

Hypoelectronic Diruthenaboranes and Diosmaboranes Having Eight to Twelve Vertices: Capped *Isocloso* and Bicapped *Closo* Structures

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Supporting Information

- Table S1.** The $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_6$ structures.
Table S2. The $\text{Cp}_2\text{Ru}_2\text{B}_7\text{H}_7$ structures.
Table S3. The $\text{Cp}_2\text{Ru}_2\text{B}_8\text{H}_8$ structures.
Table S4. The $\text{Cp}_2\text{Ru}_2\text{B}_9\text{H}_9$ structures.
Table S5. The $\text{Cp}_2\text{Ru}_2\text{B}_{10}\text{H}_{10}$ structures
Table S6. The $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_6$ structures.
Table S7. The $\text{Cp}_2\text{Os}_2\text{B}_7\text{H}_7$ structures.
Table S8. The $\text{Cp}_2\text{Os}_2\text{B}_8\text{H}_8$ structures.
Table S9. The $\text{Cp}_2\text{Os}_2\text{B}_9\text{H}_9$ structures.
Table S10. The $\text{Cp}_2\text{Os}_2\text{B}_{10}\text{H}_{10}$ structures.
Complete Gaussian09 Reference (reference 33)

The 8-vertex $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_6$ System

Table S1A. Initial structures

Table S1B Best structures distances

Table S1C. Global ranking of all structures

Table S1A. Initial $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_6$ structures (one example from each family); 84 structures in total

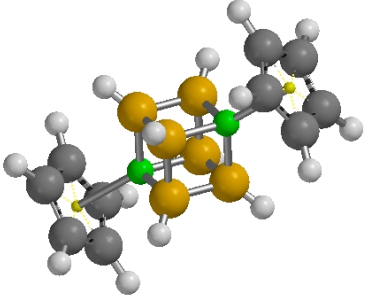
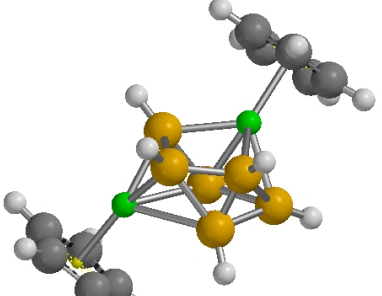
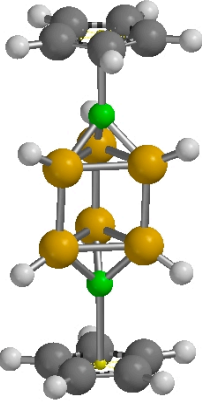
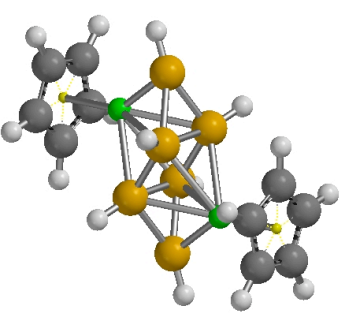
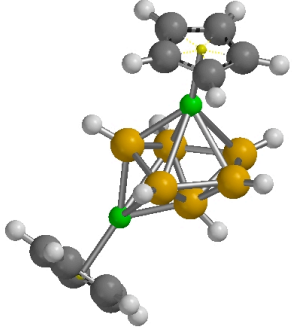
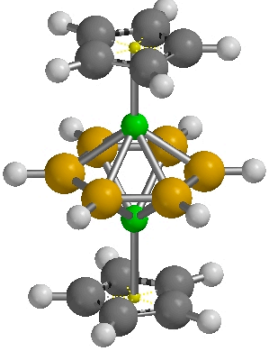
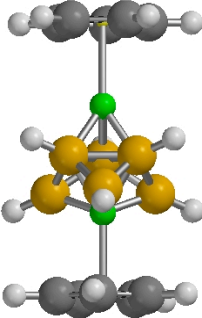
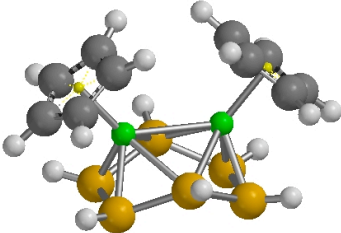
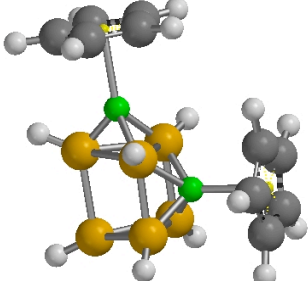
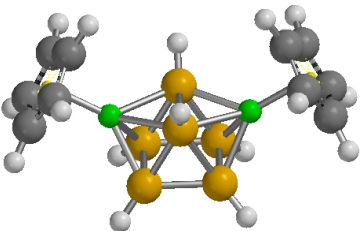
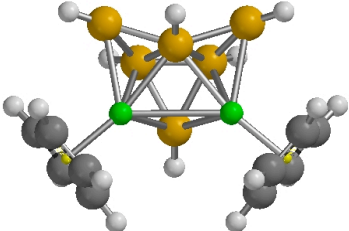
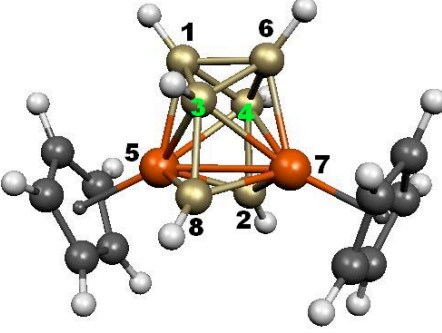
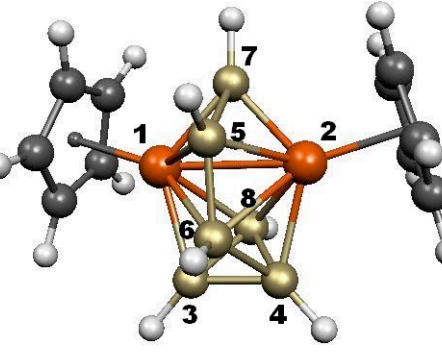
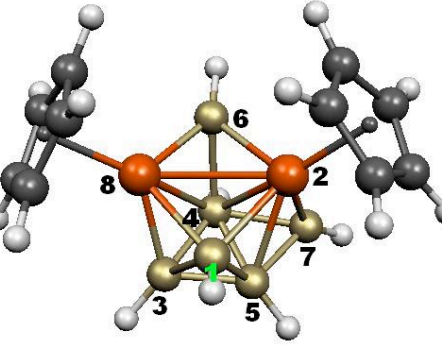
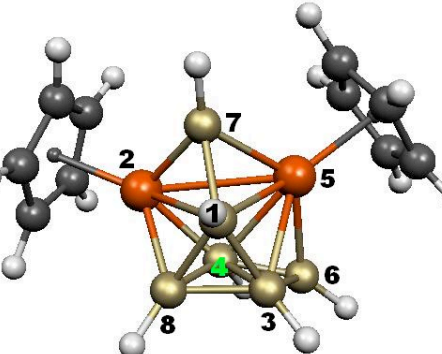
<p>Initial structures</p>	 <p>1. Cube 3</p>	 <p>2. Antiprism 4</p>
 <p>3. Trigonal Prism 6</p>	 <p>4. Trigonal Antiprism 8</p>	 <p>5. Bisdisphenoid 6</p>
 <p>6. Hexagonal bipyramid 4</p>	 <p>7. All-capped tetrahedron 5</p>	 <p>8. Nido structure 9</p>
 <p>9. Dicapped trigonal prism (C_3) 18</p>	 <p>10. Dicapped trigonal prism (C_{2v}) 10</p>	 <p>11. Dicapped octahedron 11</p>

Table S1B: Distances table for the lowest energy Cp₂Ru₂B₆H₆ structures

 <p>1 -729.79164209 0.0 kcal/mole C_{2v}</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.087090</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.740153</td><td>3.271393</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.740135</td><td>1.781833</td><td>2.557766</td><td>0.000000</td><td></td></tr> <tr><td>5 Ru</td><td>2.135975</td><td>2.059082</td><td>2.259490</td><td>2.259710</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.733525</td><td>3.087880</td><td>1.740135</td><td>1.740153</td><td>3.042886</td></tr> <tr><td>7 Ru</td><td>3.042886</td><td>2.060627</td><td>2.259710</td><td>2.259490</td><td>2.709373</td></tr> <tr><td>8 B</td><td>3.087880</td><td>2.942837</td><td>1.781833</td><td>3.271393</td><td>2.060627</td></tr> <tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Ru</td><td>2.135975</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.087090</td><td>2.059082</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.087090	0.000000				3 B	1.740153	3.271393	0.000000			4 B	1.740135	1.781833	2.557766	0.000000		5 Ru	2.135975	2.059082	2.259490	2.259710	0.000000	6 B	1.733525	3.087880	1.740135	1.740153	3.042886	7 Ru	3.042886	2.060627	2.259710	2.259490	2.709373	8 B	3.087880	2.942837	1.781833	3.271393	2.060627		6	7	8			6 B	0.000000					7 Ru	2.135975	0.000000				8 B	3.087090	2.059082	0.000000		
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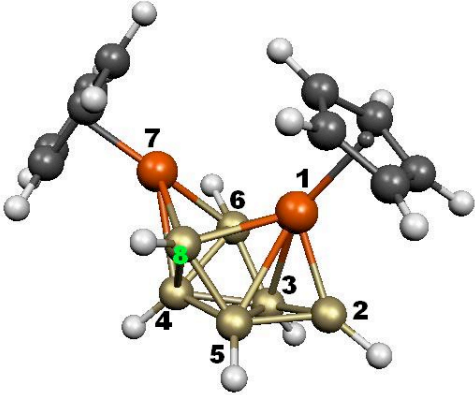
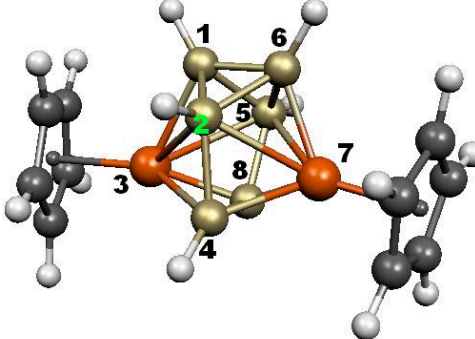
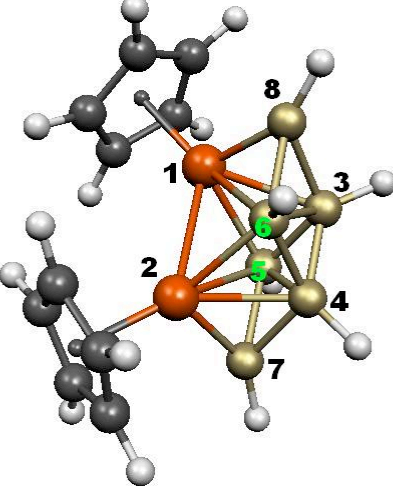
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Table S1C: Energy ranking for the $\text{Cp}_2\text{Ru}_2\text{B}_6\text{H}_6$ structures

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole
1	08-Ru-10-DicapTrPr-C2v-f_r-20	-729.79164209	0.00
2	08-Ru-01-Cub-b	-729.79149688	0.09
3	08-Ru-05-Bisdisph-d	-729.79149688	0.09
4	08-Ru-06-Bipirhex-a	-729.79149688	0.09
5	08-Ru-07-Tdallcap-d	-729.79149688	0.09
6	08-Ru-08-Nido-c	-729.79149688	0.09
7	08-Ru-08-Nido-f	-729.79149688	0.09
8	08-Ru-09-DicapTrPr-Cs-e	-729.79149688	0.09
9	08-Ru-09-DicapTrPr-Cs-i	-729.79149688	0.09
10	08-Ru-10-DicapTrPr-C2v-f_r-173	-729.79149688	0.09
11	08-Ru-09-DicapTrPr-Cs-r	-729.75565119	22.58
12	08-Ru-09-DicapTrPr-Cs-k	-729.74585282	28.73
13	08-Ru-09-DicapTrPr-Cs-a	-729.74585281	28.73
14	08-Ru-11-DicapOh-k	-729.74585281	28.73
15	08-Ru-04-AntiprTrig-c	-729.74585280	28.73
16	08-Ru-04-AntiprTrig-d	-729.74585278	28.73
17	08-Ru-09-DicapTrPr-Cs-m	-729.73344384	36.52
18	08-Ru-09-DicapTrPr-Cs-n	-729.73344379	36.52
19	08-Ru-11-DicapOh-b	-729.73344379	36.52
20	08-Ru-08-Nido-h	-729.72783064	40.04
21	08-Ru-02-Antipr-d	-729.72405327	42.41
22	08-Ru-04-AntiprTrig-g	-729.72313835	42.99
23	08-Ru-01-Cub-a	-729.72288185	43.15
24	08-Ru-03-PrTrig-d	-729.72288185	43.15
25	08-Ru-08-Nido-e	-729.72288185	43.15
26	08-Ru-08-Nido-i	-729.72288185	43.15
27	08-Ru-07-Tdallcap-b	-729.72064514	44.55
28	08-Ru-11-DicapOh-h	-729.71747737	46.54
29	08-Ru-09-DicapTrPr-Cs-f	-729.71689298	46.91
30	08-Ru-06-Bipirhex-d	-729.71435601	48.50
31	08-Ru-07-Tdallcap-e	-729.71374762	48.88
32	08-Ru-02-Antipr-c	-729.71344984	49.07
33	08-Ru-05-Bisdisph-b	-729.71344984	49.07
34	08-Ru-10-DicapTrPr-C2v-c_r-362	-729.71344984	49.07
35	08-Ru-10-DicapTrPr-C2v-b	-729.71344983	49.07
36	08-Ru-10-DicapTrPr-C2v-d	-729.71256957	49.62
37	08-Ru-09-DicapTrPr-Cs-q	-729.71156723	50.25
38	08-Ru-01-Cub-c_r-18	-729.71129097	50.42
39	08-Ru-07-Tdallcap-c	-729.71120402	50.47
40	08-Ru-11-DicapOh-i	-729.71113717	50.52
41	08-Ru-06-Bipirhex-b	-729.71108296	50.55
42	08-Ru-09-DicapTrPr-Cs-p	-729.71054527	50.89

43	08-Ru-11-DicapOh-c	-729.71054527	50.89
44	08-Ru-03-PrTrig-b	-729.71016757	51.13
45	08-Ru-04-AntiprTrig-h	-729.70791500	52.54
46	08-Ru-08-Nido-g	-729.70764036	52.71
47	08-Ru-03-PrTrig-f	-729.70595679	53.77
48	08-Ru-09-DicapTrPr-Cs-c	-729.70463600	54.60
49	08-Ru-11-DicapOh-j	-729.70463600	54.60
50	08-Ru-04-AntiprTrig-f	-729.70461225	54.61
51	08-Ru-08-Nido-d	-729.70293109	55.67
52	08-Ru-10-DicapTrPr-C2v-e	-729.70293108	55.67
53	08-Ru-05-Bisdisph-c	-729.70293107	55.67
54	08-Ru-09-DicapTrPr-Cs-j	-729.70293107	55.67
55	08-Ru-10-DicapTrPr-C2v-j_r-126	-729.70293107	55.67
56	08-Ru-10-DicapTrPr-C2v-f_r-113-61	-729.70209751	56.19
57	08-Ru-11-DicapOh-g	-729.70145995	56.59
58	08-Ru-09-DicapTrPr-Cs-d	-729.69884101	58.23
59	08-Ru-11-DicapOh-a	-729.69881727	58.25
60	08-Ru-08-Nido-b	-729.69731032	59.19
61	08-Ru-09-DicapTrPr-Cs-o	-729.69731032	59.19
62	08-Ru-05-Bisdisph-e	-729.69646205	59.73
63	08-Ru-03-PrTrig-e	-729.69598744	60.02
64	08-Ru-07-Tdallcap-a	-729.69437886	61.03
65	08-Ru-05-Bisdisph-a	-729.69368205	61.47
66	08-Ru-02-Antipr-a	-729.69368204	61.47
67	08-Ru-09-DicapTrPr-Cs-g	-729.69368204	61.47
68	08-Ru-10-DicapTrPr-C2v-a	-729.69368204	61.47
69	08-Ru-10-DicapTrPr-C2v-h_r-237-23	-729.69368204	61.47
70	08-Ru-10-DicapTrPr-C2v-h_r-237 i-23	-729.69310335	61.83
71	08-Ru-10-DicapTrPr-C2v-c i-362	-729.68311237	68.10
72	08-Ru-10-DicapTrPr-C2v-j i-126	-729.68269957	68.36
73	08-Ru-10-DicapTrPr-C2v-i	-729.67986859	70.14
74	08-Ru-02-Antipr-b	-729.67986858	70.14
75	08-Ru-09-DicapTrPr-Cs-h	-729.67946628	70.39
76	08-Ru-06-Bipirhex-c	-729.67798074	71.32
77	08-Ru-09-DicapTrPr-Cs-l	-729.67455503	73.47
78	08-Ru-03-PrTrig-c	-729.67100848	75.70
79	08-Ru-08-Nido-a	-729.67025037	76.17
80	08-Ru-11-DicapOh-e	-729.66681424	78.33
81	08-Ru-10-DicapTrPr-C2v-h i-237	-729.66445319	79.81
82	08-Ru-10-DicapTrPr-C2v-g	-729.66415404	80.00
83	08-Ru-01-Cub-c i-18	-729.66263956	80.95
84	08-Ru-11-DicapOh-f	-729.66047163	82.31

85	08-Ru-11-DicapOh-d	-729.65532661	85.54
86	08-Ru-09-DicapTrPr-Cs-b	-729.65053840	88.54
87	08-Ru-04-AntiprTrig-a	-729.65042241	88.62
88	08-Ru-04-AntiprTrig-b	-729.65042238	88.62
89	08-Ru-10-DicapTrPr-C2v-f_r-113 i-61	-729.64773420	90.30
90	08-Ru-03-PrTrig-a	-729.64279601	93.40
91	08-Ru-04-AntiprTrig-e_r-228	-729.64178217	94.04
92	08-Ru-05-Bisdisph-f_i-31	-729.62009043	107.65
93	08-Ru-05-Bisdisph-f_i-34	-729.62009043	107.65
94	08-Ru-10-DicapTrPr-C2v-f imag	-729.61870547	108.52
95	08-Ru-05-Bisdisph-f imag	-729.61654418	109.87
96	08-Ru-04-AntiprTrig-e i-228	-729.59571441	122.94

The 9-vertex $\text{Cp}_2\text{Ru}_2\text{B}_7\text{H}_7$ System

Table S2A. Initial structures

Table S2B. Best structures distances

Table S2C. Global ranking of all structures

Table S2A. Initial $\text{Cp}_2\text{Ru}_2\text{B}_7\text{H}_7$ structures (one example from each family); 43 structures in total

