2.234157 2.322288 2.209772 2.317735 2.326563 13 H 2.455952 1.328139 2.616575 3.660539 4.349311 11 12 13 11 B 0.000000 12 W 2.215314 0.000000 13 H 4.320045 3.289366 0.000000
 7. -1011.7933590 17.6 C_S	1 2 3 4 5 1 B 0.000000 2 W 2.232502 0.000000 3 B 3.686263 2.348285 0.000000 4 W 2.226709 2.604147 2.354139 0.000000 5 B 3.902459 3.559611 1.829330 2.213718 0.000000 6 B 4.687151 3.543956 1.731439 3.541177 1.851118 7 B 3.902749 2.212705 1.821403 3.557368 2.981611 8 B 3.146169 2.108288 3.182442 3.868091 3.921890 9 B 1.740210 2.316686 3.713241 3.184216 3.928472 10 B 1.736373 3.184194 3.713247 2.313465 3.152885

	11 B 3.141507 3.870264 3.189152 2.104744 1.823589 12 W 3.329716 3.147653 2.807282 3.143659 2.360602 13 H 5.035956 4.200755 2.826628 4.201681 2.419224 6 7 8 9 10 6 B 0.000000 7 B 1.856488 0.000000 8 B 3.302394 1.820874 0.000000 9 B 4.141339 3.151928 1.809934 0.000000 10 B 4.137126 3.922652 3.268714 1.835377 0.000000 11 B 3.300302 3.921683 4.044755 3.273360 1.810036 12 W 2.304320 2.361176 2.240024 2.334736 2.329816 13 H 1.229088 2.414698 3.347536 4.152942 4.151536 11 12 13 11 B 0.000000 12 W 2.238761 0.000000 13 H 3.354109 1.953131 0.000000
 8. -1011.7926460 18.0 C_1	1 2 3 4 5 1 B 0.000000 2 W 2.235451 0.000000 3 B 3.783609 2.389780 0.000000 4 W 2.241775 2.577873 2.392819 0.000000 5 B 3.915661 3.516376 1.867541 2.236403 0.000000 6 B 4.666127 3.497798 1.708967 3.461261 1.720113 7 B 3.972982 2.226491 1.812863 3.545392 2.908786 8 B 3.143734 2.109023 3.293897 3.861357 3.878389 9 B 1.732536 2.325348 3.844974 3.189474 3.917700 10 B 1.726189 3.176251 3.842733 2.327590 3.177645 11 B 3.139173 3.836171 3.275421 2.108747 1.840464 12 W 3.316911 3.125571 2.950867 3.138974 2.334922 13 H 4.605722 3.381657 2.525706 4.060599 2.708178 6 7 8 9 10 6 B 0.000000 7 B 1.832397 0.000000 8 B 3.342631 1.958901 0.000000 9 B 4.166510 3.280848 1.818655 0.000000 10 B 4.142715 4.018148 3.272377 1.830270 0.000000 11 B 3.252416 3.942634 4.021080 3.259335 1.818000 12 W 2.361995 2.465798 2.227803 2.323584 2.331851 13 H 1.368014 1.424969 2.436924 3.630512 4.092986 11 12 13 11 B 0.000000 12 W 2.216533 0.000000 13 H 3.689474 1.924079 0.000000

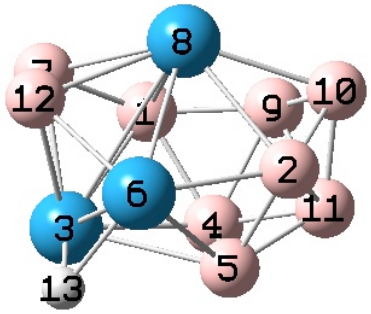


9. -1011.7918800 18.5 C_S

	1	2	3	4	5
1 W	0.000000				
2 B	3.526103	0.000000			
3 W	2.526312	2.279266	0.000000		
4 B	2.314541	1.803830	2.324530	0.000000	
5 B	4.108746	1.780033	3.559303	2.883801	0.000000
6 B	3.588483	1.797938	2.362557	2.989473	1.761557
7 B	3.536236	1.787606	3.547692	1.757618	1.756226
8 W	2.528837	3.580081	2.632339	3.631489	3.560207
9 B	2.274494	2.898894	3.546618	1.781717	2.878886
10 B	3.532549	2.894432	3.579832	3.440166	1.780146
11 B	2.321308	3.438376	3.631481	2.961923	2.883829
12 B	3.538648	2.872669	4.144790	2.875117	1.756100
13 H	3.280946	3.508683	1.846326	3.895810	4.151271