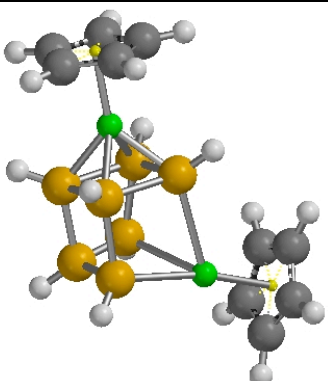
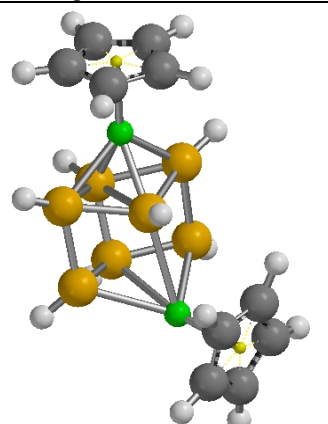
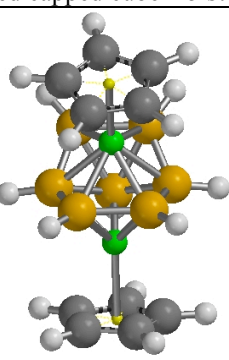
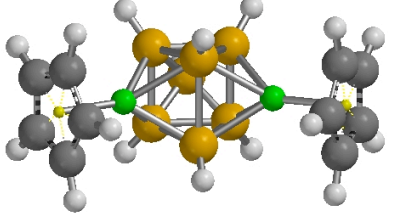
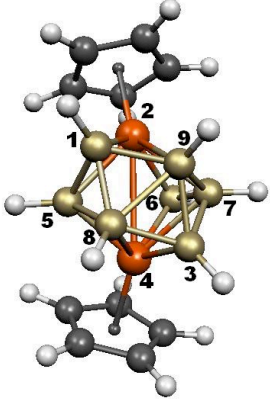
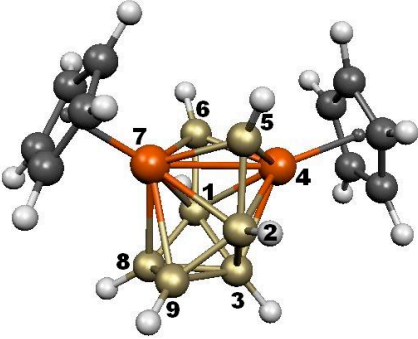
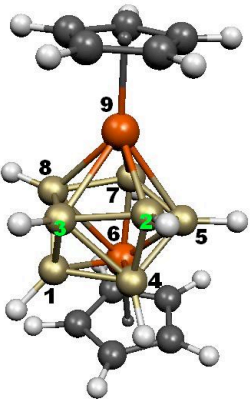
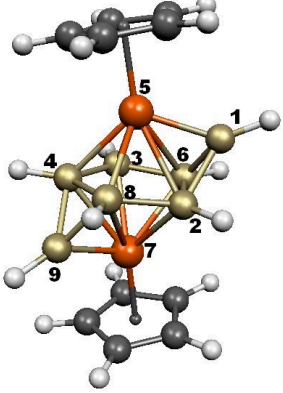
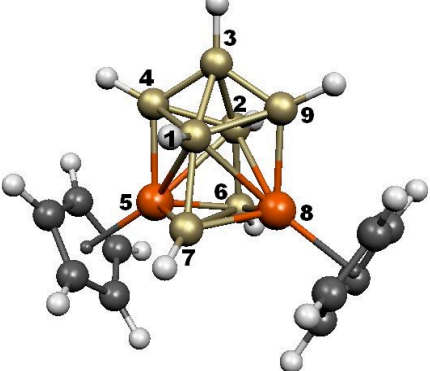
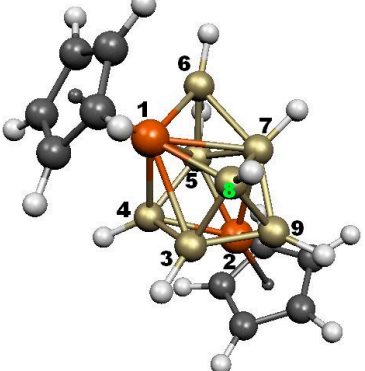
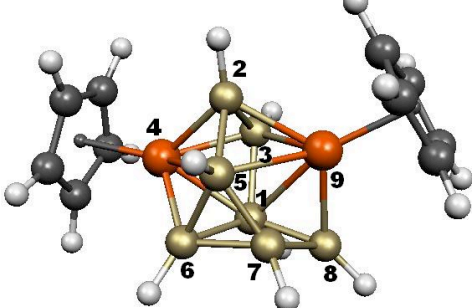
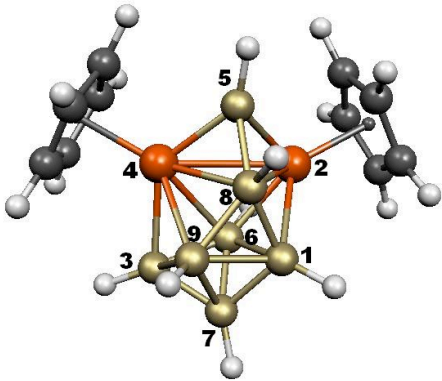
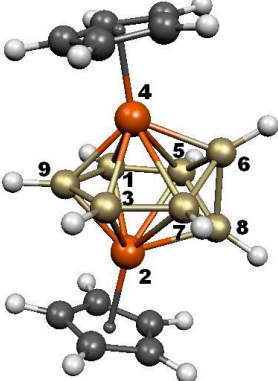
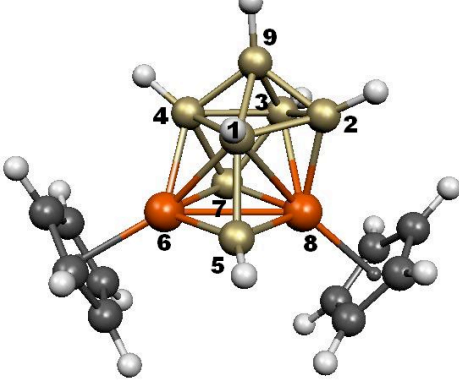
Initial structures	
	1. Capped cube 9 structures
	2. Pressed capped cube 15 structures
	3. Tl_9 -like structure 13 structures
	4. Tricapped trigonal prism 6 structures

Table S2B. Distance table for the lowest energy Cp₂Ru₂B₇H₇ structures

 <p>1. -755.23909887 0.0 kcal/mole</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Ru</td><td>2.101074</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.895737</td><td>3.246618</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Ru</td><td>3.186346</td><td>2.800694</td><td>2.074321</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.773037</td><td>2.220171</td><td>2.970139</td><td>2.083898</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.673707</td><td>2.061768</td><td>3.054122</td><td>2.038913</td><td>3.065326</td></tr> <tr><td>7 B</td><td>2.999032</td><td>2.195978</td><td>1.766088</td><td>2.275820</td><td>3.148634</td></tr> <tr><td>8 B</td><td>1.692749</td><td>2.989183</td><td>1.772447</td><td>2.329558</td><td>1.796524</td></tr> <tr><td>9 B</td><td>1.788765</td><td>2.308795</td><td>1.779719</td><td>2.982602</td><td>2.816873</td></tr> <tr><td></td><td>6</td><td>7</td><td>8</td><td>9</td><td></td></tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.781936</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.646101</td><td>2.808598</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.169338</td><td>1.729388</td><td>1.931713</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Ru	2.101074	0.000000				3 B	2.895737	3.246618	0.000000			4 Ru	3.186346	2.800694	2.074321	0.000000		5 B	1.773037	2.220171	2.970139	2.083898	0.000000	6 B	3.673707	2.061768	3.054122	2.038913	3.065326	7 B	2.999032	2.195978	1.766088	2.275820	3.148634	8 B	1.692749	2.989183	1.772447	2.329558	1.796524	9 B	1.788765	2.308795	1.779719	2.982602	2.816873		6	7	8	9		6 B	0.000000					7 B	1.781936	0.000000				8 B	3.646101	2.808598	0.000000			9 B	3.169338	1.729388	1.931713	0.000000	
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8 Ru	2.349379	2.353609	3.212659	3.437598	2.708400																																																																																						
9 B	1.893876	1.890616	1.641268	2.800243	3.437538																																																																																						
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8 Ru	2.057977	2.056562	0.000000																																																																																								
9 B	3.095200	3.101248	2.057425	0.000000																																																																																							
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7 B	2.063338	0.000000																																																																																																																	
8 Ru	2.744583	2.089686	0.000000																																																																																																																
9 B	3.435841	2.959261	3.108361	0.000000																																																																																																															

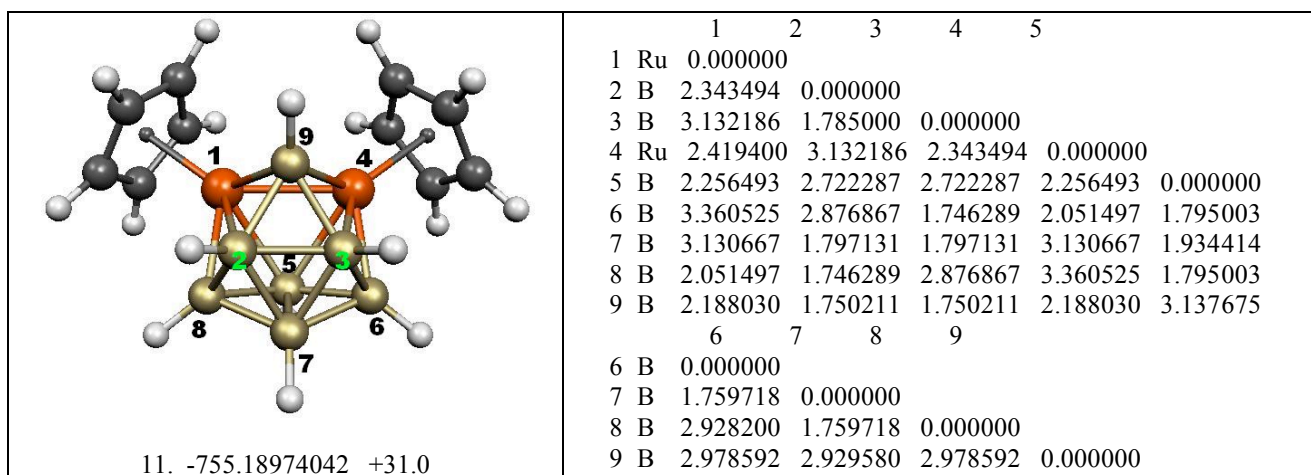


Table S2C. Energy ranking of the Cp₂Ru₂B₇H₇ structures

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole
1	09-Ru-2-PressCapCube_j_r-45-295	-755.23909887	0.00
2	09-Ru-2-PressCapCube_a_r-295	-755.23909886	0.00
3	09-Ru-2-PressCapCube_j_r-58-295	-755.23909886	0.00
4	09-Ru-1-CapCube_f	-755.23909885	0.00
5	09-Ru-2-PressCapCube_j_r-520	-755.23909884	0.00
6	09-Ru-3-TI99-b	-755.23909884	0.00
7	09-Ru-3-TI99-c	-755.22461710	9.09
8	09-Ru-3-TI99-m	-755.20969883	18.45
9	09-Ru-4-TrTrPr_e	-755.20969881	18.45
10	09-Ru-structure-5-ch3	-755.20352898	22.32
11	09-Ru-structure-f4	-755.20352898	22.32
12	09-Ru-Bipyr-hept3	-755.20230649	23.09
13	09-Ru-2-PressCapCube_f	-755.19992343	24.58
14	09-Ru-3-TI99-j_r-144	-755.19955932	24.81
15	09-Ru-3-TI99-g	-755.19717078	26.31
16	09-Ru-1-CapCube_b	-755.19717077	26.31
17	09-Ru-2-PressCapCube_j_r-178-70	-755.19610313	26.98
18	09-Ru-2-PressCapCube_j_r-62-70	-755.19610313	26.98
19	09-Ru-2-PressCapCube_j_r-566-70	-755.19610312	26.98
20	09-Ru-1-CapCube_d	-755.19540873	27.42
21	09-Ru-1-CapCube_g	-755.19540873	27.42
22	09-Ru-1-CapCube_i	-755.19385153	28.39
23	09-Ru-structure-1	-755.19377601	28.44
24	09-Ru-2-PressCapCube_e_r-340	-755.19377600	28.44
25	09-Ru-3-TI99-a-	-755.19034560	30.59
26	09-Ru-1-CapCube_c	-755.18974042	30.97
27	09-Ru-2-PressCapCube_j_r-530	-755.18974042	30.97
28	09-Ru-2-PressCapCube_j_r-91	-755.18974042	30.97
29	09-Ru-2-PressCapCube_j_r-59	-755.18974042	30.97
30	09-Ru-3-TI99-e	-755.18974042	30.97
31	09-Ru-4-TrTrPr_a	-755.18974042	30.97
32	09-Ru-4-TrTrPr_d_r-158	-755.18974042	30.97
33	09-Ru-4-TrTrPr_d_r-29	-755.18974042	30.97
34	09-Ru-2-PressCapCube_e_i-340	-755.18939515	31.19
35	09-Ru-2-PressCapCube_h	-755.18649186	33.01
36	09-Ru-3-TI99-i	-755.18488766	34.02
37	09-Ru-4-TrTrPr_c	-755.17441952	40.59
38	09-Ru-2-PressCapCube_n	-755.17366258	41.06
39	09-Ru-1-CapCube_h	-755.17231461	41.91
40	09-Ru-4-TrTrPr_f_r-160	-755.17122513	42.59
41	09-Ru-3-TI99-d_r-16-158-81	-755.17031968	43.16

42	09-Ru-3-Tl99-d_r-196-93	-755.17031965	43.16
43	09-Ru-3-Tl99-d_r-196-31	-755.17031965	43.16
44	09-Ru-3-Tl99-d_r-32-176	-755.17031965	43.16
45	09-Ru-3-Tl99-d_r-16-158-48	-755.17031965	43.16
46	09-Ru-1-CapCube_e	-755.17031964	43.16
47	09-Ru-4-TrTrPr_d imag	-755.16665698	45.46
48	09-Ru-4-TrTrPr_f i-160	-755.16559481	46.12
49	09-Ru-2-PressCapCube_l	-755.16511373	46.43
50	09-Ru-2-PressCapCube_i	-755.16085100	49.10
51	09-Ru-2-PressCapCube_c	-755.15409989	53.34
52	09-Ru-2-PressCapCube_j_r-566-360	-755.15409989	53.34
53	09-Ru-2-PressCapCube_j_r-178-360	-755.15409989	53.34
54	09-Ru-2-PressCapCube_j_r-62-360	-755.15409989	53.34
55	09-Ru-4-TrTrPr_b	-755.15409989	53.34
56	09-Ru-3-Tl99-k_r-49	-755.15298130	54.04
57	09-Ru-3-Tl99-j i-144	-755.15139667	55.03
58	09-Ru-3-Tl99-f	-755.15115205	55.19
59	09-Ru-3-Tl99-k_r-221	-755.15080678	55.40
60	09-Ru-2-PressCapCube_g	-755.14660298	58.04
61	09-Ru-3-Tl99-h	-755.14276478	60.45
62	09-Ru-1-CapCube_a	-755.14276477	60.45
63	09-Ru-2-PressCapCube_m	-755.14248991	60.62
64	09-Ru-2-PressCapCube_k	-755.13862112	63.05
65	09-Ru-3-Tl99-l_r-655	-755.13314471	66.49
66	09-Ru-3-Tl99-d_r-16-158 imag	-755.13209352	67.15
67	09-Ru-3-Tl99-d_r-196	-755.13157174	67.47
68	09-Ru-3-Tl99-d_r-32 i-176	-755.13148898	67.53
69	09-Ru-3-Tl99-d_r-16-40 i-176	-755.13148467	67.53
70	09-Ru-3-Tl99-d_r-16 imag	-755.13122407	67.69
71	09-Ru-2-PressCapCube_j_r-58 i-295	-755.13099849	67.83
72	09-Ru-2-PressCapCube_a i-295	-755.13099848	67.83
73	09-Ru-2-PressCapCube_j_r-45 i-295	-755.13099848	67.83
74	09-Ru-2-PressCapCube_d	-755.12975981	68.61
75	09-Ru-3-Tl99-d imag	-755.12969808	68.65
76	09-Ru-2-PressCapCube_o	-755.12804650	69.69
77	09-Ru-2-PressCapCube_b	-755.12326473	72.69
78	09-Ru-Bipyr-hept1	-755.12130343	73.92
79	09-Ru-Bipyr-hept2	-755.11956666	75.01
80	09-Ru-3-Tl99-l i-655	-755.09151406	92.61
81	09-Ru-3-Tl99-k imag	-755.08279867	98.08
82	09-Ru-2-PressCapCube_j_r-178 imag	-755.04601606	121.16
83	09-Ru-2-PressCapCube_j_r-62 imag	-755.04601606	121.16
84	09-Ru-2-PressCapCube_j_r-566 imag	-755.04601605	121.16
85	09-Ru-3-Tl99-a	-755.03436909	128.47
86	09-Ru-2-PressCapCube_j imag	-754.97413669	166.26

The 10-vertex $\text{Cp}_2\text{Ru}_2\text{B}_8\text{H}_8$ Structures

Table S3A. Initial structures

Table S3B. Lowest energy structure distances

Table S3C. Global ranking of all structures

Table S3A. Initial $\text{Cp}_2\text{Ru}_2\text{B}_8\text{H}_8$ structures (one example from each family) 62 structures in total

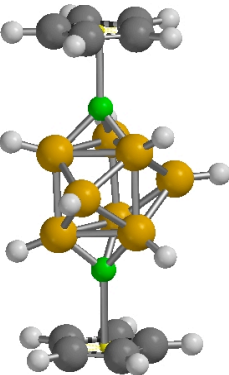
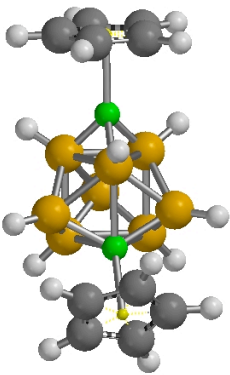
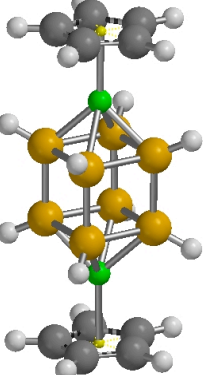
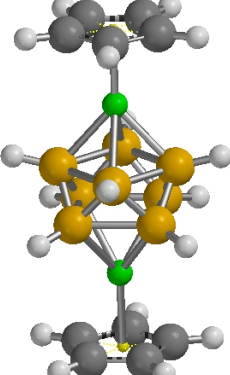
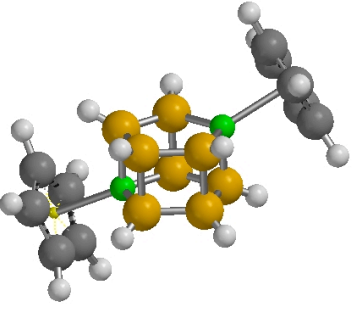
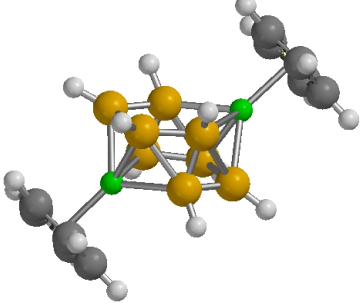
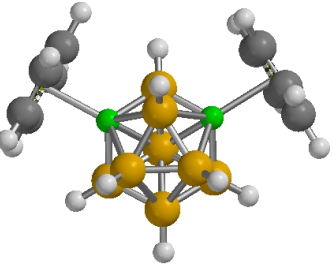
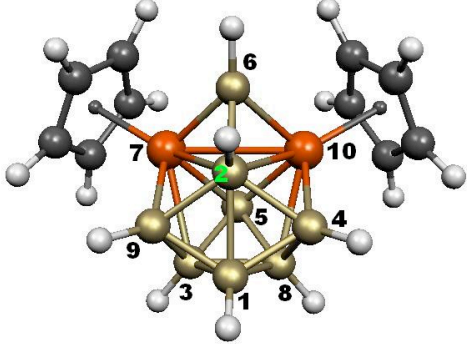
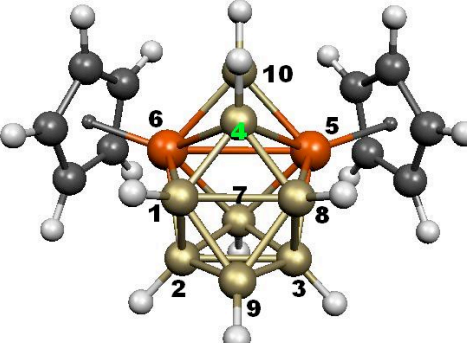
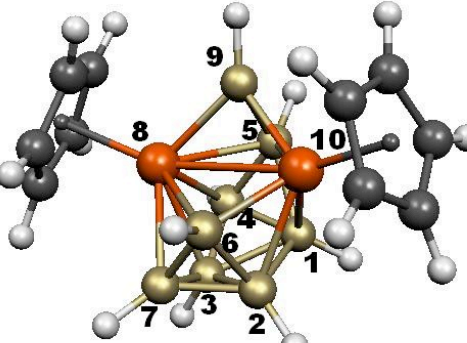
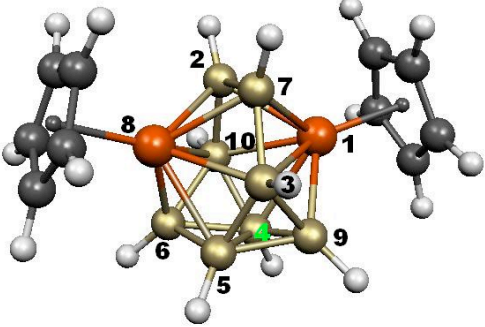
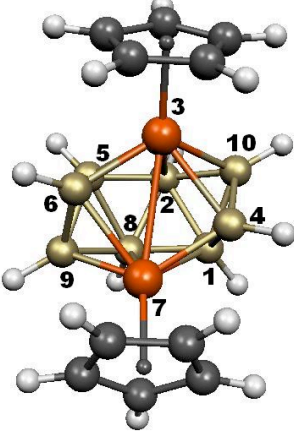
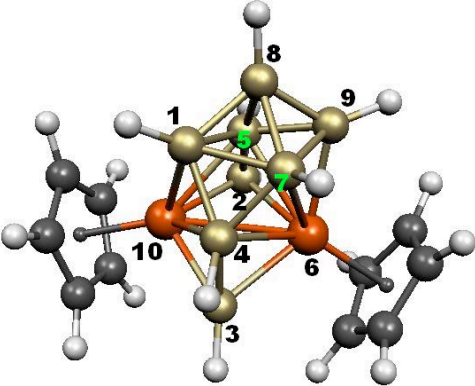
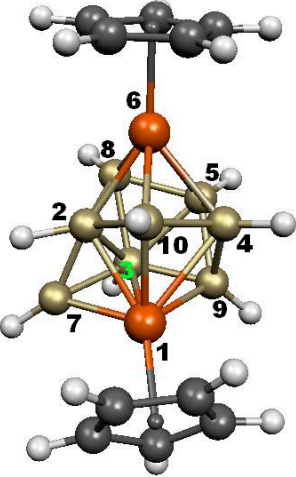
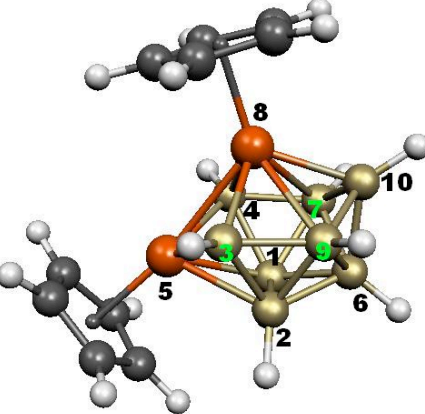
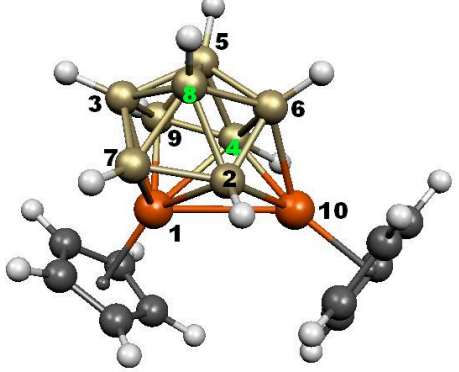
<p>Initial structures</p>	 <p>1. Tetracapped trigonal prism (C_{2v}) 16</p>
 <p>2. Tetracapped trigonal prism (C_{3v}) 9</p>	 <p>3. Bicapped cube 8</p>
 <p>4. Bicapped square antiprism 7</p>	 <p>5. Pentagonal prism 5</p>
 <p>6. Pentagonal antiprism 5</p>	 <p>7. Isocloso structure 12</p>

Table S3B. Distance table for the lowest energy Cp₂Ru₂B₈H₈ structures

 <p>1. -780.71376957 0.0 kcal/mole Cs</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.972300</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.784489</td><td>2.719156</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.748677</td><td>1.839151</td><td>2.889244</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.914655</td><td>3.003423</td><td>1.789502</td><td>2.966391</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.627249</td><td>1.841428</td><td>3.681823</td><td>3.079926</td><td>3.116466</td></tr> <tr><td>7 Ru</td><td>3.152953</td><td>2.305427</td><td>2.312358</td><td>3.521707</td><td>2.129254</td></tr> <tr><td>8 B</td><td>1.784418</td><td>2.719065</td><td>1.776400</td><td>1.756515</td><td>1.789525</td></tr> <tr><td>9 B</td><td>1.748677</td><td>1.839151</td><td>1.756609</td><td>2.962200</td><td>2.966391</td></tr> <tr><td>10 Ru</td><td>3.152953</td><td>2.305427</td><td>3.204425</td><td>2.048400</td><td>2.129254</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Ru</td><td>2.044644</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.681754</td><td>3.204389</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.079926</td><td>2.048400</td><td>2.889186</td><td>0.000000</td><td></td></tr> <tr><td>10 Ru</td><td>2.044644</td><td>2.770400</td><td>2.312309</td><td>3.521707</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.972300	0.000000				3 B	1.784489	2.719156	0.000000			4 B	1.748677	1.839151	2.889244	0.000000		5 B	2.914655	3.003423	1.789502	2.966391	0.000000	6 B	3.627249	1.841428	3.681823	3.079926	3.116466	7 Ru	3.152953	2.305427	2.312358	3.521707	2.129254	8 B	1.784418	2.719065	1.776400	1.756515	1.789525	9 B	1.748677	1.839151	1.756609	2.962200	2.966391	10 Ru	3.152953	2.305427	3.204425	2.048400	2.129254		6	7	8	9	10	6 B	0.000000					7 Ru	2.044644	0.000000				8 B	3.681754	3.204389	0.000000			9 B	3.079926	2.048400	2.889186	0.000000		10 Ru	2.044644	2.770400	2.312309	3.521707	0.000000
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9 B	3.366948	2.883868	1.790640	0.000000																																																																																																			
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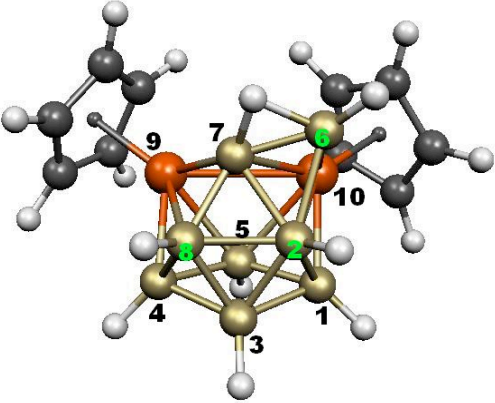
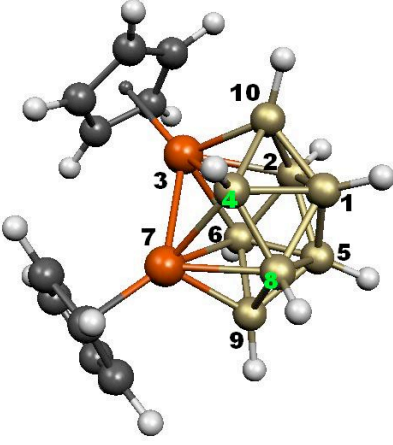
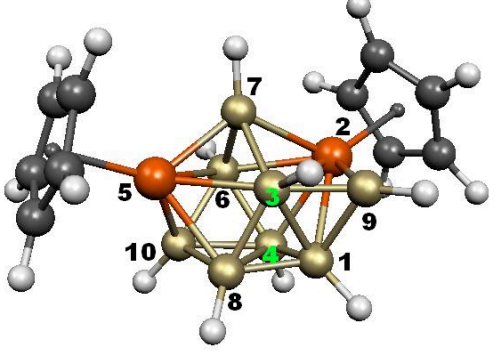
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 <p>11. -780.66831913 +28.5 C₂</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.811467</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Ru</td><td>3.086430</td><td>2.275490</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.850618</td><td>2.721343</td><td>2.353190</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.789576</td><td>1.786482</td><td>3.361821</td><td>2.860819</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.860819</td><td>1.759209</td><td>2.223939</td><td>3.044067</td><td>1.850618</td></tr> <tr><td>7 Ru</td><td>3.361821</td><td>3.358841</td><td>2.396652</td><td>2.223939</td><td>3.086430</td></tr> <tr><td>8 B</td><td>1.786482</td><td>2.821250</td><td>3.358841</td><td>1.759209</td><td>1.811467</td></tr> <tr><td>9 B</td><td>2.983015</td><td>2.975712</td><td>3.440647</td><td>3.012100</td><td>1.745895</td></tr> <tr><td>10 B</td><td>1.745895</td><td>1.780880</td><td>2.017858</td><td>1.856973</td><td>2.983015</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Ru</td><td>2.353190</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.721343</td><td>2.275490</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.856973</td><td>2.017858</td><td>1.780880</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.012100</td><td>3.440647</td><td>2.975712</td><td>3.870931</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.811467	0.000000				3 Ru	3.086430	2.275490	0.000000			4 B	1.850618	2.721343	2.353190	0.000000		5 B	1.789576	1.786482	3.361821	2.860819	0.000000	6 B	2.860819	1.759209	2.223939	3.044067	1.850618	7 Ru	3.361821	3.358841	2.396652	2.223939	3.086430	8 B	1.786482	2.821250	3.358841	1.759209	1.811467	9 B	2.983015	2.975712	3.440647	3.012100	1.745895	10 B	1.745895	1.780880	2.017858	1.856973	2.983015		6	7	8	9	10	6 B	0.000000					7 Ru	2.353190	0.000000				8 B	2.721343	2.275490	0.000000			9 B	1.856973	2.017858	1.780880	0.000000		10 B	3.012100	3.440647	2.975712	3.870931	0.000000
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Table S3C Energy ranking of the $\text{Cp}_2\text{Ru}_2\text{B}_8\text{H}_8$ structures

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole
1	10-Ru-1-TetrTriPri1-e	-780.71376957	0.00
2	10-Ru-2-TetrTriPri2_c	-780.71376957	0.00
3	10-Ru-2-TetrTriPri2_d	-780.71376957	0.00
4	10-Ru-7-Isocloso-i	-780.71376956	0.00
5	10-Ru-1-TetrTriPri1-i	-780.70044535	8.36
6	10-Ru-5-PentagPrism-b	-780.69577525	11.29
7	10-Ru-2-TetrTriPri2_f	-780.68713236	16.71
8	10-Ru-1-TetrTriPri1-l	-780.68713235	16.71
9	10-Ru-7-Isocloso-c	-780.68713235	16.71
10	10-Ru-structure-2	-780.68713235	16.71
11	10-Ru-3-BicapCub_g	-780.68027389	21.02
12	10-Ru-3-BicapCub_b	-780.67970267	21.38
13	10-Ru-6-AntiPr-d	-780.67970267	21.38
14	10-Ru-7-Isocloso-k	-780.67258719	25.84
15	10-Ru-2-TetrTriPri2_h	-780.67258707	25.84
16	10-Ru-7-Isocloso-b	-780.67256369	25.86
17	10-Ru-2-TetrTriPri2_e	-780.67142058	26.57
18	10-Ru-5-PentagPrism-a	-780.66957763	27.73
19	10-Ru-4-BicapSqAntipr-f	-780.66831913	28.52
20	10-Ru-7-Isocloso-j	-780.66828079	28.54
21	10-Ru-7-Isocloso-l_r-18	-780.66828079	28.54
22	10-Ru-7-Isocloso-l_r-189	-780.66828078	28.54
23	10-Ru-1-TetrTriPri1-j	-780.66719501	29.23
24	10-Ru-6-AntiPr-e	-780.66719496	29.23
25	10-Ru-1-TetrTriPri1-h	-780.66615832	29.88
26	10-Ru-1-TetrTriPri1-o	-780.66278476	31.99
27	10-Ru-5-PentagPrism-c	-780.66278475	31.99
28	10-Ru-1-TetrTriPri1-f	-780.66083248	33.22
29	10-Ru-5-PentagPrism-e	-780.66059464	33.37
30	10-Ru-1-TetrTriPri1-g	-780.66016175	33.64
31	10-Ru-1-TetrTriPri1-n	-780.65926036	34.20
32	10-Ru-2-TetrTriPri2_g_r-20	-780.65898373	34.38
33	10-Ru-2-TetrTriPri2_g_r-152	-780.65898372	34.38
34	10-Ru-2-TetrTriPri2_g_i-152-20	-780.65769755	35.19
35	10-Ru-3-BicapCub_h	-780.65515020	36.78
36	10-Ru-4-BicapSqAntipr-e_r-98-17	-780.65352165	37.81
37	10-Ru-4-BicapSqAntipr-e_r-98	-780.65286149	38.22
38	10-Ru-6-AntiPr-c	-780.64987845	40.09
39	10-Ru-3-BicapCub_e	-780.64987782	40.09
40	10-Ru-1-TetrTriPri1-c	-780.64708309	41.85

41	10-Ru-6-AntiPr-b	-780.64509424	43.09
42	10-Ru-1-TetrTriPri1-d	-780.64413085	43.70
43	10-Ru-2-TetrTriPri2_a	-780.64256418	44.68
44	10-Ru-7-Isocloso-a	-780.64256418	44.68
45	10-Ru-5-PentagPrism-d	-780.64252186	44.71
46	10-Ru-4-BicapSqAntipr-g	-780.64102700	45.65
47	10-Ru-7-Isocloso-h	-780.64102697	45.65
48	10-Ru-1-TetrTriPri1-b	-780.64021436	46.16
49	10-Ru-1-TetrTriPri1-p	-780.64010083	46.23
50	10-Ru-4-BicapSqAntipr-b	-780.63822484	47.40
51	10-Ru-7-Isocloso-f	-780.63815645	47.45
52	10-Ru-1-TetrTriPri1-m	-780.63375820	50.21
53	10-Ru-7-Isocloso-g	-780.63371452	50.23
54	10-Ru-4-BicapSqAntipr-d	-780.63371451	50.23
55	10-Ru-4-BicapSqAntipr-a	-780.63299180	50.69
56	10-Ru-7-Isocloso-e	-780.63299180	50.69
57	10-Ru-1-TetrTriPri1-k	-780.62308168	56.91
58	10-Ru-7-Isocloso-d	-780.62200365	57.58
59	10-Ru-4-BicapSqAntipr-e_r-57	-780.62200364	57.58
60	10-Ru-7-Isocloso-l imag	-780.62160644	57.83
61	10-Ru-4-BicapSqAntipr-e imag	-780.62160206	57.84
62	10-Ru-2-TetrTriPri2_i_r-116	-780.61890797	59.53
63	10-Ru-2-TetrTriPri2_i_i-116	-780.61678901	60.86
64	10-Ru-3-BicapCub_d	-780.60999390	65.12
65	10-Ru-6-AntiPr-a	-780.60990119	65.18
66	10-Ru-3-BicapCub_a	-780.59182375	76.52
67	10-Ru-3-BicapCub_f	-780.59034043	77.45
68	10-Ru-1-TetrTriPri1-a	-780.58797781	78.93
69	10-Ru-3-BicapCub_c	-780.56571140	92.91
70	10-Ru-4-BicapSqAntipr-c	-780.56089687	95.93
71	10-Ru-Bipypr-octag	-780.54853452	103.68

The 11-vertex $\text{Cp}_2\text{Ru}_2\text{B}_9\text{H}_9$ Structures

Table S4A. Initial structures

Table S4B. Distances in the lowest energy structures.

Table S4C. Global ranking of all structures

Table S4A. Initial $\text{Cp}_2\text{Re}_2\text{B}_9\text{H}_9$ structures (one example from each family) 89 structures in total