	6	7	8	9	10
6 B	0.000000				
7 B	2.894192	0.000000			
8 W	2.365564	4.144478	0.000000		
9 B	3.450073	1.787783	3.542233	0.000000	
10 B	1.798111	2.873672	2.280113	2.898574	0.000000
11 B	2.988550	2.875478	2.319137	1.779406	1.804772
12 B	2.893477	1.748222	3.544864	1.786163	1.787307
13 H	2.476335	4.751475	1.848728	4.582898	3.508281

	11	12	13
11 B	0.000000		
12 B	1.757628	0.000000	
13 H	3.893382	4.750147	0.000000



10. -1011.7904873 19.4 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	3.455504	0.000000			
3 W	2.315594	3.511154	0.000000		
4 B	1.817931	2.843149	2.288419	0.000000	
5 B	3.092867	1.795142	2.413732	1.818455	0.000000
6 W	3.779122	2.274686	2.604853	3.582362	2.348655
7 B	1.790749	4.054699	2.186041	3.230550	3.843221
8 W	2.279702	2.403890	3.137396	3.131486	3.196388
9 B	1.760021	2.714931	3.484980	1.815350	2.880399
10 B	3.082998	1.692941	4.198070	2.874751	2.871363
11 B	2.984993	1.825230	3.585227	1.774068	1.767005
12 B	3.076800	3.636788	2.313322	3.887404	3.637393
13 H	3.959846	3.530696	1.851366	3.517130	2.520617

	6	7	8	9	10
6 W	0.000000				
7 B	3.406397	0.000000			
8 W	2.722444	2.243695	0.000000		
9 B	4.090449	3.305063	2.398483	0.000000	

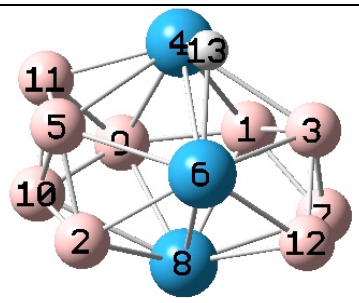
	10 B 3.667057 4.100523 2.248985 1.699087 0.000000 11 B 3.620122 4.306744 3.158301 1.793624 1.716406 12 B 2.160330 1.755570 2.295645 4.133008 4.288433 13 H 1.816833 3.573753 3.904793 4.708747 4.831676 11 12 13 11 B 0.000000 12 B 4.561131 0.000000 13 H 4.202628 2.659508 0.000000
 11. -1011.7872476 21.4 C_1	1 2 3 4 5 1 B 0.000000 2 B 3.852821 0.000000 3 B 1.874399 3.892501 0.000000 4 W 2.218855 3.400987 2.362170 0.000000 5 B 3.775739 1.728343 3.891315 2.407676 0.000000 6 W 3.431816 2.207672 2.444030 2.657604 2.388640 7 B 1.762343 4.113764 1.706661 3.483232 4.626964 8 W 2.342455 2.250357 2.857661 3.321755 3.222322 9 B 1.898048 3.008156 3.332032 2.358208 2.794224 10 B 3.429377 1.725709 4.239773 3.111139 1.810933 11 B 3.215820 2.916278 4.102911 2.153184 1.782504 12 B 2.839300 3.355732 1.741054 3.555889 4.093421 13 H 3.546857 3.482589 2.581184 1.843120 2.619015 6 7 8 9 10 6 W 0.000000 7 B 3.406653 0.000000 8 W 2.822219 2.218595 0.000000 9 B 3.646667 3.242060 2.204425 0.000000 10 B 3.354748 4.295971 2.406334 1.848503 0.000000 11 B 3.635246 4.607348 3.398813 1.768218 1.707184 12 B 2.199596 1.711975 2.268314 3.841521 4.211982 13 H 1.825307 4.107862 4.016911 3.894323 4.010828 11 12 13 11 B 0.000000 12 B 4.733921 0.000000 13 H 3.440974 3.406539 0.000000