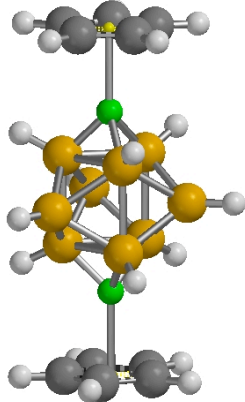
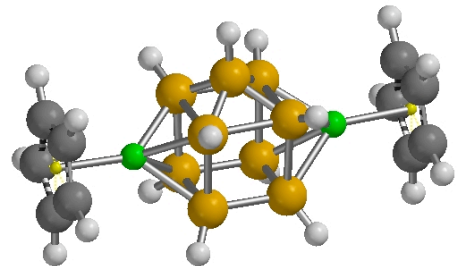
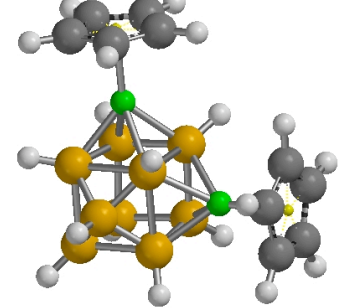
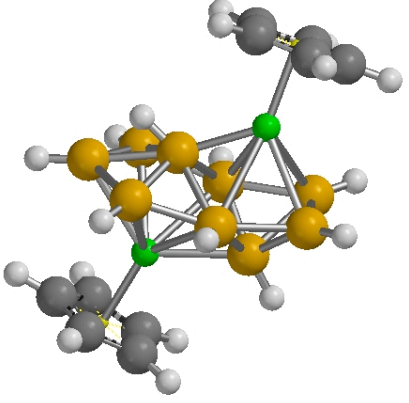
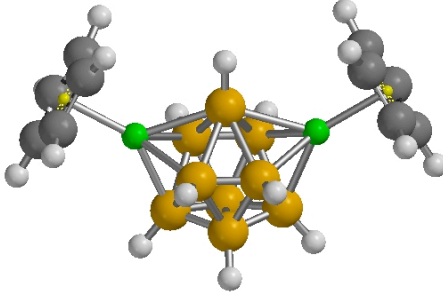
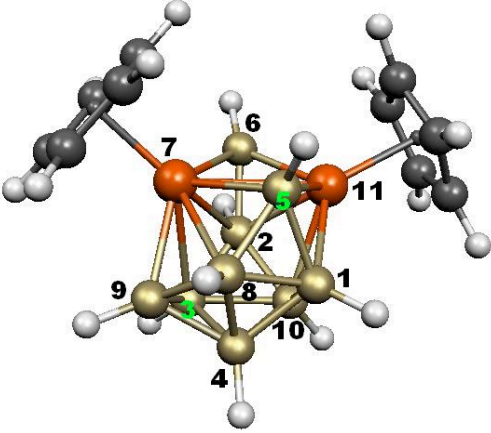
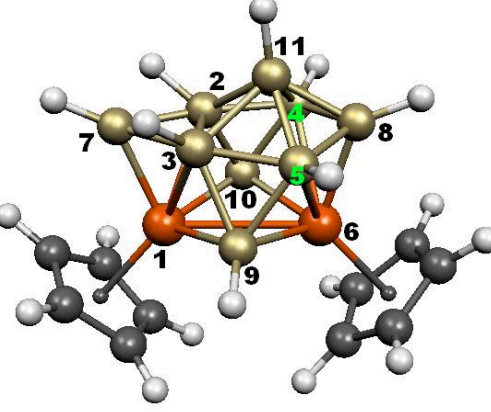
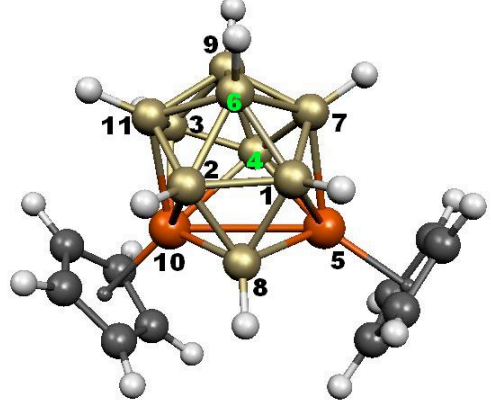
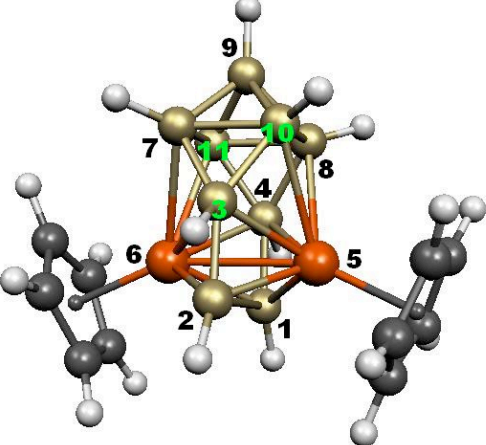
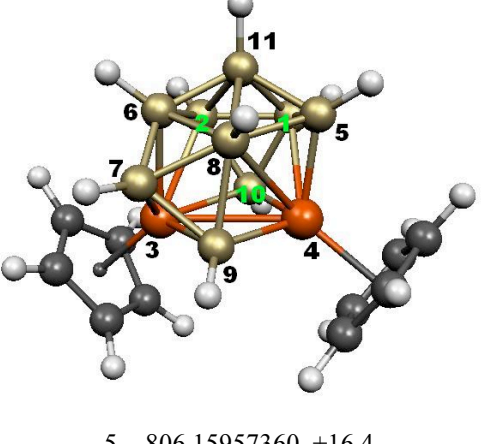
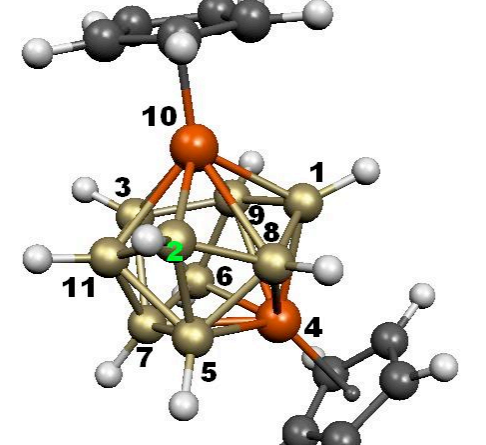
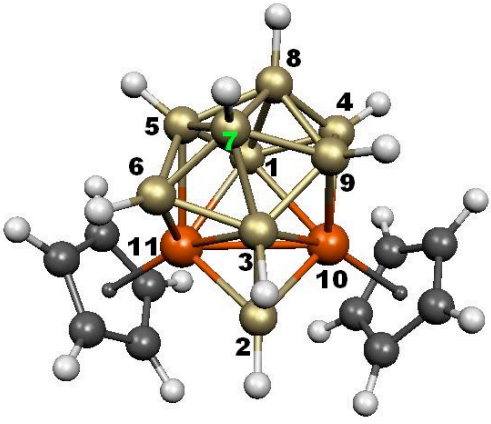
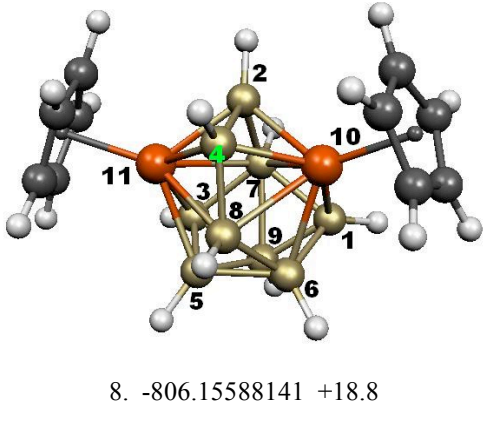
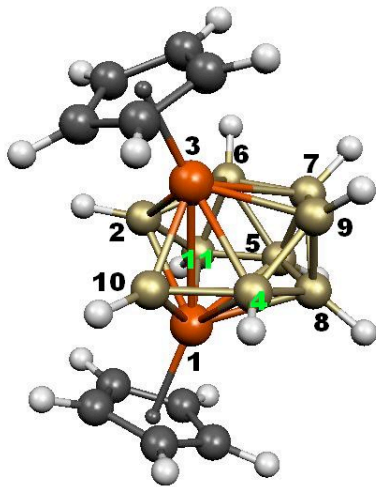
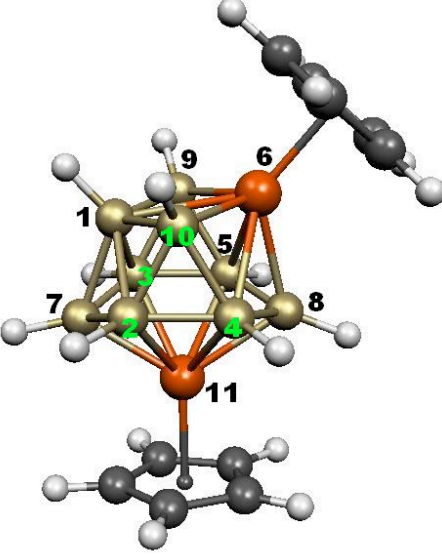
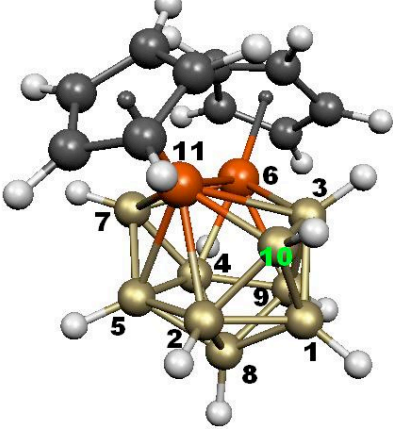
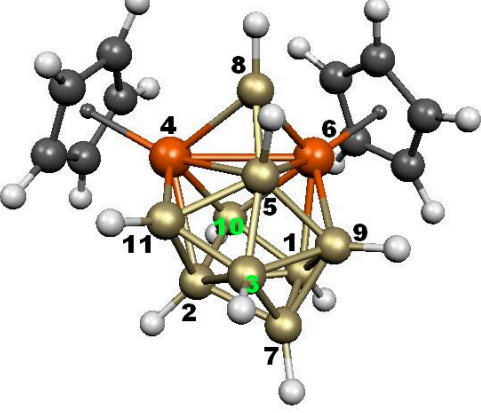
<p style="text-align: center;">Initial structures</p>	 <p style="text-align: center;">1. Pentacapped trigonal prism 11 structures</p>
 <p style="text-align: center;">2a. Tricapped cubeA (C_{2v}) 18 structures</p>	 <p style="text-align: center;">2b. Tricapped cubeA (C_{3v}) 16 structures</p>
 <p style="text-align: center;">3. Octahedron fused to pentagonal bipyramid 24 structures</p>	 <p style="text-align: center;">4. Edge-coalesced icosahedrons (icosahedron without a vertex) 20 structures</p>

Table S4B Distance table for the lowest energy $Cp_2Ru_2B_9H_9$ structures

 <p>1. -806.18577798 0.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.879232</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.904612</td><td>1.667209</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.801954</td><td>2.825829</td><td>1.819653</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.812285</td><td>3.094118</td><td>3.465630</td><td>2.981294</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.774689</td><td>1.621804</td><td>3.099274</td><td>4.183330</td><td>3.225677</td></tr> <tr><td>7 Ru</td><td>3.124955</td><td>2.238792</td><td>2.429385</td><td>3.120504</td><td>2.221184</td></tr> <tr><td>8 B</td><td>1.775871</td><td>3.302953</td><td>2.767569</td><td>1.801049</td><td>1.740453</td></tr> <tr><td>9 B</td><td>2.882319</td><td>2.942458</td><td>1.729133</td><td>1.725402</td><td>3.034798</td></tr> <tr><td>10 B</td><td>1.796572</td><td>1.724790</td><td>1.896858</td><td>1.817258</td><td>3.012434</td></tr> <tr><td>11 Ru</td><td>2.250886</td><td>2.110714</td><td>3.344389</td><td>3.455689</td><td>2.088379</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Ru</td><td>2.258152</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>4.056614</td><td>2.382126</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.950243</td><td>2.181681</td><td>1.713598</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.128218</td><td>3.188551</td><td>2.871527</td><td>2.941475</td><td>0.000000</td></tr> <tr><td>11 Ru</td><td>2.093811</td><td>2.825805</td><td>3.263641</td><td>3.941333</td><td>2.266609</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.879232	0.000000				3 B	2.904612	1.667209	0.000000			4 B	1.801954	2.825829	1.819653	0.000000		5 B	1.812285	3.094118	3.465630	2.981294	0.000000	6 B	3.774689	1.621804	3.099274	4.183330	3.225677	7 Ru	3.124955	2.238792	2.429385	3.120504	2.221184	8 B	1.775871	3.302953	2.767569	1.801049	1.740453	9 B	2.882319	2.942458	1.729133	1.725402	3.034798	10 B	1.796572	1.724790	1.896858	1.817258	3.012434	11 Ru	2.250886	2.110714	3.344389	3.455689	2.088379		6	7	8	9	10	6 B	0.000000					7 Ru	2.258152	0.000000				8 B	4.056614	2.382126	0.000000			9 B	3.950243	2.181681	1.713598	0.000000		10 B	3.128218	3.188551	2.871527	2.941475	0.000000	11 Ru	2.093811	2.825805	3.263641	3.941333	2.266609
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5 Ru	2.152051	2.155666	2.181881	2.181874	0.000000																																																																																																														
6 Ru	2.149818	2.146709	2.183091	2.182776	2.721608																																																																																																														
7 B	3.987951	3.170626	1.704791	2.914080	3.359401																																																																																																														
8 B	3.170990	3.986102	2.911874	1.705782	2.508393																																																																																																														
9 B	4.306285	4.305970	2.802958	2.803383	3.585598																																																																																																														
10 B	3.986695	3.172904	1.705335	2.913727	2.510649																																																																																																														
11 B	3.172822	3.987663	2.914679	1.704629	3.359228																																																																																																														
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6 Ru	0.000000																																																																																																																		
7 B	2.517504	0.000000																																																																																																																	
8 B	3.362063	2.664686	0.000000																																																																																																																
9 B	3.592265	1.693719	1.693393	0.000000																																																																																																															
10 B	3.362587	1.828225	1.936401	1.692500	0.000000																																																																																																														
11 B	2.519030	1.940602	1.828044	1.692865	2.664425																																																																																																														
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 <p>8. -806.15588141 +18.8</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.075183</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.927400</td><td>3.075183</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.603561</td><td>1.826179</td><td>3.603561</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.925434</td><td>3.504426</td><td>1.769066</td><td>3.119365</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.769066</td><td>3.504426</td><td>2.925434</td><td>3.119365</td><td>1.854400</td></tr> <tr><td>7 B</td><td>1.845113</td><td>1.825506</td><td>1.845113</td><td>2.977321</td><td>2.704091</td></tr> <tr><td>8 B</td><td>2.979264</td><td>2.864241</td><td>2.979264</td><td>1.743549</td><td>1.750163</td></tr> <tr><td>9 B</td><td>1.722242</td><td>3.581416</td><td>1.722242</td><td>3.928777</td><td>1.794848</td></tr> <tr><td>10 Ru</td><td>2.042974</td><td>2.127671</td><td>3.739447</td><td>2.113732</td><td>3.379770</td></tr> <tr><td>11 Ru</td><td>3.739447</td><td>2.127671</td><td>2.042974</td><td>2.113732</td><td>2.282269</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.704091</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.750163</td><td>2.928975</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.794848</td><td>2.017861</td><td>2.856745</td><td>0.000000</td><td></td></tr> <tr><td>10 Ru</td><td>2.282269</td><td>2.405815</td><td>2.305544</td><td>3.219728</td><td>0.000000</td></tr> <tr><td>11 Ru</td><td>3.379770</td><td>2.405815</td><td>2.305544</td><td>3.219728</td><td>3.351000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.075183	0.000000				3 B	2.927400	3.075183	0.000000			4 B	3.603561	1.826179	3.603561	0.000000		5 B	2.925434	3.504426	1.769066	3.119365	0.000000	6 B	1.769066	3.504426	2.925434	3.119365	1.854400	7 B	1.845113	1.825506	1.845113	2.977321	2.704091	8 B	2.979264	2.864241	2.979264	1.743549	1.750163	9 B	1.722242	3.581416	1.722242	3.928777	1.794848	10 Ru	2.042974	2.127671	3.739447	2.113732	3.379770	11 Ru	3.739447	2.127671	2.042974	2.113732	2.282269		6	7	8	9	10	6 B	0.000000					7 B	2.704091	0.000000				8 B	1.750163	2.928975	0.000000			9 B	1.794848	2.017861	2.856745	0.000000		10 Ru	2.282269	2.405815	2.305544	3.219728	0.000000	11 Ru	3.379770	2.405815	2.305544	3.219728	3.351000
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3 B	1.860846	2.780893	0.000000																																																																																																																
4 B	2.811431	2.686835	2.670265	0.000000																																																																																																															
5 B	2.978780	1.746235	3.324107	1.724956	0.000000																																																																																																														
6 Ru	3.579472	3.906784	2.246811	2.018559	3.306782																																																																																																														
7 B	3.878628	3.130103	3.276410	1.725694	1.800191																																																																																																														
8 B	1.783907	1.783371	2.837792	1.727664	1.863277																																																																																																														
9 B	1.767426	2.849302	1.764465	1.790225	2.973328																																																																																																														
10 B	1.719885	1.782284	1.790978	3.375611	3.064029																																																																																																														
11 Ru	3.140022	2.318870	2.449200	2.804505	2.296323																																																																																																														
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6 Ru	0.000000																																																																																																																		
7 B	2.207674	0.000000																																																																																																																	
8 B	3.413646	3.077388	0.000000																																																																																																																
9 B	2.336209	3.243158	1.777738	0.000000																																																																																																															
10 B	3.645494	3.656680	2.910395	2.897138	0.000000																																																																																																														
11 Ru	2.859238	2.078411	3.290790	3.382989	2.057855																																																																																																														
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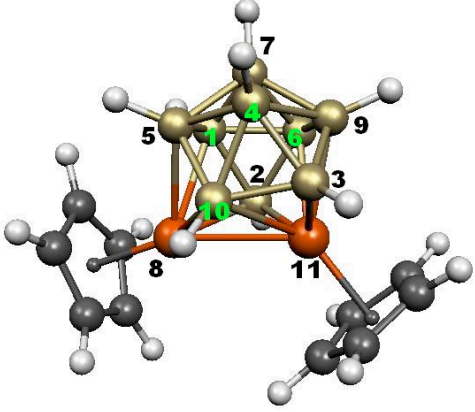
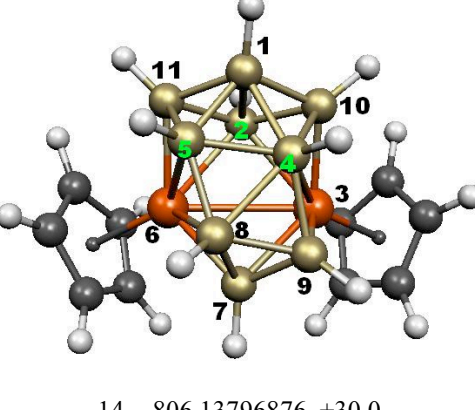
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Table 4C. Energy ranking of the $Cp_2Ru_2B_9H_9$ structures

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole
1	11-Ru-2-TricapCubeA-e	-806.18577798	0.00
2	11-Ru-4-Icos-1vx-l_r-10-53	-806.17167862	8.85
3	11-Ru-1-PentaCapTrPr-f	-806.17167861	8.85
4	11-Ru-4-Icos-1vx-l_r-47-225	-806.17167861	8.85
5	11-Ru-4-Icos-1vx-l_r-47-33	-806.17146474	8.98
6	11-Ru-4-Icos-1vx-l_r-47 i	-806.17015438	9.80
7	11-Ru-4-Icos-1vx-o	-806.16658996	12.04
8	11-Ru-1-PentaCapTrPr-c	-806.16592762	12.46
9	11-Ru-3-OhfusetopentBipyr-o	-806.16244262	14.64
10	11-Ru-1-PentaCapTrPr-d	-806.15957922	16.44
11	11-Ru-2-TricapCubeA-q	-806.15957361	16.44
12	11-Ru-2-TricapCubeA-k	-806.15957360	16.44
13	11-Ru-2-TricapCubeB-g	-806.15957359	16.44
14	11-Ru-2-TricapCubeB-j	-806.15798640	17.44
15	11-Ru-4-Icos-1vx-d	-806.15743681	17.78
16	11-Ru-2-TricapCubeA-c	-806.15614275	18.60
17	11-Ru-1-PentaCapTrPr-k	-806.15588141	18.76
18	11-Ru-2-TricapCubeA-j	-806.15193641	21.24
19	11-Ru-1-PentaCapTrPr-j	-806.15074442	21.98
20	11-Ru-2-TricapCubeB-b	-806.15074442	21.98
21	11-Ru-2-TricapCubeB-o	-806.15074442	21.98
22	11-Ru-1-PentaCapTrPr-b	-806.14911142	23.01
23	11-Ru-2-TricapCubeB-p	-806.14813148	23.62
24	11-Ru-1-PentaCapTrPr-e	-806.14736585	24.10
25	11-Ru-4-Icos-1vx-l_r-10 i-53	-806.14631573	24.76
26	11-Ru-4-Icos-1vx-l imag	-806.14566785	25.17
27	11-Ru-4-Icos-1vx-c	-806.14064632	28.32
28	11-Ru-2-TricapCubeA-r	-806.14064631	28.32
29	11-Ru-2-TricapCubeA-m	-806.13796876	30.00
30	11-Ru-4-Icos-1vx-i	-806.13632364	31.03
31	11-Ru-2-TricapCubeB-n	-806.13632363	31.03
32	11-Ru-2-TricapCubeA-n	-806.13210259	33.68
33	11-Ru-1-PentaCapTrPr-g_r-9	-806.13019532	34.88
34	11-Ru-1-PentaCapTrPr-g	-806.13019251	34.88
35	11-Ru-2-TricapCubeB-h	-806.12882833	35.74
36	11-Ru-4-Icos-1vx-h_r-152-334	-806.12881419	35.74
37	11-Ru-4-Icos-1vx-p	-806.12881419	35.74
38	11-Ru-Ig-3	-806.12694362	36.92
39	11-Ru-2-TricapCubeA-a	-806.12396186	38.79
40	11-Ru-2-TricapCubeA-p	-806.12396186	38.79
41	11-Ru-2-TricapCubeB-i	-806.12396186	38.79

42	11-Ru-4-Icos-1vx-k	-806.12396186	38.79
43	11-Ru-4-Icos-1vx-r	-806.12396186	38.79
44	11-Ru-2-TricapCubeA-g	-806.12169168	40.21
45	11-Ru-4-Icos-1vx-a_r-59	-806.12111654	40.58
46	11-Ru-2-TricapCubeA-d	-806.12111651	40.58
47	11-Ru-2-TricapCubeB-e	-806.12111650	40.58
48	11-Ru-2-TricapCubeB-k	-806.12111649	40.58
49	11-Ru-4-Icos-1vx-b	-806.11938853	41.66
50	11-Ru-2-TricapCubeA-i	-806.11840841	42.27
51	11-Ru-4-Icos-1vx-a i-59	-806.11748571	42.85
52	11-Ru-2-TricapCubeB-m	-806.11695789	43.18
53	11-Ru-3-OhfusettoPentBipyr-h	-806.11496331	44.44
54	11-Ru-2-TricapCubeB-l	-806.11254322	45.95
55	11-Ru-1-PentaCapTrPr-i	-806.11205559	46.26
56	11-Ru-3-OhfusettoPentBipyr-j	-806.11038951	47.31
57	11-Ru-4-Icos-1vx-h_r-76	-806.11025619	47.39
58	11-Ru-3-OhfusettoPentBipyr-e	-806.10981804	47.66
59	11-Ru-4-Icos-1vx-f	-806.10610709	49.99
60	11-Ru-2-TricapCubeB-c	-806.10522783	50.55
61	11-Ru-3-OhfusettoPentBipyr-w	-806.10483905	50.79
62	11-Ru-3-OhfusettoPentBipyr-f_r-211	-806.10169955	52.76
63	11-Ru-3-OhfusettoPentBipyr-i	-806.10124237	53.05
64	11-Ru-3-OhfusettoPentBipyr-c	-806.09905074	54.42
65	11-Ru-2-TricapCubeB-f	-806.09734474	55.49
66	11-Ru-2-TricapCubeA-f	-806.09637365	56.10
67	11-Ru-4-Icos-1vx-s	-806.09631470	56.14
68	11-Ru-2-TricapCubeA-l	-806.09599142	56.34
69	11-Ru-2-TricapCubeB-a	-806.09500243	56.96
70	11-Ru-3-OhfusettoPentBipyr-l	-806.09438947	57.35
71	11-Ru-3-OhfusettoPentBipyr-lf	-806.09438947	57.35
72	11-Ru-2-TricapCubeA-h	-806.09411876	57.52
73	11-Ru-4-Icos-1vx-g	-806.09221183	58.71
74	11-Ru-3-OhfusettoPentBipyr-m	-806.08781702	61.47
75	11-Ru-3-OhfusettoPentBipyr-g	-806.08743202	61.71
76	11-Ru-4-Icos-1vx-q_r-35	-806.08500130	63.24
77	11-Ru-4-Icos-1vx-q_r-42	-806.08487297	63.32
78	11-Ru-4-Icos-1vx-q i-35-42	-806.08486515	63.32
79	11-Ru-4-Icos-1vx-m	-806.08475709	63.39
80	11-Ru-4-Icos-1vx-e	-806.08355833	64.14
81	11-Ru-3-OhfusettoPentBipyr-s	-806.08261883	64.73
82	11-Ru-4-Icos-1vx-n	-806.08245813	64.83
83	11-Ru-2-TricapCubeB-df	-806.08242324	64.86
84	11-Ru-2-TricapCubeB-d	-806.08223737	64.97
85	11-Ru-4-Icos-1vx-j	-806.08029591	66.19
86	11-Ru-4-Icos-1vx-h_r-195	-806.07611091	68.82

87	11-Ru-4-Icos-1vx-h_r-26	-806.07611091	68.82
88	11-Ru-3-OhfusettoPentBipyr-v	-806.07286410	70.85
89	11-Ru-4-Icos-1vx-t	-806.06952713	72.95
90	11-Ru-3-OhfusettoPentBipyr-a	-806.06816446	73.80
91	11-Ru-3-OhfusettoPentBipyr-x_r-76	-806.05947564	79.25
92	11-Ru-4-Icos-1vx-h_r-15	-806.05870958	79.74
93	11-Ru-4-Icos-1vx-h_r-152 i-334	-806.05870958	79.74
94	11-Ru-1-PentaCapTrPr-a	-806.05657987	81.07
95	11-Ru-3-OhfusettoPentBipyr-n	-806.05372195	82.87
96	11-Ru-3-OhfusettoPentBipyr-k_r-77	-806.04993874	85.24
97	11-Ru-3-OhfusettoPentBipyr-k_r-78_r-368	-806.04993874	85.24
98	11-Ru-3-OhfusettoPentBipyr-k_r-388	-806.04993872	85.24
99	11-Ru-3-OhfusettoPentBipyr-b	-806.04681601	87.20
100	11-Ru-3-OhfusettoPentBipyr-d	-806.03792843	92.78
101	11-Ru-3-OhfusettoPentBipyr-k_r-78 i-368	-806.03628766	93.81
102	11-Ru-3-OhfusettoPentBipyr-f i-211	-806.03079439	97.25
103	11-Ru-3-OhfusettoPentBipyr-x	-806.02845915	98.72
104	11-Ru-3-OhfusettoPentBipyr-r	-806.02670835	99.82
105	11-Ru-3-OhfusettoPentBipyr-k imag	-806.02497022	100.91
106	11-Ru-3-OhfusettoPentBipyr-u	-806.01240318	108.79
107	11-Ru-3-OhfusettoPentBipyr-p	-806.00875599	111.08
108	11-Ru-3-OhfusettoPentBipyr-t	-806.00402102	114.05
109	11-Ru-3-OhfusettoPentBipyr-q	-806.00340763	114.44
110	11-Ru-4-Icos-1vx-h imag	-806.00110243	115.88

The 12-vertex $\text{Cp}_2\text{Ru}_2\text{B}_{10}\text{H}_{10}$ System

Table S5A. Initial structures

Table S5B. Lowest energy structure distances

Table S5C Global ranking of all structures

Table S5A. Initial $\text{Cp}_2\text{Ru}_2\text{B}_{10}\text{H}_{10}$ structures (one example from each family) 22 structures in total

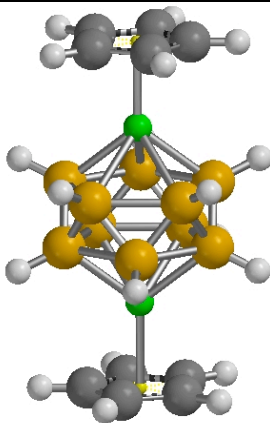
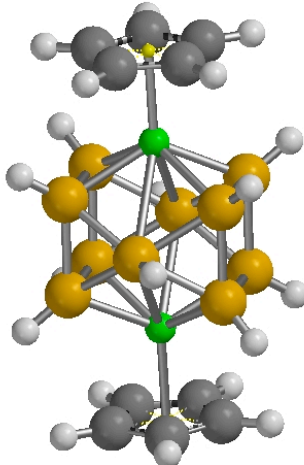
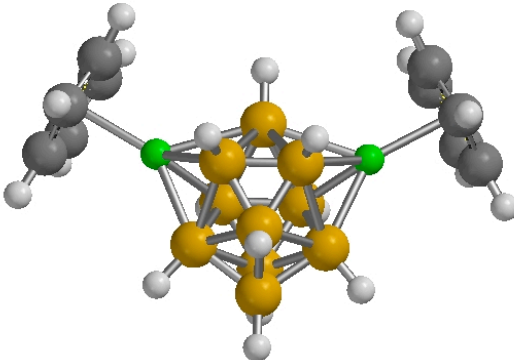
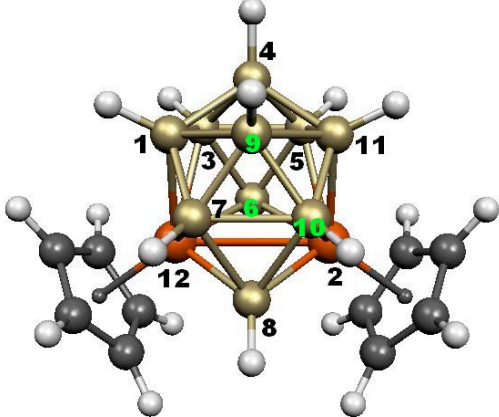
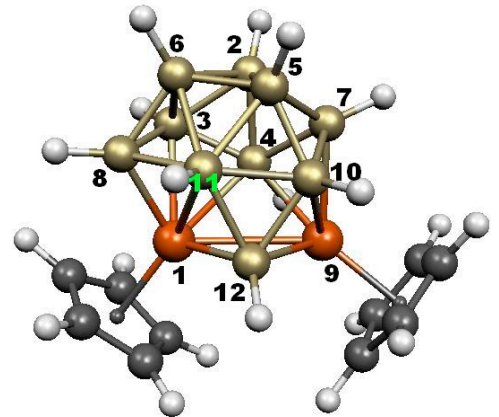
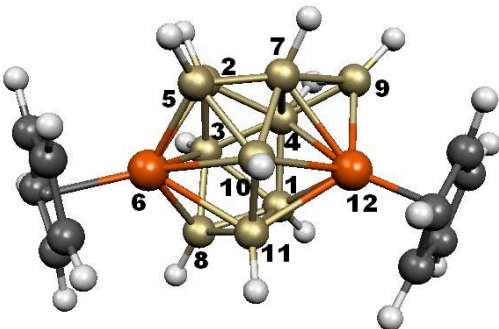
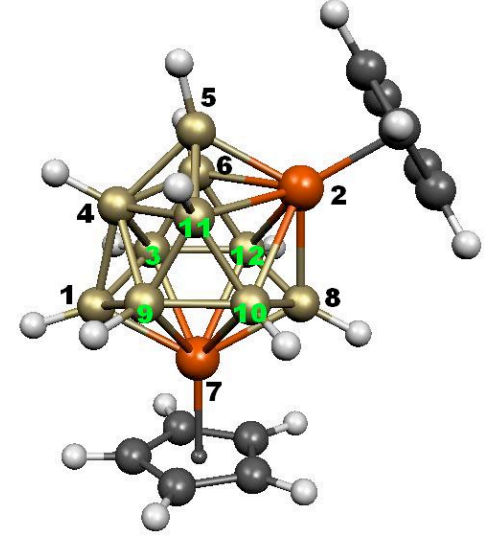
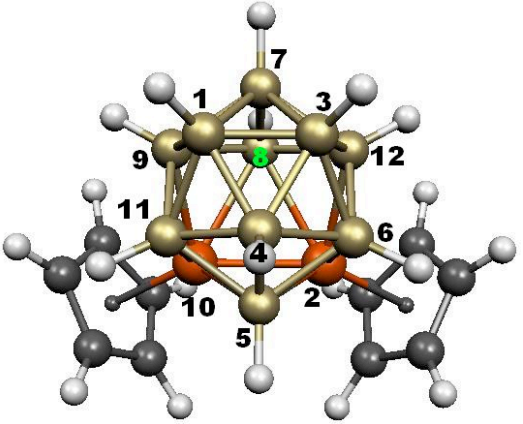
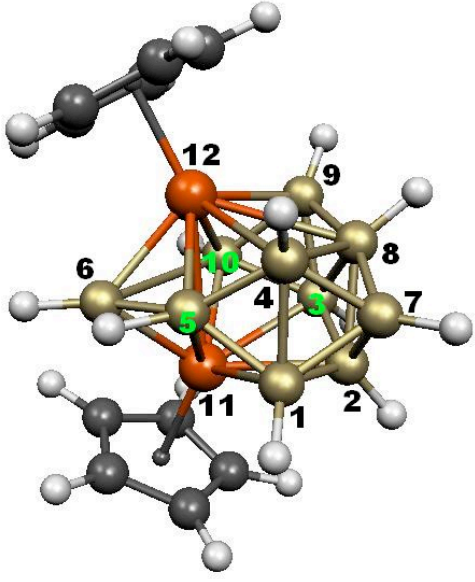
Initial structures
 <p>1. Icosahedron 3 structures</p>
 <p>2. Cubeoctahedron 9 structures</p>
 <p>3. Anticubeoctahedron 10 structures</p>

Table S5B. Distances table for the lowest energy Cp₂Ru₂B₁₀H₁₀ structures

 <p>1. -831.64407734 0.0 kcal/mole C_{2v}</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Ru</td><td>3.645993</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.743253</td><td>3.214187</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.792353</td><td>3.330371</td><td>1.758933</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.912984</td><td>2.226514</td><td>1.888800</td><td>1.758933</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.120228</td><td>2.098316</td><td>1.857324</td><td>3.007100</td><td>1.857324</td></tr> <tr><td>7 B</td><td>1.749812</td><td>3.224543</td><td>3.031668</td><td>2.925792</td><td>3.601930</td></tr> <tr><td>8 B</td><td>3.230406</td><td>2.055600</td><td>3.606285</td><td>3.891948</td><td>3.606285</td></tr> <tr><td>9 B</td><td>1.826906</td><td>3.303362</td><td>2.945269</td><td>1.829595</td><td>2.945269</td></tr> <tr><td>10 B</td><td>2.972729</td><td>2.167882</td><td>3.601930</td><td>2.925792</td><td>3.031668</td></tr> <tr><td>11 B</td><td>2.883600</td><td>2.255975</td><td>2.912984</td><td>1.792353</td><td>1.743253</td></tr> <tr><td>12 Ru</td><td>2.255975</td><td>2.845000</td><td>2.226514</td><td>3.330371</td><td>3.214187</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.562972</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.013239</td><td>2.000236</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.807411</td><td>1.746708</td><td>3.095030</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.562972</td><td>2.002800</td><td>2.000236</td><td>1.746708</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.120228</td><td>2.972729</td><td>3.230406</td><td>1.826906</td><td>1.749812</td></tr> <tr><td>12 Ru</td><td>2.098316</td><td>2.167882</td><td>2.055600</td><td>3.303362</td><td>3.224543</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Ru</td><td>3.645993</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Ru	3.645993	0.000000				3 B	1.743253	3.214187	0.000000			4 B	1.792353	3.330371	1.758933	0.000000		5 B	2.912984	2.226514	1.888800	1.758933	0.000000	6 B	3.120228	2.098316	1.857324	3.007100	1.857324	7 B	1.749812	3.224543	3.031668	2.925792	3.601930	8 B	3.230406	2.055600	3.606285	3.891948	3.606285	9 B	1.826906	3.303362	2.945269	1.829595	2.945269	10 B	2.972729	2.167882	3.601930	2.925792	3.031668	11 B	2.883600	2.255975	2.912984	1.792353	1.743253	12 Ru	2.255975	2.845000	2.226514	3.330371	3.214187		6	7	8	9	10	6 B	0.000000					7 B	3.562972	0.000000				8 B	3.013239	2.000236	0.000000			9 B	3.807411	1.746708	3.095030	0.000000		10 B	3.562972	2.002800	2.000236	1.746708	0.000000	11 B	3.120228	2.972729	3.230406	1.826906	1.749812	12 Ru	2.098316	2.167882	2.055600	3.303362	3.224543		11	12				11 B	0.000000					12 Ru	3.645993	0.000000			
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11 B	2.723200	3.364555	3.058172	1.699800	1.754992																																																																																																																																												
12 B	1.754992	2.308940	1.776344	3.287536	2.837800																																																																																																																																												
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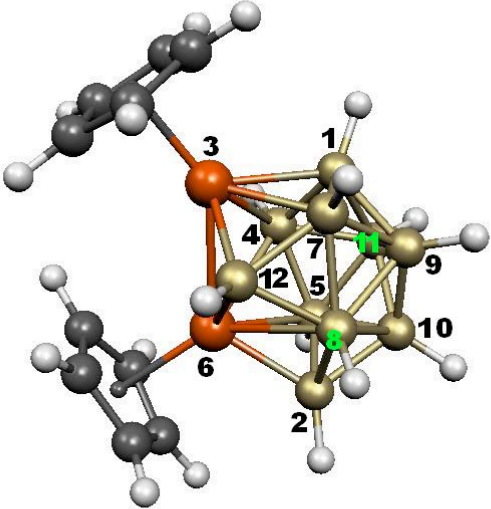
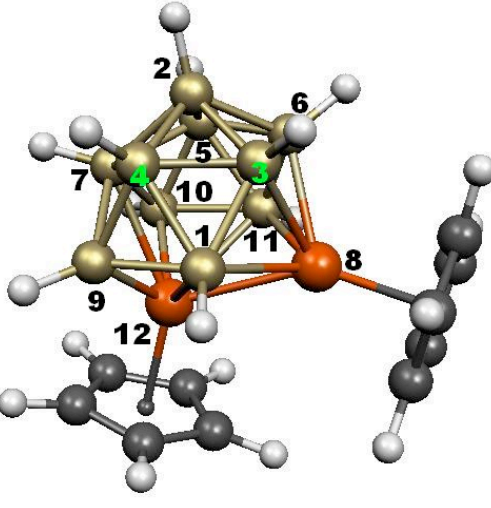
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9 B	1.814608	2.962211	3.405850	2.828903	2.865589																																																																																																																																												
10 B	2.936986	1.737002	4.141003	2.863368	1.801863																																																																																																																																												
11 B	1.788066	2.950792	3.483424	1.753203	1.789862																																																																																																																																												
12 B	3.062024	3.071577	2.066579	3.288088	3.680040																																																																																																																																												
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7 B	3.175715	0.000000																																																																																																																																															
8 B	2.453810	1.891199	0.000000																																																																																																																																														
9 B	3.569365	1.722694	1.860682	0.000000																																																																																																																																													
10 B	3.154281	3.042405	1.946240	1.740865	0.000000																																																																																																																																												
11 B	3.376738	2.909525	2.888319	1.797117	1.762920																																																																																																																																												
12 B	2.182602	1.802175	1.873829	3.059178	3.594331																																																																																																																																												
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 <p>8. -831.59410049 +31.4 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.900521</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.790275</td><td>1.789790</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.828703</td><td>1.734929</td><td>1.787969</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.670105</td><td>1.734929</td><td>2.953245</td><td>3.022000</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.054612</td><td>1.789790</td><td>1.828200</td><td>2.953245</td><td>1.787969</td></tr> <tr><td>7 B</td><td>2.837771</td><td>1.850137</td><td>2.882666</td><td>1.877179</td><td>1.877179</td></tr> <tr><td>8 Ru</td><td>2.177163</td><td>3.329157</td><td>2.190512</td><td>3.384149</td><td>3.384149</td></tr> <tr><td>9 B</td><td>1.801672</td><td>3.018619</td><td>2.965970</td><td>1.753690</td><td>3.504432</td></tr> <tr><td>10 B</td><td>3.667781</td><td>3.018619</td><td>3.790256</td><td>3.504432</td><td>1.753690</td></tr> <tr><td>11 B</td><td>3.350600</td><td>2.900521</td><td>3.054612</td><td>3.670105</td><td>1.828703</td></tr> <tr><td>12 Ru</td><td>2.347849</td><td>3.505881</td><td>3.347198</td><td>3.100298</td><td>3.100298</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.882666</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Ru</td><td>2.190512</td><td>3.665946</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.790256</td><td>1.903185</td><td>3.493588</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.965970</td><td>1.903185</td><td>3.493588</td><td>3.046200</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.790275</td><td>2.837771</td><td>2.177163</td><td>3.667781</td><td>1.801672</td></tr> <tr><td>12 Ru</td><td>3.347198</td><td>2.422584</td><td>2.587724</td><td>2.010440</td><td>2.010440</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Ru</td><td>2.347849</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.900521	0.000000				3 B	1.790275	1.789790	0.000000			4 B	1.828703	1.734929	1.787969	0.000000		5 B	3.670105	1.734929	2.953245	3.022000	0.000000	6 B	3.054612	1.789790	1.828200	2.953245	1.787969	7 B	2.837771	1.850137	2.882666	1.877179	1.877179	8 Ru	2.177163	3.329157	2.190512	3.384149	3.384149	9 B	1.801672	3.018619	2.965970	1.753690	3.504432	10 B	3.667781	3.018619	3.790256	3.504432	1.753690	11 B	3.350600	2.900521	3.054612	3.670105	1.828703	12 Ru	2.347849	3.505881	3.347198	3.100298	3.100298		6	7	8	9	10	6 B	0.000000					7 B	2.882666	0.000000				8 Ru	2.190512	3.665946	0.000000			9 B	3.790256	1.903185	3.493588	0.000000		10 B	2.965970	1.903185	3.493588	3.046200	0.000000	11 B	1.790275	2.837771	2.177163	3.667781	1.801672	12 Ru	3.347198	2.422584	2.587724	2.010440	2.010440		11	12				11 B	0.000000					12 Ru	2.347849	0.000000			
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Table S5C Energy ranking of the $\text{Cp}_2\text{Ru}_2\text{B}_{10}\text{H}_{10}$ structures.