Table S8C. Energy ranking for all of the $Cp_3W_3(H)B_9H_9$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE(kcal/mol)
1	12v-03-AnticubeOh------128	-1011.4763651	0.00
2	12v-02-CubeOh------52	-1011.4761322	0.15
3	12v-01-Icos----------1	-1011.4761049	0.16
4	12v-01-Icos----------2	-1011.4761039	0.16
5	12v-02-CubeOh------54	-1011.4761004	0.17
6	12v-03-AnticubeOh------156	-1011.4616852	9.21
7	12v-02-CubeOh------55	-1011.4598112	10.39
8	12v-02-CubeOh------82	-1011.4487455	17.33
9	12v-02-CubeOh------81	-1011.4487416	17.33
10	12v-02-CubeOh------46	-1011.4445499	19.96
11	12v-03-AnticubeOh------179	-1011.4368107	24.82
12	12v-02-CubeOh------51	-1011.4367017	24.89
13	12v-01-Icos----------3	-1011.4366086	24.95
14	12v-03-AnticubeOh------99	-1011.4356862	25.53
15	12v-02-CubeOh------67	-1011.4350829	25.90
16	12v-02-CubeOh------89_r-15	-1011.4350781	25.91
17	12v-02-CubeOh------89_i-15	-1011.4350637	25.92
18	12v-02-CubeOh------60	-1011.4350636	25.92
19	12v-03-AnticubeOh------167	-1011.4332546	27.05
20	12v-03-AnticubeOh------101	-1011.4330289	27.19
21	12v-02-CubeOh------39	-1011.4328135	27.33
22	12v-03-AnticubeOh------103	-1011.4327193	27.39
23	12v-02-CubeOh------30	-1011.4326756	27.42
24	12v-03-AnticubeOh------178	-1011.4317652	27.99
25	12v-03-AnticubeOh------143	-1011.4308767	28.54
26	12v-02-CubeOh------53	-1011.4287268	29.89
27	12v-03-AnticubeOh------175	-1011.4279619	30.37
28	12v-03-AnticubeOh------110	-1011.4279133	30.40
29	12v-03-AnticubeOh------173	-1011.4277831	30.49
30	12v-02-CubeOh------56	-1011.4277625	30.50
31	12v-02-CubeOh------49	-1011.4254093	31.98
32	12v-03-AnticubeOh------133	-1011.4247675	32.38
33	12v-02-CubeOh------87	-1011.4238400	32.96
34	12v-03-AnticubeOh------134	-1011.4232465	33.33
35	12v-03-AnticubeOh------189	-1011.4231966	33.36
36	12v-03-AnticubeOh------150	-1011.4216971	34.30
37	12v-03-AnticubeOh------114	-1011.4183558	36.40
38	12v-03-AnticubeOh------165	-1011.4178872	36.70
39	12v-03-AnticubeOh------162	-1011.4166107	37.50

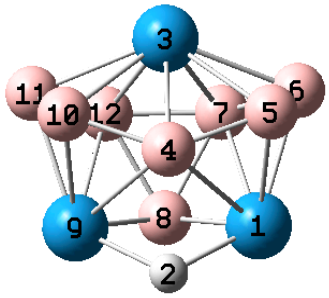
40	12v-02-CubeOh------28	-1011.4158689	37.96
41	12v-02-CubeOh------27	-1011.4158413	37.98
42	12v-03-AnticubeOh------154	-1011.4156898	38.07
43	12v-01-Icos----------8	-1011.4156377	38.11
44	12v-01-Icos----------9	-1011.4156375	38.11
45	12v-02-CubeOh------20	-1011.4156003	38.13
46	12v-02-CubeOh------19	-1011.4156002	38.13
47	12v-03-AnticubeOh------139	-1011.4147907	38.64
48	12v-03-AnticubeOh------148	-1011.4138409	39.23
49	12v-02-CubeOh------88	-1011.4138307	39.24
50	12v-03-AnticubeOh------191	-1011.4135031	39.45
51	12v-02-CubeOh------59	-1011.4133695	39.53
52	12v-03-AnticubeOh------104	-1011.4129134	39.82
53	12v-03-AnticubeOh------135	-1011.4126922	39.96
54	12v-03-AnticubeOh------190	-1011.4126790	39.96
55	12v-03-AnticubeOh------145	-1011.4115541	40.67
56	12v-03-AnticubeOh------159	-1011.4106218	41.25
57	12v-03-AnticubeOh------95	-1011.4104313	41.37
58	12v-01-Icos----------4	-1011.4082697	42.73
59	12v-03-AnticubeOh------140	-1011.4078983	42.96
60	12v-03-AnticubeOh------174	-1011.4077006	43.09
61	12v-03-AnticubeOh------109	-1011.4074264	43.26
62	12v-03-AnticubeOh------168	-1011.4069345	43.57
63	12v-01-Icos----------7	-1011.4063417	43.94
64	12v-02-CubeOh------29	-1011.4063015	43.97
65	12v-01-Icos----------11	-1011.4061747	44.05
66	12v-02-CubeOh------61	-1011.4061324	44.07
67	12v-01-Icos----------15	-1011.4061271	44.08
68	12v-02-CubeOh------80	-1011.4052931	44.60
69	12v-03-AnticubeOh------111	-1011.4032414	45.89
70	12v-03-AnticubeOh------172	-1011.4027527	46.19
71	12v-02-CubeOh------84	-1011.4018552	46.76
72	12v-03-AnticubeOh------153	-1011.4014191	47.03
73	12v-03-AnticubeOh------105	-1011.4008296	47.40
74	12v-03-AnticubeOh------107	-1011.4005608	47.57
75	12v-03-AnticubeOh------142	-1011.4004961	47.61
76	12v-01-Icos----------13	-1011.3993211	48.35
77	12v-01-Icos----------14	-1011.3992918	48.36
78	12v-02-CubeOh------25	-1011.3990051	48.54
79	12v-02-CubeOh------74	-1011.3989572	48.57
80	12v-02-CubeOh------73	-1011.3989462	48.58
81	12v-02-CubeOh------66	-1011.3988995	48.61
82	12v-03-AnticubeOh------124	-1011.3988523	48.64