No	Initial structure	Final energy (a.u.)	$\Delta E_{\text{kcal/mole}}$
1	12-Ru-2-Cuboctaedru-g_r-91	-831.64407734	0.00
2	12-Ru-2-Cuboctaedru-g_r-11-93	-831.64403184	0.03
3	12-Ru-2-Cuboctaedru-g_r-25	-831.64397722	0.06
4	12-Ru-2-Cuboctaedru-f	-831.64397153	0.07
5	12-Ru-2-Cuboctaedru-g_r-11 i-93	-831.64396481	0.07
6	12-Ru-2-Cuboctaedru-g imag	-831.64391304	0.10
7	12-Ru-1-Icos-b_r-97	-831.64382989	0.16
8	12-Ru-1-Icos-b i-97	-831.64374350	0.21
9	12-Ru-3-Anticuboh-j_r-21	-831.63961592	2.80
10	12-Ru-3-Anticuboh-j_r-1063	-831.63950945	2.87
11	12-Ru-3-Anticuboh-h_r-46	-831.62282569	13.34
12	12-Ru-3-Anticuboh-e	-831.61923852	15.59
13	12-Ru-2-Cuboctaedru-h	-831.61473009	18.42
14	12-Ru-3-Anticuboh-i_r-205	-831.61473009	18.42
15	12-Ru-2-Cuboctaedru-e	-831.61266881	19.71
16	12-Ru-3-Anticuboh-a_r-133	-831.61266881	19.71
17	12-Ru-3-Anticuboh-a_r-26	-831.61266881	19.71
18	12-Ru-1-Icos-a	-831.61266880	19.71
19	12-Ru-Ig-4	-831.59955086	27.94
20	12-Ru-2-Cuboctaedru-b	-831.59725636	29.38
21	12-Ru-3-Anticuboh-d	-831.59410049	31.36
22	12-Ru-3-Anticuboh-c	-831.58802219	35.17
23	12-Ru-2-Cuboctaedru-a	-831.58764729	35.41
24	12-Ru-3-Anticuboh-i_r-130	-831.58734550	35.60
25	12-Ru-3-Anticuboh-i_r-156-89	-831.58217815	38.84
26	12-Ru-3-Anticuboh-i_r-81-89	-831.58217815	38.84
27	12-Ru-2-Cuboctaedru-d	-831.57537914	43.11
28	12-Ru-2-Cuboctaedru-i_r-34	-831.57407692	43.93
29	12-Ru-2-Cuboctaedru-i_r-40	-831.57393838	44.01
30	12-Ru-1-Icos-c	-831.57370521	44.16
31	12-Ru-2-Cuboctaedru-i imag	-831.57124356	45.70
32	12-Ru-3-Anticuboh-i_r-156 i-89	-831.56169036	51.70
33	12-Ru-3-Anticuboh-i_r-81 i-89	-831.56169035	51.70
34	12-Ru-3-Anticuboh-f	-831.55226961	57.61
35	12-Ru-2-Cuboctaedru-c	-831.55212860	57.70
36	12-Ru-3-Anticuboh-j imag	-831.53105406	70.92
37	12-Ru-3-Anticuboh-g	-831.51884452	78.58
38	12-Ru-3-Anticuboh-i_r-325	-831.51882755	78.59
39	12-Ru-3-Anticuboh-a imag	-831.50834023	85.18

40	12-Ru-3-Anticuboh-h i-46	-831.50678548	86.15
41	12-Ru-3-Anticuboh-b	-831.49490665	93.60
42	12-Ru-Bipypr-decag	-831.46397792	113.01
43	12-Ru-3-Anticuboh-l imag	-831.40793232	148.18

The 8-vertex $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_6$ Structures

Table S6A. Initial structures

Table S6B. Best structures distances

Table S6C. Global ranking of all structures

Table S6A Initial $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_6$ structures (one example from each family); 84 structures in total

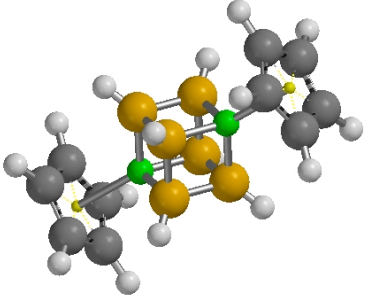
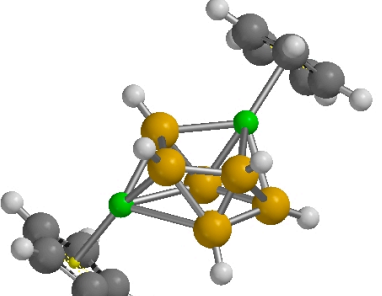
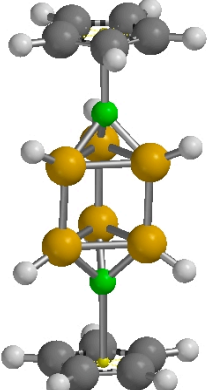
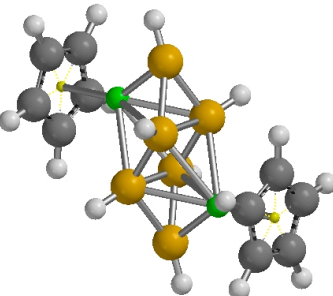
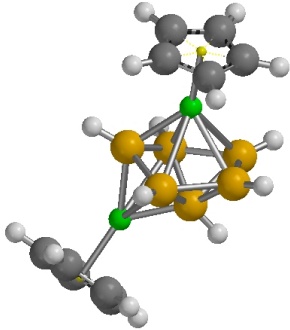
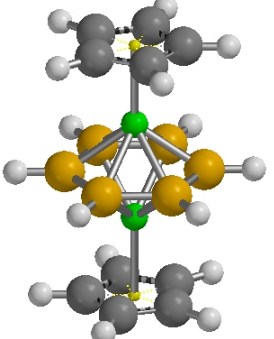
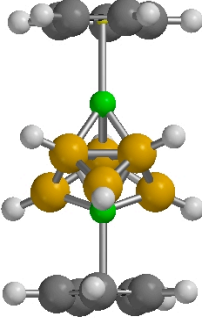
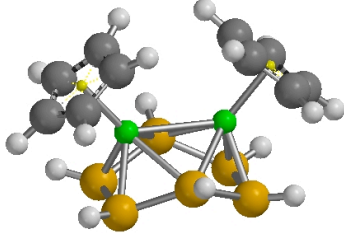
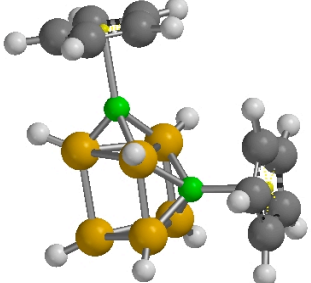
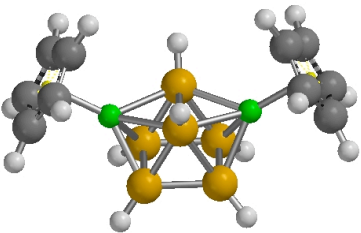
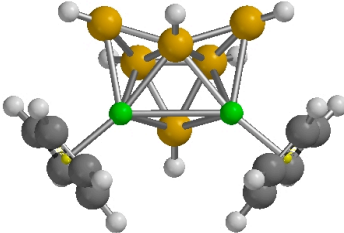
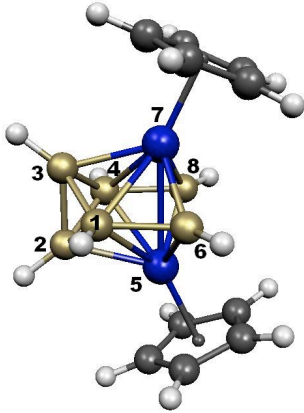
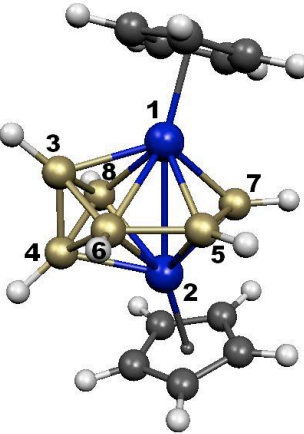
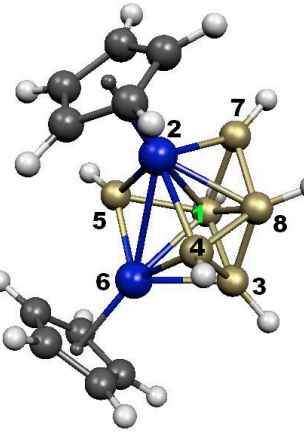
<p>Initial structures</p>	 <p>1. Cube 3</p>	 <p>2. Antiprism 4</p>
 <p>3. Trigonal Prism 6</p>	 <p>4. Trigonal Antiprism 8</p>	 <p>5. Bisdisphenoid 6</p>
 <p>6. Hexagonal bipyramid 4</p>	 <p>7. All-capped tetrahedron 5</p>	 <p>8. Nido structure 9</p>
 <p>9. Dicapped trigonal prism (C_3) 18</p>	 <p>10. Dicapped trigonal prism (C_{2v}) 10</p>	 <p>11. Dicapped octahedron 11</p>

Table S6B. Distance table for the lowest energy Cp₂Os₂B₆H₆ structures

 <p>1. -721.39864397 0.0 C_{2v}</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.744278</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.744328</td><td>1.729700</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.566400</td><td>1.744278</td><td>1.744328</td><td>0.000000</td><td></td></tr> <tr><td>5 Os</td><td>2.282213</td><td>2.154528</td><td>3.068854</td><td>2.282213</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.819109</td><td>3.120440</td><td>3.120468</td><td>3.292260</td><td>2.081176</td></tr> <tr><td>7 Os</td><td>2.282213</td><td>3.068781</td><td>2.154504</td><td>2.282213</td><td>2.761000</td></tr> <tr><td>8 B</td><td>3.292260</td><td>3.120440</td><td>3.120468</td><td>1.819109</td><td>2.081176</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td></td> <td></td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Os</td><td>2.081176</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.934000</td><td>2.081176</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.744278	0.000000				3 B	1.744328	1.729700	0.000000			4 B	2.566400	1.744278	1.744328	0.000000		5 Os	2.282213	2.154528	3.068854	2.282213	0.000000	6 B	1.819109	3.120440	3.120468	3.292260	2.081176	7 Os	2.282213	3.068781	2.154504	2.282213	2.761000	8 B	3.292260	3.120440	3.120468	1.819109	2.081176		6	7	8			6 B	0.000000					7 Os	2.081176	0.000000				8 B	2.934000	2.081176	0.000000		
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 <p>2. -721.36451489 +21.4 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Os</td><td>2.780800</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.178377</td><td>3.061375</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.061375</td><td>2.178377</td><td>1.663800</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.130116</td><td>2.130116</td><td>3.132565</td><td>3.132565</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.292604</td><td>2.292604</td><td>1.767820</td><td>1.767820</td><td>1.772809</td></tr> <tr><td>7 B</td><td>2.047052</td><td>2.047052</td><td>3.698277</td><td>3.698277</td><td>1.961541</td></tr> <tr><td>8 B</td><td>2.233130</td><td>2.233130</td><td>1.755706</td><td>1.755706</td><td>3.275324</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td></td> <td></td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.123571</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.574465</td><td>2.923562</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Os	0.000000					2 Os	2.780800	0.000000				3 B	2.178377	3.061375	0.000000			4 B	3.061375	2.178377	1.663800	0.000000		5 B	2.130116	2.130116	3.132565	3.132565	0.000000	6 B	2.292604	2.292604	1.767820	1.767820	1.772809	7 B	2.047052	2.047052	3.698277	3.698277	1.961541	8 B	2.233130	2.233130	1.755706	1.755706	3.275324		6	7	8			6 B	0.000000					7 B	3.123571	0.000000				8 B	2.574465	2.923562	0.000000		
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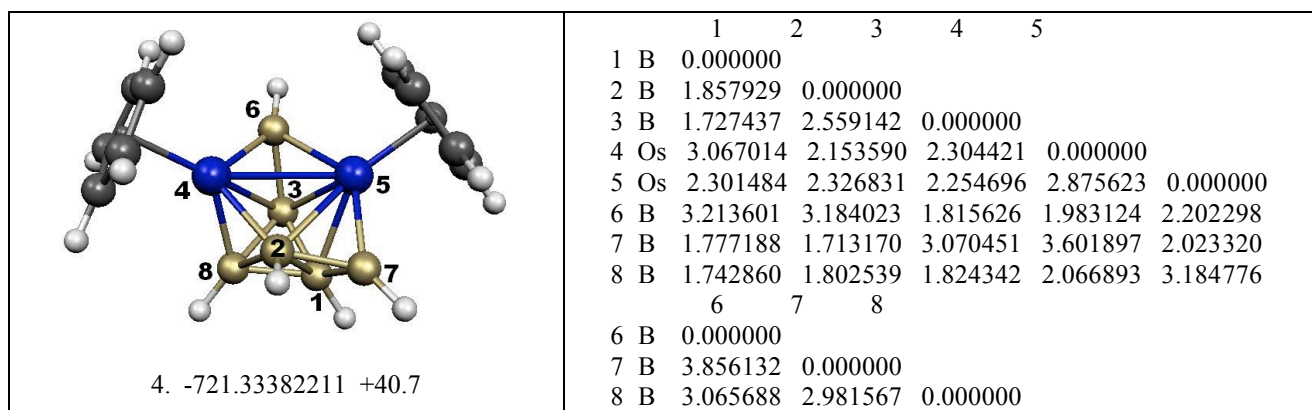


Table S6C. Energy ranking of the $\text{Cp}_2\text{Os}_2\text{B}_6\text{H}_6$ structures.

No	Initial structure	Final energy (a.u.)	D kcal/mole
1	01-Os-Cub-b	-721.39864397	0.00
2	03-Os-PrTrig-f	-721.39864397	0.00
3	05-Os-Bisdisph-d	-721.39864397	0.00
4	09-Os-DicapTrPr-Cs-e	-721.39864397	0.00
5	09-Os-DicapTrPr-Cs-i	-721.39864397	0.00
6	07-Os-Tdallcap-d	-721.39864396	0.00
7	08-Os-Nido-c	-721.39864396	0.00
8	08-Os-Nido-f	-721.39864396	0.00
9	09-Os-DicapTrPr-Cs-r	-721.36451489	21.42
10	09-Os-DicapTrPr-Cs-k	-721.34916678	31.05
11	09-Os-DicapTrPr-Cs-a	-721.34916677	31.05
12	11-Os-DicapOh-c	-721.34916676	31.05
13	04-Os-AntiprTrig-d	-721.34916675	31.05
14	08-Os-Nido-i	-721.34916675	31.05
15	04-Os-AntiprTrig-c	-721.34903970	31.13
16	09-Os-DicapTrPr-Cs-n	-721.33382211	40.68
17	08-Os-Nido-b	-721.33382210	40.68
18	09-Os-DicapTrPr-Cs-m	-721.33376081	40.71
19	11-Os-DicapOh-b	-721.33376079	40.71
20	04-Os-AntiprTrig-g	-721.32691398	45.01
21	03-Os-PrTrig-d	-721.32691172	45.01
22	01-Os-Cub-a	-721.32691171	45.01
23	08-Os-Nido-e	-721.32691171	45.01
24	02-Os-Antipr-d	-721.32414669	46.75
25	10-Os-DicapTrPr-C2v-g	-721.32414669	46.75
26	05-Os-Bisdisph-f_r-180	-721.31974759	49.51
27	10-Os-DicapTrPr-C2v-c_r-353	-721.31974759	49.51
28	10-Os-DicapTrPr-C2v-i	-721.31974759	49.51
29	02-Os-Antipr-b	-721.31974260	49.51
30	02-Os-Antipr-c	-721.31974260	49.51
31	10-Os-DicapTrPr-C2v-b	-721.31974260	49.51
32	05-Os-Bisdisph-b	-721.31973567	49.51
33	06-Os-Bipirhex-d	-721.31948224	49.67
34	08-Os-Nido-h	-721.31921756	49.84
35	09-Os-DicapTrPr-Cs-p	-721.31516753	52.38
36	09-Os-DicapTrPr-Cs-h	-721.31516752	52.38
37	07-Os-Tdallcap-e	-721.31464226	52.71
38	09-Os-DicapTrPr-Cs-q	-721.31403204	53.09
39	11-Os-DicapOh-i	-721.31384762	53.21
40	07-Os-Tdallcap-c	-721.31307904	53.69
41	06-Os-Bipirhex-b	-721.31296355	53.76

42	10-Os-DicapTrPr-C2v-f_r-165	-721.31262646	53.98
43	04-Os-AntiprTrig-h	-721.31116813	54.89
44	08-Os-Nido-g	-721.31084123	55.10
45	06-Os-Bipirhex-a	-721.30996870	55.64
46	05-Os-Bisdisph-c	-721.30865138	56.47
47	08-Os-Nido-d	-721.30865138	56.47
48	10-Os-DicapTrPr-C2v-e	-721.30865137	56.47
49	10-Os-DicapTrPr-C2v-j_r-45	-721.30865137	56.47
50	11-Os-DicapOh-d	-721.30865137	56.47
51	09-Os-DicapTrPr-Cs-j	-721.30865136	56.47
52	10-Os-DicapTrPr-C2v-f_r-262-32	-721.30860593	56.50
53	11-Os-DicapOh-g	-721.30860593	56.50
54	11-Os-DicapOh-j	-721.30860593	56.50
55	02-Os-Antipr-a	-721.30773380	57.05
56	05-Os-Bisdisph-a	-721.30773380	57.05
57	09-Os-DicapTrPr-Cs-g	-721.30773380	57.05
58	09-Os-DicapTrPr-Cs-l	-721.30773380	57.05
59	10-Os-DicapTrPr-C2v-a	-721.30773380	57.05
60	10-Os-DicapTrPr-C2v-h_r-272	-721.30773380	57.05
61	03-Os-PrTrig-b	-721.30760342	57.13
62	11-Os-DicapOh-k	-721.30732384	57.30
63	11-Os-DicapOh-e	-721.30732382	57.30
64	04-Os-AntiprTrig-f	-721.30715898	57.41
65	10-Os-DicapTrPr-C2v-j i-45	-721.30320680	59.89
66	07-Os-Tdallcap-b	-721.30285638	60.11
67	09-Os-DicapTrPr-Cs-o	-721.30280622	60.14
68	10-Os-DicapTrPr-C2v-d	-721.30199494	60.65
69	11-Os-DicapOh-a	-721.30060936	61.52
70	09-Os-DicapTrPr-Cs-d	-721.30056827	61.54
71	03-Os-PrTrig-e	-721.29840227	62.90
72	04-Os-AntiprTrig-e	-721.29281405	66.41
73	05-Os-Bisdisph-e	-721.29281404	66.41
74	03-Os-PrTrig-a	-721.29188025	66.99
75	09-Os-DicapTrPr-Cs-f	-721.29039114	67.93
76	10-Os-DicapTrPr-C2v-c i-353	-721.29031563	67.98
77	07-Os-Tdallcap-a	-721.29017227	68.07
78	11-Os-DicapOh-h	-721.28200085	73.19
79	08-Os-Nido-a	-721.28019230	74.33
80	09-Os-DicapTrPr-Cs-c	-721.27323602	78.69
81	10-Os-DicapTrPr-C2v-h i-272	-721.27036285	80.50
82	01-Os-Cub-c	-721.26569335	83.43
83	10-Os-DicapTrPr-C2v-f_r-262 i-32	-721.26555245	83.51
84	05-Os-Bisdisph-f i-180	-721.26460859	84.11
85	11-Os-DicapOh-f	-721.25801630	88.24
86	06-Os-Bipirhex-c	-721.25398606	90.77

87	09-Os-DicapTrPr-Cs-b_r-19	-721.25068712	92.84
88	09-Os-DicapTrPr-Cs-b i-19	-721.25063749	92.87
89	04-Os-AntiprTrig-a	-721.24099369	98.93
90	04-Os-AntiprTrig-b	-721.24092061	98.97
91	10-Os-DicapTrPr-C2v-f imag	-721.22634461	108.12
92	03-Os-PrTrig-c	-721.20472312	121.69

The 9-vertex $\text{Cp}_2\text{Os}_2\text{B}_7\text{H}_7$ System

Table S7A. Initial structures

Table S7B. Best structures distances

Table S7C. Global ranking of all structures

Table S7A. Initial $\text{Cp}_2\text{Os}_2\text{B}_7\text{H}_7$ structures (one example from each family); 43 structures in total

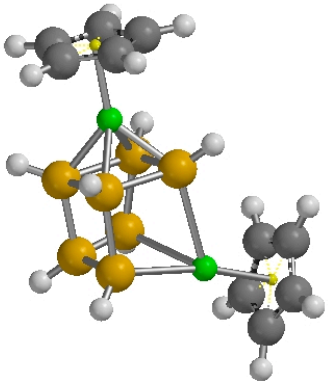
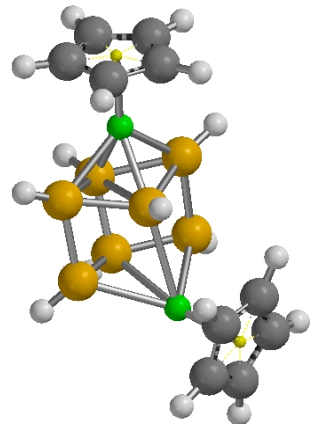
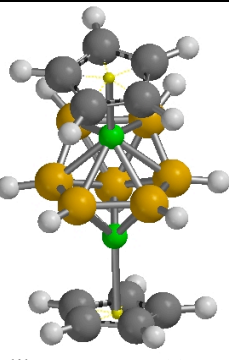
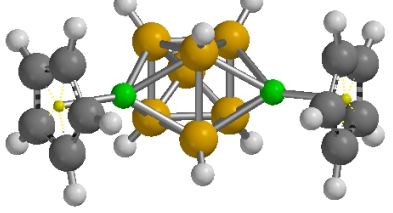
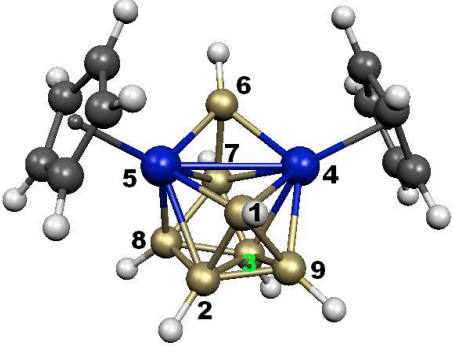
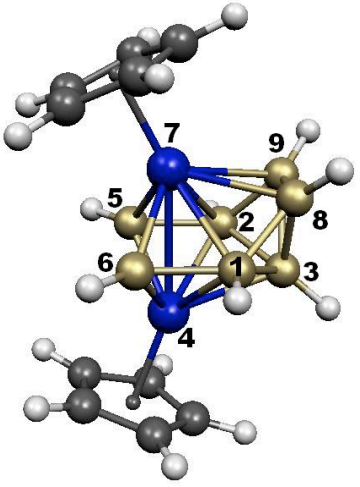
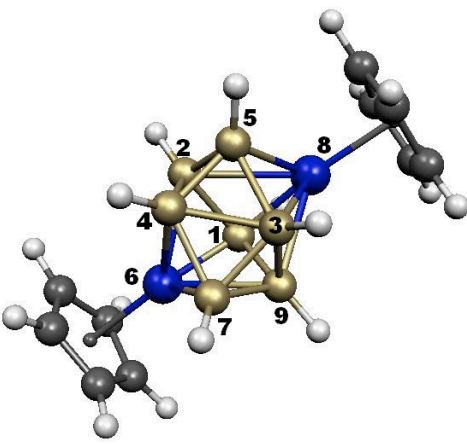
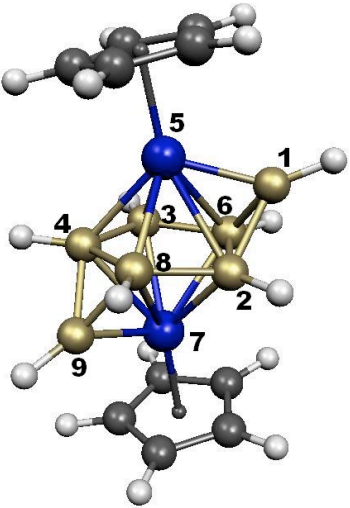
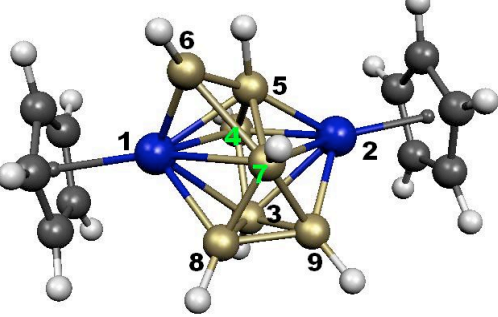
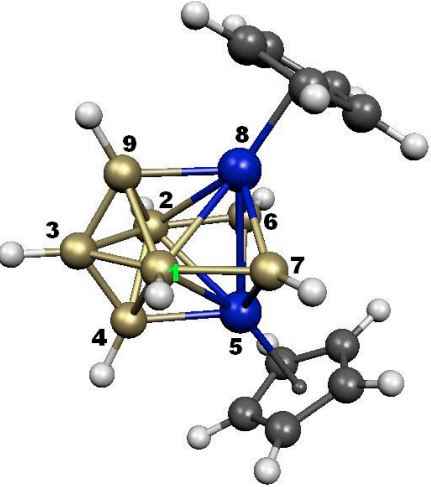
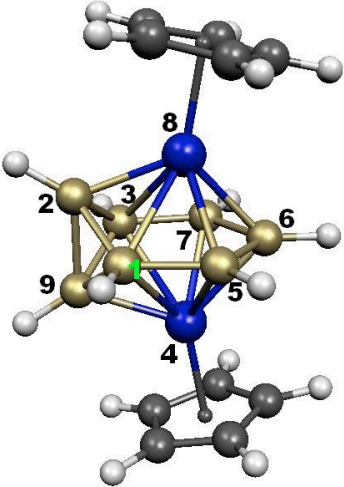
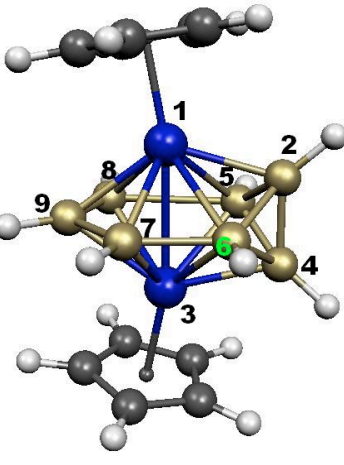
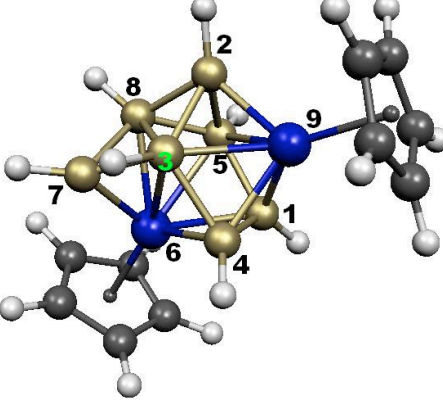
Initial structures	
	1. Capped cube 9 structures
	2. Pressed capped cube 15 structures
	3. Tl_9^{9-} -like structure 13 structures
	4. Tricapped trigonal prism 6 structures

Table S7B. Distance table for the lowest energy Cp₂Os₂B₇H₇ structures

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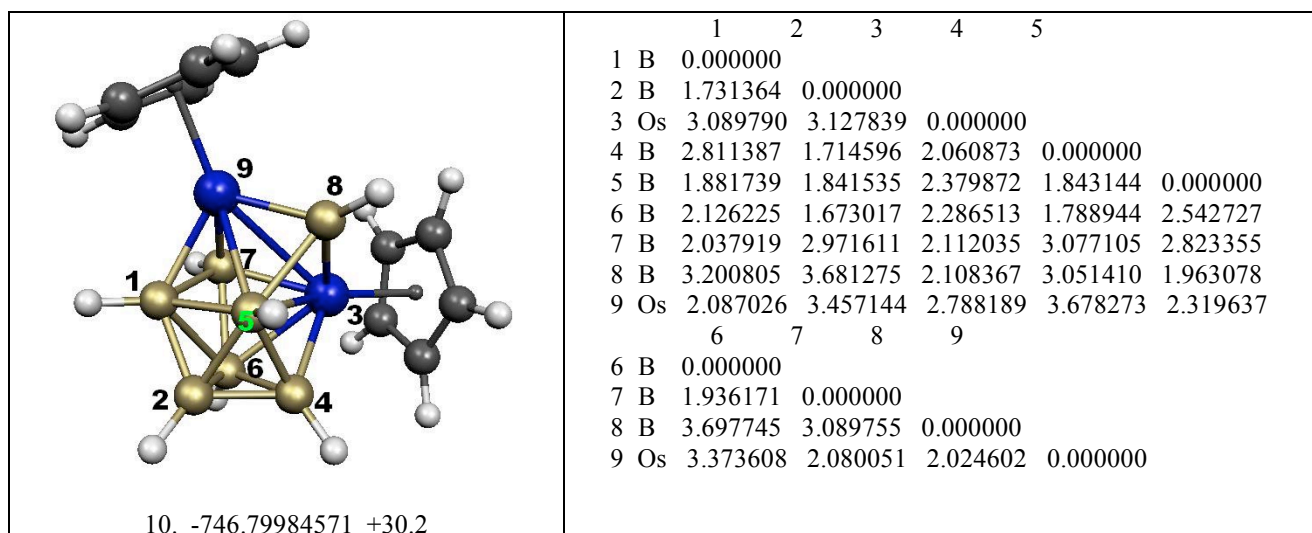


Table S7C. Energy ranking of the Cp₂Os₂B₇H₇ structures

No	Initial structure	Final energy (a.u.)	D kcal/mole
1	09-Os-1-CapCube_f	-746.84793009	0.00
2	09-Os-3-Tl99-b	-746.84793009	0.00
3	09-Os-3-Tl99-c	-746.82879378	12.01
4	09-Os-1-CapCube_d	-746.82879377	12.01
5	09-Os-4-TrTrPr_c_r-34	-746.82879377	12.01
6	09-Os-4-TrTrPr_c_i-34	-746.82802994	12.49
7	09-Os-2-PressCapCube_m	-746.81376772	21.44
8	09-Os-3-Tl99-g	-746.81376772	21.44
9	09-Os-3-Tl99-m	-746.81376772	21.44
10	09-Os-4-TrTrPr_e_r-213	-746.81376771	21.44
11	09-Os-5-structure-5	-746.80721256	25.55
12	09-Os-5-structure-4	-746.80721256	25.55
13	09-Os-3-Tl99-j_r-136	-746.80552785	26.61
14	09-Os-5-Bipyr-hept3	-746.80536618	26.71
15	09-Os-1-CapCube_g	-746.80279011	28.33
16	09-Os-2-PressCapCube_o	-746.80279011	28.33
17	09-Os-2-PressCapCube_e_r-348	-746.80240548	28.57
18	09-Os-5-structure-1	-746.80240548	28.57
19	09-Os-2-PressCapCube_f	-746.80197481	28.84
20	09-Os-1-CapCube_b	-746.80100499	29.45
21	09-Os-2-PressCapCube_a_r-44	-746.79984571	30.17
22	09-Os-2-PressCapCube_a_r-277	-746.79984570	30.17
23	09-Os-1-CapCube_i	-746.79976676	30.22
24	09-Os-1-CapCube_c	-746.79972140	30.25
25	09-Os-2-PressCapCube_j_r-551-142	-746.79972140	30.25
26	09-Os-3-Tl99-e	-746.79972139	30.25
27	09-Os-4-TrTrPr_a	-746.79972139	30.25
28	09-Os-4-TrTrPr_d_r-209	-746.79972139	30.25
29	09-Os-4-TrTrPr_d_r-45	-746.79972139	30.25
30	09-Os-2-PressCapCube_e_i-348	-746.79632437	32.38
31	09-Os-3-Tl99-l_r-724	-746.79270898	34.65
32	09-Os-2-PressCapCube_j_r-551-368	-746.79102841	35.71
33	09-Os-2-PressCapCube_j_r-551-55	-746.79102841	35.71
34	09-Os-2-PressCapCube_b	-746.78932408	36.78
35	09-Os-2-PressCapCube_h	-746.78856124	37.25
36	09-Os-3-Tl99-i	-746.78314180	40.65
37	09-Os-4-TrTrPr_e_i-213	-746.78195391	41.40
38	09-Os-2-PressCapCube_i	-746.78149856	41.69
39	09-Os-2-PressCapCube_j_r-92-450	-746.77973293	42.79
40	09-Os-2-PressCapCube_j_r-68	-746.77973292	42.79
41	09-Os-4-TrTrPr_f_r-115	-746.77950082	42.94

42	09-Os-1-CapCube_h	-746.77769598	44.07
43	09-Os-1-CapCube_e	-746.77675950	44.66
44	09-Os-3-Tl99-d_r-343-75	-746.77675950	44.66
45	09-Os-3-Tl99-d_r-19-316-48	-746.77675950	44.66
46	09-Os-2-PressCapCube_g	-746.77675949	44.66
47	09-Os-3-Tl99-d_r-343-34	-746.77675949	44.66
48	09-Os-3-Tl99-d_r-46-320	-746.77675949	44.66
49	09-Os-3-Tl99-d_r-33-320	-746.77675949	44.66
50	09-Os-3-Tl99-d_r-19-316-81	-746.77675949	44.66
51	09-Os-3-Tl99-d_r-19-40	-746.77675949	44.66
52	09-Os-4-TrTrPr_f i-115	-746.77651588	44.81
53	09-Os-3-Tl99-a	-746.77291234	47.07
54	09-Os-4-TrTrPr_d imag	-746.77176847	47.79
55	09-Os-2-PressCapCube_j_r-551 imag	-746.76393245	52.71
56	09-Os-2-PressCapCube_n	-746.76373662	52.83
57	09-Os-2-PressCapCube_j_r-636-314	-746.76224369	53.77
58	09-Os-2-PressCapCube_j_r-188-314	-746.76224369	53.77
59	09-Os-2-PressCapCube_j_r-72-314	-746.76224369	53.77
60	09-Os-4-TrTrPr_b	-746.76224369	53.77
61	09-Os-3-Tl99-k_r-48	-746.76224368	53.77
62	09-Os-2-PressCapCube_c	-746.76224312	53.77
63	09-Os-3-Tl99-j i-136	-746.76072521	54.72
64	09-Os-2-PressCapCube_j_r-507-52	-746.75949824	55.49
65	09-Os-2-PressCapCube_j_r-57-52	-746.75949824	55.49
66	09-Os-3-Tl99-f	-746.75949824	55.49
67	09-Os-2-PressCapCube_j_r-507-81	-746.75949823	55.49
68	09-Os-2-PressCapCube_j_r-57-81	-746.75949823	55.49
69	09-Os-3-Tl99-h	-746.75465885	58.53
70	09-Os-1-CapCube_a	-746.75465219	58.53
71	09-Os-2-PressCapCube_k	-746.75047608	61.15
72	09-Os-2-PressCapCube_j_r-507-521	-746.74664718	63.56
73	09-Os-2-PressCapCube_j_r-57-521	-746.74664718	63.56
74	09-Os-2-PressCapCube_l	-746.74183023	66.58
75	09-Os-3-Tl99-d_r-19-316 imag	-746.74010769	67.66
76	09-Os-3-Tl99-d_r-343 imag	-746.73936656	68.12
77	09-Os-3-Tl99-d_r-46 i-320	-746.73453444	71.16
78	09-Os-3-Tl99-d_r-33 i-320	-746.73453443	71.16
79	09-Os-3-Tl99-d_r-19 imag	-746.73441766	71.23
80	09-Os-2-PressCapCube_a imag	-746.73237503	72.51
81	09-Os-3-Tl99-d imag	-746.73196086	72.77
82	09-Os-2-PressCapCube_j_r-92 i-450	-746.73001104	73.99
83	09-Os-5-Bipyr-hept1_r-27	-746.72592812	76.56
84	09-Os-5-Bipyr-hept1 i-27	-746.72436914	77.53
85	09-Os-3-Tl99-l_r-67	-746.72258334	78.66
86	09-Os-2-PressCapCube_d	-746.72258333	78.66

87	09-Os-2-PressCapCube_j_r-507-404	-746.72049360	79.97
88	09-Os-2-PressCapCube_j_r-57-404	-746.72049358	79.97
89	09-Os-3-Tl99-k_r-445	-746.71989520	80.34
90	09-Os-5-Bipyr-hept2	-746.69149704	98.16
91	09-Os-2-PressCapCube_j_r-72 i-314	-746.67488424	108.59
92	09-Os-2-PressCapCube_j_r-636 i-314	-746.67488423	108.59
93	09-Os-2-PressCapCube_j_r-188 i-314	-746.67488422	108.59
94	09-Os-3-Tl99-l imag	-746.67296576	109.79
95	09-Os-3-Tl99-k imag	-746.66111169	117.23
96	09-Os-2-PressCapCube_j_r-507 imag	-746.59722570	157.32
97	09-Os-2-PressCapCube_j_r-57 imag	-746.59722569	157.32
98	09-Os-2-PressCapCube_j imag	-746.58409054	165.56

The 10-vertex $\text{Cp}_2\text{Os}_2\text{B}_8\text{H}_8$ System

Table S8A. Initial structures

Table S8B. Best structures distances

Table S8C. Global ranking of all structures

Table S8A. Initial $\text{Cp}_2\text{Os}_2\text{B}_8\text{H}_8$ structures (one example from each family); 62 structures in total

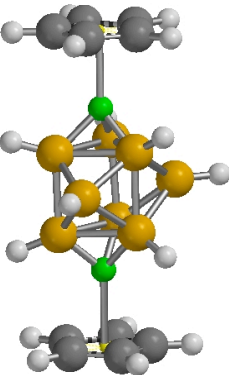
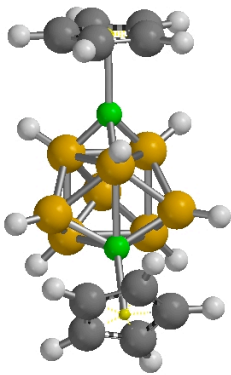
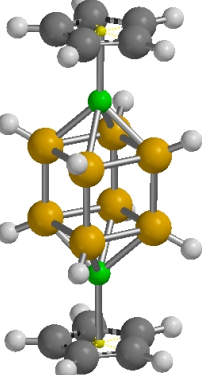
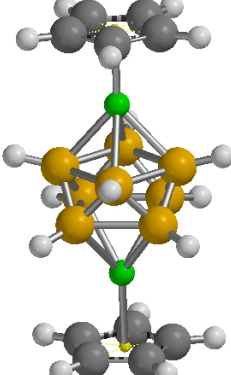
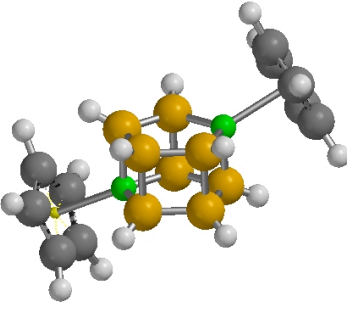
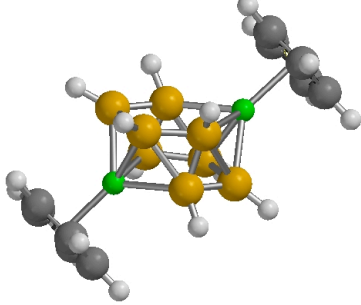
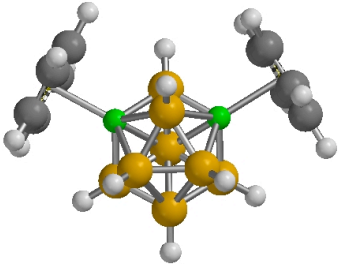
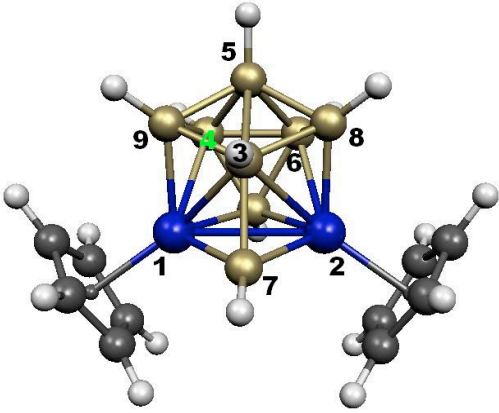
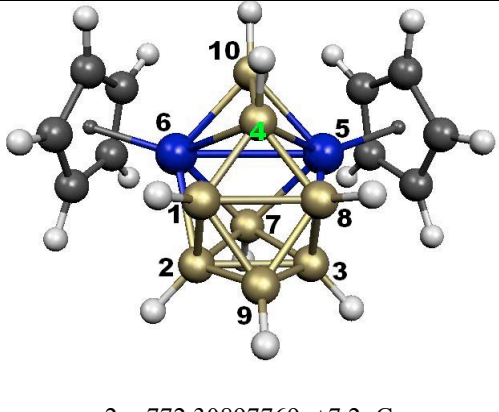
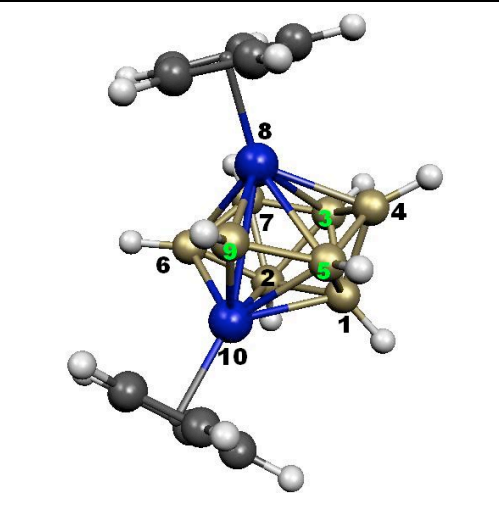
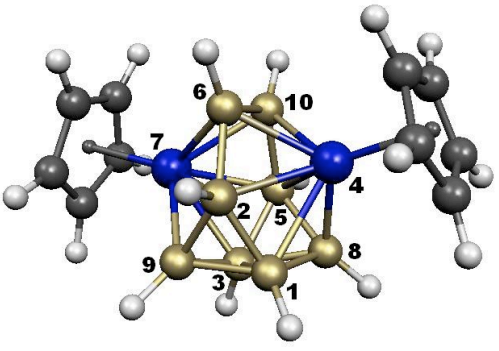
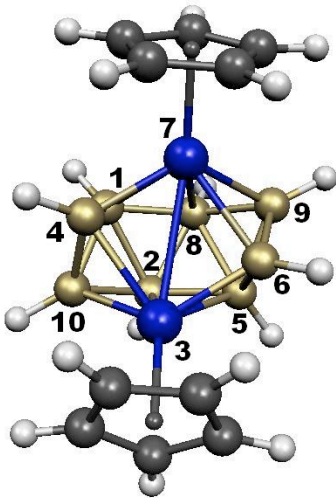
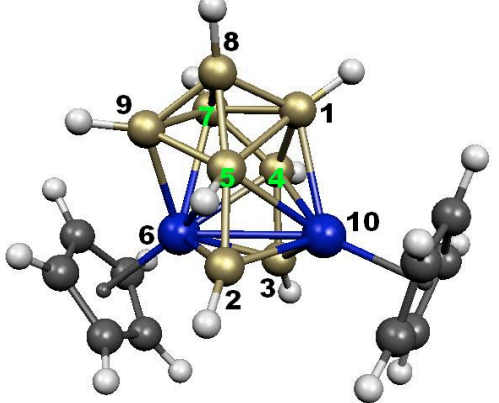
<p>Initial structures</p>	 <p>1. Tetrapped trigonal prism (C_{2v}) 16</p>
 <p>2. Tetrapped trigonal prism (C_{3v}) 9</p>	 <p>3. Bicapped cube 8</p>
 <p>4. Bicapped square antiprism 7</p>	 <p>5. Pentagonal prism 5</p>
 <p>6. Pentagonal antiprism 5</p>	 <p>7. Isocloso structure 12</p>