83	12v-03-AnticubeOh------152	-1011.3985157	48.85
84	12v-03-AnticubeOh------112	-1011.3977272	49.35
85	12v-03-AnticubeOh------166	-1011.3969150	49.86
86	12v-02-CubeOh------48	-1011.3967255	49.97
87	12v-03-AnticubeOh------149	-1011.3966402	50.03
88	12v-02-CubeOh------47	-1011.3956673	50.64
89	12v-02-CubeOh------26	-1011.3953066	50.87
90	12v-02-CubeOh------69	-1011.3952993	50.87
91	12v-03-AnticubeOh------155	-1011.3944304	51.41
92	12v-03-AnticubeOh------180	-1011.3938805	51.76
93	12v-01-Icos----------5	-1011.3935064	51.99
94	12v-03-AnticubeOh------171	-1011.3924614	52.65
95	12v-03-AnticubeOh------170	-1011.3923267	52.73
96	12v-02-CubeOh------63	-1011.3903010	54.01
97	12v-03-AnticubeOh------161	-1011.3898648	54.28
98	12v-02-CubeOh------44	-1011.3896952	54.39
99	12v-02-CubeOh------62	-1011.3888301	54.93
100	12v-02-CubeOh------78	-1011.3887497	54.98
101	12v-02-CubeOh------58	-1011.3886511	55.04
102	12v-02-CubeOh------83	-1011.3885481	55.11
103	12v-01-Icos----------6	-1011.3885167	55.13
104	12v-02-CubeOh------90	-1011.3883711	55.22
105	12v-02-CubeOh------72	-1011.3874875	55.77
106	12v-03-AnticubeOh------151	-1011.3873829	55.84
107	12v-03-AnticubeOh------123	-1011.3862519	56.55
108	12v-03-AnticubeOh------116	-1011.3845411	57.62
109	12v-02-CubeOh------64	-1011.3839866	57.97
110	12v-03-AnticubeOh------160	-1011.3835606	58.24
111	12v-02-CubeOh------24	-1011.3808254	59.95
112	12v-02-CubeOh------41	-1011.3803517	60.25
113	12v-03-AnticubeOh------113	-1011.3800026	60.47
114	12v-03-AnticubeOh------176	-1011.3796339	60.70
115	12v-02-CubeOh------57	-1011.3796259	60.70
116	12v-02-CubeOh------18	-1011.3796181	60.71
117	12v-02-CubeOh------68	-1011.3794446	60.82
118	12v-02-CubeOh------71	-1011.3794402	60.82
119	12v-01-Icos----------10	-1011.3779511	61.76
120	12v-03-AnticubeOh------147	-1011.3777305	61.89
121	12v-03-AnticubeOh------144	-1011.3772378	62.20
122	12v-02-CubeOh------77	-1011.3766180	62.59
123	12v-01-Icos----------12	-1011.3765834	62.61
124	12v-03-AnticubeOh------138	-1011.3753590	63.38
125	12v-02-CubeOh------75	-1011.3746710	63.81

126	12v-02-CubeOh------45	-1011.3745958	63.86
127	12v-02-CubeOh------50	-1011.3743128	64.04
128	12v-02-CubeOh------33	-1011.3735547	64.51
129	12v-03-AnticubeOh------108_i-67	-1011.3732911	64.68
130	12v-03-AnticubeOh------108_r-67	-1011.3731578	64.76
131	12v-03-AnticubeOh------177	-1011.3720232	65.48
132	12v-02-CubeOh------42	-1011.3717050	65.68
133	12v-03-AnticubeOh------188	-1011.3716547	65.71
134	12v-03-AnticubeOh------158	-1011.3711690	66.01
135	12v-03-AnticubeOh------100	-1011.3708430	66.22
136	12v-03-AnticubeOh------187	-1011.3707221	66.29
137	12v-03-AnticubeOh------169	-1011.3704928	66.44
138	12v-03-AnticubeOh------157	-1011.3686964	67.56
139	12v-02-CubeOh------32	-1011.3681445	67.91
140	12v-03-AnticubeOh------146_r-24	-1011.3676282	68.23
141	12v-02-CubeOh------35	-1011.3676058	68.25
142	12v-02-CubeOh------36	-1011.3675991	68.25
143	12v-03-AnticubeOh------146_i-24	-1011.3673687	68.40
144	12v-02-CubeOh------34	-1011.3660842	69.20
145	12v-02-CubeOh------31	-1011.3660426	69.23
146	12v-02-CubeOh------37	-1011.3633515	70.92
147	12v-03-AnticubeOh------117	-1011.3631892	71.02
148	12v-02-CubeOh------85	-1011.3626188	71.38
149	12v-03-AnticubeOh------115	-1011.3621539	71.67
150	12v-03-AnticubeOh------102	-1011.3617841	71.90
151	12v-02-CubeOh------38	-1011.3617747	71.91
152	12v-02-CubeOh------43	-1011.3604602	72.73
153	12v-01-Icos----------17	-1011.3604256	72.75
154	12v-02-CubeOh------91	-1011.3598099	73.14
155	12v-02-CubeOh------23	-1011.3584877	73.97
156	12v-03-AnticubeOh------98	-1011.3577934	74.40
157	12v-03-AnticubeOh------163	-1011.3570394	74.88
158	12v-03-AnticubeOh------164	-1011.3569785	74.92
159	12v-03-AnticubeOh------184	-1011.3558345	75.63
160	12v-01-Icos----------16	-1011.3557779	75.67
161	12v-02-CubeOh------22_r-44	-1011.3529833	77.42
162	12v-02-CubeOh------21	-1011.3527547	77.57
163	12v-03-AnticubeOh------181	-1011.3524991	77.73
164	12v-03-AnticubeOh------131	-1011.3524117	77.78
165	12v-02-CubeOh------22_i-44	-1011.3502810	79.12
166	12v-03-AnticubeOh------136	-1011.3484619	80.26
167	12v-02-CubeOh------65	-1011.3458643	81.89
168	12v-03-AnticubeOh------183	-1011.3453467	82.22

169	12v-03-AnticubeOh------96	-1011.3443030	82.87
170	12v-02-CubeOh------70	-1011.3430659	83.65
171	12v-02-CubeOh------86	-1011.3426366	83.92
172	12v-02-CubeOh------76	-1011.3421944	84.19
173	12v-03-AnticubeOh------97	-1011.3401817	85.46
174	12v-03-AnticubeOh------106	-1011.3399232	85.62
175	12v-03-AnticubeOh------119	-1011.3392004	86.07
176	12v-03-AnticubeOh------122	-1011.3376313	87.06
177	12v-03-AnticubeOh------141	-1011.3368173	87.57
178	12v-03-AnticubeOh------127	-1011.3365591	87.73
179	12v-03-AnticubeOh------130	-1011.3361532	87.98
180	12v-03-AnticubeOh------185	-1011.3359003	88.14
181	12v-03-AnticubeOh------137	-1011.3358084	88.20
182	12v-03-AnticubeOh------118	-1011.3335207	89.64
183	12v-03-AnticubeOh------182	-1011.3331303	89.88
184	12v-02-CubeOh------79	-1011.3330081	89.96
185	12v-03-AnticubeOh------126	-1011.3322178	90.45
186	12v-03-AnticubeOh------125	-1011.3321745	90.48
187	12v-03-AnticubeOh------129	-1011.3311549	91.12
188	12v-02-CubeOh------40	-1011.3274212	93.46
189	12v-03-AnticubeOh------93	-1011.3253169	94.78
190	12v-03-AnticubeOh------132	-1011.3252864	94.80
191	12v-03-AnticubeOh------120	-1011.3235043	95.92
192	12v-03-AnticubeOh------121	-1011.3210564	97.46
193	12v-03-AnticubeOh------94	-1011.3195860	98.38
194	12v-03-AnticubeOh------186	-1011.3193695	98.52
195	12v-03-AnticubeOh------92	-1011.3012490	109.89

Table S9A. Distance table for the lowest-lying $Cp_3^*W_3(H)B8H8$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.



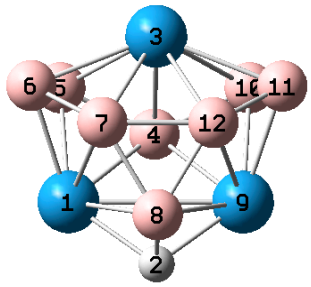
1. -1575.814106 0.0 C_S

Experimental structure Lowest energy structure as Cp_3W_3H

		1	2	3	4	5
1	W	0.000000				
2	H	1.869100	0.000000			
3	W	3.076582	3.527337	0.000000		
4	B	2.508608	1.942528	2.263275	0.000000	
5	B	2.194870	2.894403	2.231654	1.743219	0.000000
6	B	2.111481	3.631784	2.237801	3.058840	1.790572
7	B	2.326014	3.613537	2.337377	3.545051	3.084315
8	B	2.231617	2.871690	3.297775	3.657327	3.859511
9	W	2.793448	1.869100	3.076582	2.508608	3.701394
10	B	3.701394	2.894403	2.231654	1.743219	3.179892
11	B	3.981449	3.631784	2.237801	3.058840	4.021929
12	B	3.227385	3.613537	2.337377	3.545051	3.900148

		6	7	8	9	10
6	B	0.000000				
7	B	1.771624	0.000000			
8	B	3.131570	1.766240	0.000000		
9	W	3.981449	3.227385	2.231617	0.000000	
10	B	4.021929	3.900148	3.859511	2.194870	0.000000
11	B	4.078682	3.232241	3.131570	2.111481	1.790572
12	B	3.232241	1.791934	1.766240	2.326014	3.084315

		11	12
11	B	0.000000	
12	B	1.771624	0.000000

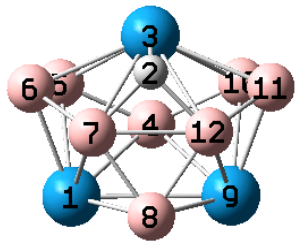
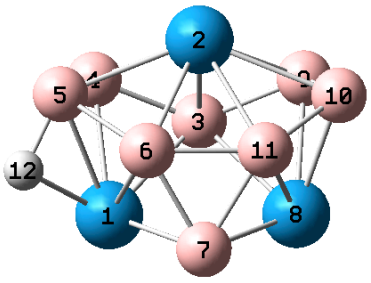


2. -1575.797242 +10.6 C_S

Corresponds to B8H9W3-3 in the Cp_3W_3H rankings

		1	2	3	4	5
1	W	0.000000				
2	H	1.900200	0.000000			
3	W	3.055733	3.729859	0.000000		
4	B	2.356647	3.083035	2.349630	0.000000	
5	B	2.164849	3.741697	2.210859	1.766872	0.000000
6	B	2.087872	3.548378	2.249095	3.081002	1.831022
7	B	2.324660	2.710808	2.342283	3.499799	3.096753
8	B	2.351345	1.368798	3.325608	3.610854	3.930768
9	W	2.862951	1.900454	3.052644	2.349498	3.678242
10	B	3.690468	3.747043	2.211012	1.774021	3.104747
11	B	4.021454	3.548104	2.253502	3.083894	4.017266
12	B	3.259374	2.709597	2.343447	3.500367	3.903974

		6	7	8	9	10
6	B	0.000000				
7	B	1.775954	0.000000			
8	B	3.173312	1.751523	0.000000		
9	W	4.016048	3.259916	2.355827	0.000000	
10	B	4.016950	3.906090	3.935515	2.164498	0.000000

	11 B 4.118128 3.265673 3.175241 2.088451 1.830370 12 B 3.263499 1.821294 1.751509 2.327665 3.098290 11 12 11 B 0.000000 12 B 1.777749 0.000000
 3. -1575.787637 +16.6 C_S Corresponds to B8H9W3-4 in the Cp_3W_3H rankings	1 W 0.000000 2 H 3.312217 0.000000 3 W 3.070804 1.891122 0.000000 4 B 2.335094 3.692847 2.340345 0.000000 5 B 2.166993 3.515687 2.216776 1.768899 0.000000 6 B 2.097357 2.526923 2.275710 3.057242 1.793896 7 B 2.275842 1.450423 2.502263 3.550421 3.120542 8 B 2.237271 2.482801 3.355079 3.532354 3.866968 9 W 2.750313 3.305537 3.068412 2.330043 3.643387 10 B 3.652382 3.512924 2.219036 1.770573 3.128550 11 B 3.975157 2.522280 2.281957 3.057107 4.021041 12 B 3.271988 1.441167 2.497086 3.542883 3.999560 6 7 8 9 10 6 B 0.000000 7 B 1.793754 0.000000 8 B 3.167132 1.762222 0.000000 9 W 3.969167 3.274283 2.239686 0.000000 10 B 4.020730 4.009611 3.874026 2.170097 0.000000 11 B 4.138588 3.404121 3.172241 2.095817 1.794848 12 B 3.395929 2.016525 1.764622 2.270522 3.117391 11 12 11 B 0.000000 12 B 1.792142 0.000000
 4. -1575.786968 +17.0 C_1 Corresponds to B8H9W3-2 in the Cp_3W_3H rankings	1 W 0.000000 2 W 3.017869 0.000000 3 B 2.320697 2.320261 0.000000 4 B 2.161791 2.215534 1.761197 0.000000 5 B 2.190804 2.242343 3.111732 1.846942 0.000000 6 B 2.397602 2.315552 3.518286 3.159713 1.893737 7 B 2.247706 3.270352 3.520256 3.863083 3.211786 8 W 2.782438 3.046971 2.376555 3.688405 4.062263 9 B 3.629792 2.229318 1.758573 3.126676 4.055813 10 B 3.961466 2.245586 3.051337 4.013248 4.142511 11 B 3.254018 2.347859 3.511701 3.935459 3.326163 12 H 1.841593 3.289441 3.641500 2.554758 1.266218 6 7 8 9 10 6 B 0.000000 7 B 1.753446 0.000000 8 W 3.211524 2.228692 0.000000 9 B 3.885299 3.843360 2.169883 0.000000 10 B 3.205142 3.139227 2.086001 1.800885 0.000000

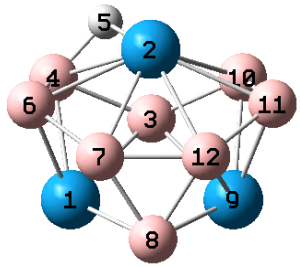
	11 B 1.760657 1.781387 2.315683 3.097144 1.778935 12 H 2.096766 2.973678 4.264217 4.800811 4.825603 11 12 11 B 0.000000 12 H 3.720383 0.000000
 5. -1575.781384 +20.5 C_1 Corresponds to B8H9W3-5 in the Cp_3W_3H rankings	1 W 0.000000 2 W 3.065863 0.000000 3 B 2.302557 2.474403 0.000000 4 B 2.179166 2.297781 1.914206 0.000000 5 H 3.170139 1.849580 1.914354 1.303380 0.000000 6 B 2.102905 2.257050 3.140606 1.820241 2.624438 7 B 2.310909 2.348673 3.524013 3.118706 3.623360 8 B 2.223507 3.314374 3.484794 3.889203 4.422777 9 W 2.768063 3.097000 2.296191 3.736749 3.795511 10 B 3.647694 2.252544 1.816617 3.215004 2.524908 11 B 3.953226 2.275375 3.089638 4.090212 3.613437 12 B 3.203789 2.358859 3.505324 3.953993 3.982025 6 7 8 9 10 6 B 0.000000 7 B 1.770079 0.000000 8 B 3.132228 1.764717 0.000000 9 W 3.988599 3.224631 2.227210 0.000000 10 B 4.029837 3.894912 3.842138 2.172988 0.000000 11 B 4.109825 3.249177 3.125251 2.088729 1.797682 12 B 3.250052 1.806294 1.757257 2.307062 3.076411 11 12 11 B 0.000000 12 B 1.771927 0.000000

Table 10. HOMO-LUMO gaps of all optimized structures.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	Gap (eV)
B2HW3-1	-0.168089	-0.094138	2.01
B2HW3-2	-0.164530	-0.096721	1.85
B2HW3-3	-0.166980	-0.081916	2.31
B2HW3-4	-0.158141	-0.101462	1.54
B2HW3-5	-0.154017	-0.117308	1.00
B3HW3-1	-0.164495	-0.104201	1.64
B3HW3-2	-0.171301	-0.100645	1.92
B3HW3-3	-0.170527	-0.093239	2.10
B3HW3-4	-0.168106	-0.096107	1.96
B3HW3-5	-0.163543	-0.096405	1.83
B3HW3-6	-0.167258	-0.092343	2.04
B3HW3-7	-0.152806	-0.111651	1.12
B3HW3-8	-0.168427	-0.099846	1.87
B4HW3-1	-0.172975	-0.090110	2.25
B4HW3-2	-0.175369	-0.095539	2.17
B4HW3-3	-0.167935	-0.099283	1.87
B4HW3-4	-0.169354	-0.101703	1.84
B4HW3-5	-0.169053	-0.113543	1.51
B4HW3-6	-0.176392	-0.111144	1.78
B4HW3-7	-0.161442	-0.095101	1.81
B4HW3-8	-0.173028	-0.113285	1.63
B5HW3-1	-0.178017	-0.101259	2.09
B5HW3-2	-0.175430	-0.096229	2.16
B5HW3-3	-0.176279	-0.093444	2.25
B5HW3-4	-0.182810	-0.087507	2.59
B5HW3-5	-0.174473	-0.096026	2.13
B5HW3-6	-0.183010	-0.087638	2.60
B5HW3-7	-0.167599	-0.099459	1.85
B5HW3-8	-0.173660	-0.101639	1.96
B5HW3-9	-0.161442	-0.104543	1.55
B5HW3-10	-0.174508	-0.115825	1.60
B5HW3-11	-0.178549	-0.086099	2.52
B5HW3-12	-0.156757	-0.102062	1.49
B5HW3-13	-0.182383	-0.088962	2.54
B6HW3-1	-0.178517	-0.106737	1.95
B6HW3-2	-0.179654	-0.095433	2.29
B6HW3-3	-0.183183	-0.108224	2.04
B6HW3-4	-0.178050	-0.115502	1.70

B6HW3-5	-0.181767	-0.100818	2.20
B6HW3-6	-0.178973	-0.098553	2.19
B6HW3-7	-0.175166	-0.110339	1.76
B6HW3-8	-0.169654	-0.096029	2.00
B6HW3-9	-0.186202	-0.104466	2.22
B6HW3-10	-0.187849	-0.108272	2.17
B6HW3-11	-0.187080	-0.106946	2.18
B6HW3-12	-0.174745	-0.111221	1.73
B6HW3-13	-0.183157	-0.103194	2.18
B7HW3-1	-0.178292	-0.110250	1.85
B7HW3-2	-0.175755	-0.106836	1.88
B7HW3-3	-0.186516	-0.120343	1.80
B7HW3-4	-0.175493	-0.097250	2.13
B7HW3-5	-0.173992	-0.100919	1.99
B7HW3-6	-0.178458	-0.098738	2.17
B7HW3-7	-0.196353	-0.110079	2.35
B7HW3-8	-0.173323	-0.085655	2.39
B7HW3-9	-0.169160	-0.088209	2.20
B7HW3-10	-0.168208	-0.094760	2.00
B8HW3-1	-0.187140	-0.089965	2.64
B8HW3-2	-0.185587	-0.089232	2.62
B8HW3-3	-0.183343	-0.085524	2.66
B8HW3-4	-0.188677	-0.081695	2.91
B8HW3-5	-0.181062	-0.082931	2.67
B8HW3-6	-0.183522	-0.088692	2.58
B8HW3-7	-0.185846	-0.114551	1.94
B9HW3-1	-0.188270	-0.091778	2.63
B9HW3-2	-0.181915	-0.097648	2.29
B9HW3-3	-0.184517	-0.099209	2.32
B9HW3-4	-0.182867	-0.093223	2.44
B9HW3-5	-0.182568	-0.093569	2.42
B9HW3-6	-0.179809	-0.102514	2.10
B9HW3-7	-0.178889	-0.091027	2.39
B9HW3-8	-0.182864	-0.100284	2.25
B9HW3-9	-0.200065	-0.118376	2.22
B9HW3-10	-0.180351	-0.115259	1.77
B9HW3-11	-0.192300	-0.121018	1.94