Table S8B. Distance table for the lowest energy Cp₂Os₂B₈H₈ structures

 <p>1. -772.32049989 +0.0 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Os</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Os</td><td>2.813000</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.326819</td><td>2.326819</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.324591</td><td>3.228853</td><td>2.724559</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.182018</td><td>3.182018</td><td>1.988548</td><td>1.787587</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.228853</td><td>2.324591</td><td>2.724559</td><td>1.785200</td><td>1.787587</td></tr> <tr><td>7 B</td><td>2.067467</td><td>2.067467</td><td>1.894208</td><td>3.715093</td><td>3.688356</td></tr> <tr><td>8 B</td><td>3.549145</td><td>2.070059</td><td>1.838285</td><td>2.894865</td><td>1.749516</td></tr> <tr><td>9 B</td><td>2.070059</td><td>3.549145</td><td>1.838285</td><td>1.762298</td><td>1.749516</td></tr> <tr><td>10 B</td><td>2.150369</td><td>2.150369</td><td>3.016690</td><td>1.796622</td><td>2.928043</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.715093</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.762298</td><td>3.126935</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.894865</td><td>3.126935</td><td>2.954600</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.796622</td><td>3.135015</td><td>2.983771</td><td>2.983771</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 Os	0.000000					2 Os	2.813000	0.000000				3 B	2.326819	2.326819	0.000000			4 B	2.324591	3.228853	2.724559	0.000000		5 B	3.182018	3.182018	1.988548	1.787587	0.000000	6 B	3.228853	2.324591	2.724559	1.785200	1.787587	7 B	2.067467	2.067467	1.894208	3.715093	3.688356	8 B	3.549145	2.070059	1.838285	2.894865	1.749516	9 B	2.070059	3.549145	1.838285	1.762298	1.749516	10 B	2.150369	2.150369	3.016690	1.796622	2.928043		6	7	8	9	10	6 B	0.000000					7 B	3.715093	0.000000				8 B	1.762298	3.126935	0.000000			9 B	2.894865	3.126935	2.954600	0.000000		10 B	1.796622	3.135015	2.983771	2.983771	0.000000
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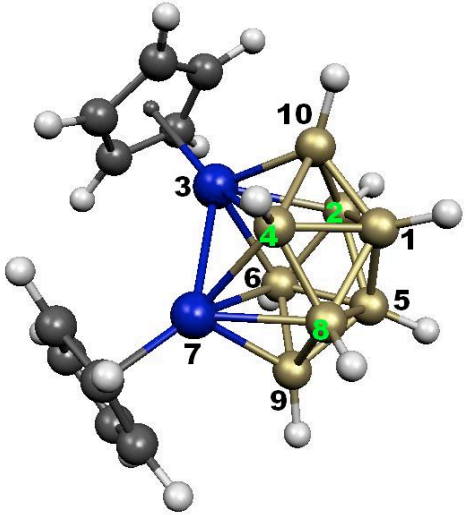
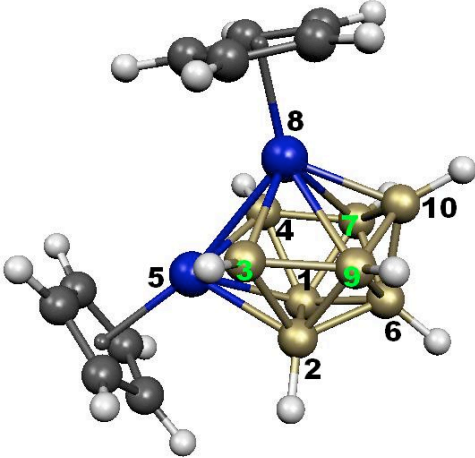
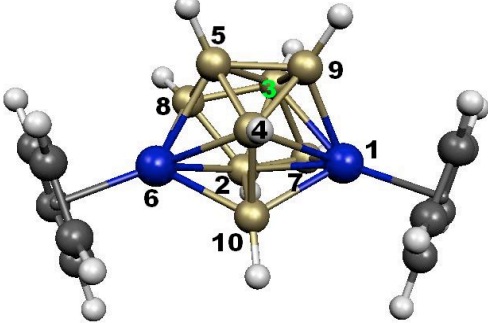
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 <p>8. -772.27815302 +26.6 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.893871</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.127627</td><td>1.884611</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.814560</td><td>3.074375</td><td>3.271835</td><td>0.000000</td><td></td></tr> <tr><td>5 Os</td><td>2.257484</td><td>2.265786</td><td>2.115336</td><td>2.103245</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.812112</td><td>1.790814</td><td>3.036790</td><td>2.984775</td><td>3.396446</td></tr> <tr><td>7 B</td><td>1.781448</td><td>2.911674</td><td>3.529552</td><td>1.733799</td><td>3.242244</td></tr> <tr><td>8 Os</td><td>3.052613</td><td>3.031478</td><td>2.159163</td><td>2.208301</td><td>2.645368</td></tr> <tr><td>9 B</td><td>2.925428</td><td>1.761644</td><td>1.781079</td><td>3.507488</td><td>3.248099</td></tr> <tr><td>10 B</td><td>2.886178</td><td>2.863242</td><td>3.039156</td><td>3.023553</td><td>3.829836</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.826429</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Os</td><td>3.031181</td><td>2.383651</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.816043</td><td>2.840662</td><td>2.374239</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.729661</td><td>1.753242</td><td>2.108944</td><td>1.746900</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.893871	0.000000				3 B	3.127627	1.884611	0.000000			4 B	1.814560	3.074375	3.271835	0.000000		5 Os	2.257484	2.265786	2.115336	2.103245	0.000000	6 B	1.812112	1.790814	3.036790	2.984775	3.396446	7 B	1.781448	2.911674	3.529552	1.733799	3.242244	8 Os	3.052613	3.031478	2.159163	2.208301	2.645368	9 B	2.925428	1.761644	1.781079	3.507488	3.248099	10 B	2.886178	2.863242	3.039156	3.023553	3.829836		6	7	8	9	10	6 B	0.000000					7 B	1.826429	0.000000				8 Os	3.031181	2.383651	0.000000			9 B	1.816043	2.840662	2.374239	0.000000		10 B	1.729661	1.753242	2.108944	1.746900	0.000000
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Table S8C. Energy ranking of the $\text{Cp}_2\text{Os}_2\text{B}_8\text{H}_8$ structures

No	Initial structure	Final energy (a.u.)	D kcal/mole
1	2-Os-TetrcTriPri2_d	-772.32049989	0.00
2	2-Os-TetrcTriPri2_c	-772.32049987	0.00
3	1-Os-TetrcTriPri1-e	-772.32047902	0.01
4	7-Os-Isocloso-i	-772.32047902	0.01
5	1-Os-TetrcTriPri1-i	-772.30897769	7.23
6	5-Os-PentagPrism-b	-772.30445470	10.07
7	1-Os-TetrcTriPri1-l	-772.29616981	15.27
8	2-Os-TetrcTriPri2_b	-772.29616981	15.27
9	2-Os-TetrcTriPri2_f	-772.29616981	15.27
10	5-Os-PentagPrism-d	-772.29616981	15.27
11	7-Os-Isocloso-c	-772.29616981	15.27
12	8-Os-Structure-2	-772.29616981	15.27
13	6-Os-AntiPr-d	-772.29616980	15.27
14	3-Os-BicapCub_g	-772.29041583	18.88
15	6-Os-AntiPr-c	-772.29041583	18.88
16	3-Os-BicapCub_b	-772.28157680	24.42
17	4-Os-BicapSqAntipr-f	-772.28138188	24.55
18	7-Os-Isocloso-l-238	-772.28137536	24.55
19	2-Os-TetrcTriPri2_a	-772.28137535	24.55
20	7-Os-Isocloso-j	-772.28137534	24.55
21	7-Os-Isocloso-b_r-22	-772.27815302	26.57
22	7-Os-Isocloso-b i-22	-772.27811343	26.60
23	3-Os-BicapCub_c	-772.27589175	27.99
24	1-Os-TetrcTriPri1-k	-772.27392349	29.23
25	2-Os-TetrcTriPri2_h	-772.27392348	29.23
26	6-Os-AntiPr-e	-772.27392348	29.23
27	7-Os-Isocloso-k	-772.26995959	31.71
28	1-Os-TetrcTriPri1-j	-772.26995956	31.71
29	1-Os-TetrcTriPri1-h	-772.26855865	32.59
30	1-Os-TetrcTriPri1-o	-772.26663111	33.80
31	5-Os-PentagPrism-c	-772.26663111	33.80
32	1-Os-TetrcTriPri1-f	-772.26615530	34.10
33	3-Os-BicapCub_h	-772.26542659	34.56
34	1-Os-TetrcTriPri1-n	-772.26239897	36.46
35	2-Os-TetrcTriPri2_g_r-88	-772.26226078	36.55
36	2-Os-TetrcTriPri2_g_r-29	-772.26226077	36.55
37	5-Os-PentagPrism-e	-772.26075906	37.49
38	1-Os-TetrcTriPri1-g	-772.26075905	37.49
39	2-Os-TetrcTriPri2_g imag	-772.26001821	37.95
40	6-Os-AntiPr-b	-772.25243114	42.71
41	3-Os-BicapCub_e	-772.25163552	43.21

42	1-Os-TetrTriPri1-m	-772.25087581	43.69
43	7-Os-Isocloso-g	-772.25087581	43.69
44	4-Os-BicapSqAntipr-d	-772.25087580	43.69
45	5-Os-PentagPrism-a	-772.25005962	44.20
46	7-Os-Isocloso-h	-772.24959391	44.49
47	4-Os-BicapSqAntipr-g	-772.24959361	44.49
48	7-Os-Isocloso-a	-772.24574050	46.91
49	4-Os-BicapSqAntipr-b	-772.24298497	48.64
50	4-Os-BicapSqAntipr-a	-772.24285236	48.72
51	7-Os-Isocloso-e	-772.24285236	48.72
52	1-Os-TetrTriPri1-d	-772.24196118	49.28
53	1-Os-TetrTriPri1-p	-772.24188186	49.33
54	4-Os-BicapSqAntipr-e_r-31	-772.23533589	53.44
55	7-Os-Isocloso-d	-772.23533587	53.44
56	4-Os-BicapSqAntipr-e i-31	-772.23502672	53.63
57	7-Os-Isocloso-f	-772.23226845	55.37
58	1-Os-TetrTriPri1-b	-772.23160269	55.78
59	7-Os-Isocloso-l i-238	-772.23112878	56.08
60	2-Os-TetrTriPri2_i_r-323	-772.22714054	58.58
61	2-Os-TetrTriPri2_i i-323	-772.22489004	60.00
62	2-Os-TetrTriPri2_e	-772.22034531	62.85
63	3-Os-BicapCub_d	-772.21745873	64.66
64	6-Os-AntiPr-a	-772.21745873	64.66
65	1-Os-TetrTriPri1-c	-772.20846353	70.30
66	3-Os-BicapCub_a	-772.20844644	70.31
67	3-Os-BicapCub_f	-772.19718997	77.38
68	1-Os-TetrTriPri1-a	-772.17138095	93.57
69	8-Os-Bipypr-octag	-772.16919231	94.95

The 11-vertex $\text{Cp}_2\text{Os}_2\text{B}_9\text{H}_9$ Structures

Table S9A. Initial structures

Table S9B. Lowest energy structure distances

Table S9C. Global ranking of all structures

Table S9A. Initial structures (one example from each family); 89 structures in total

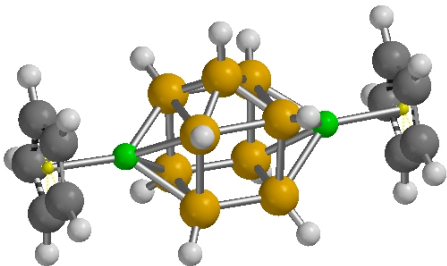
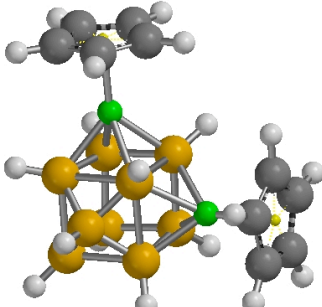
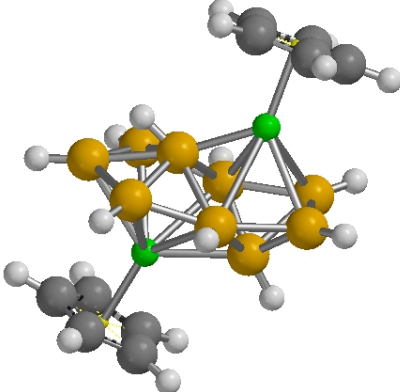
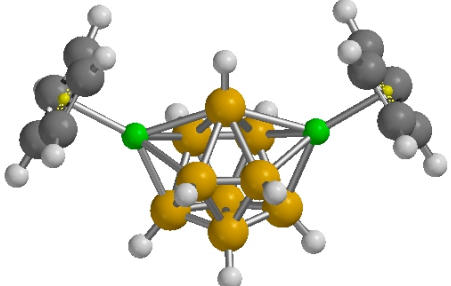
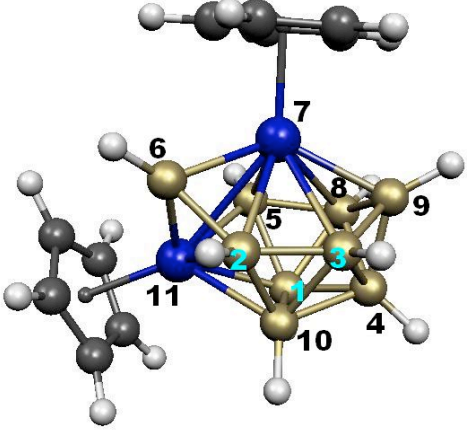
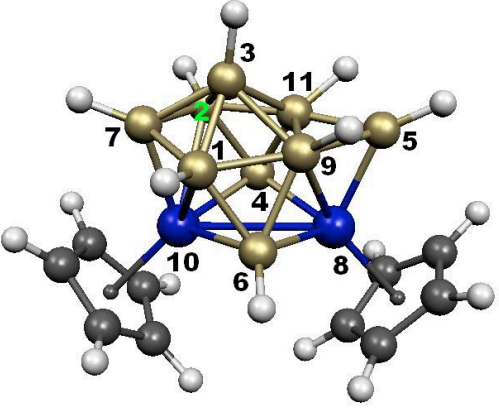
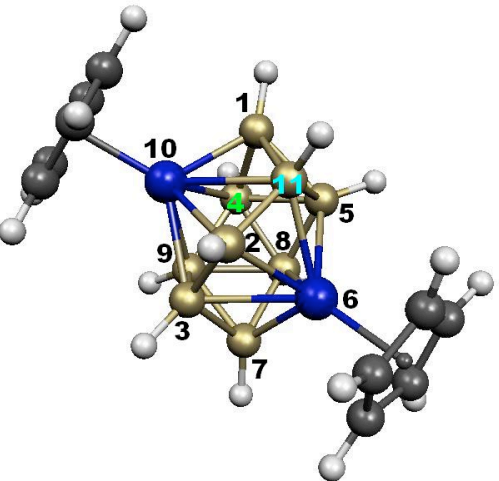
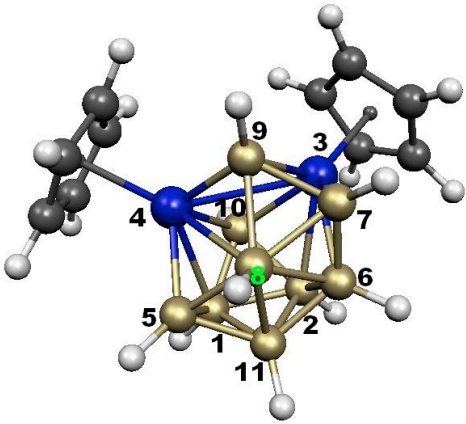
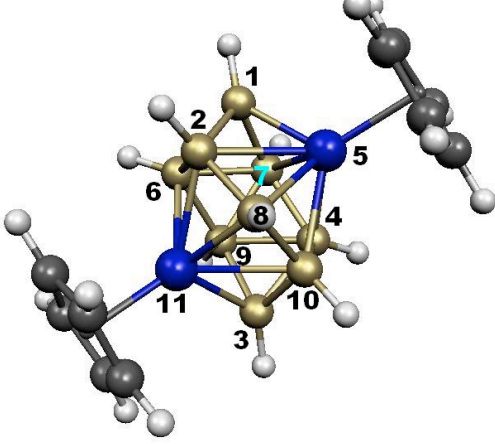
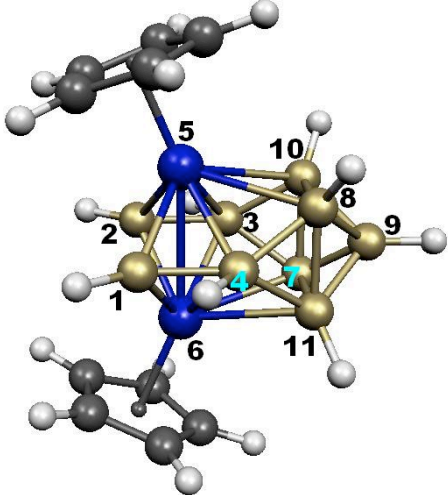
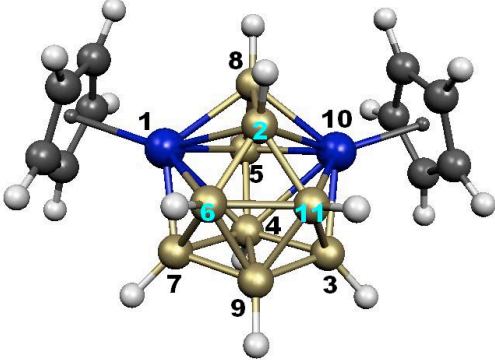
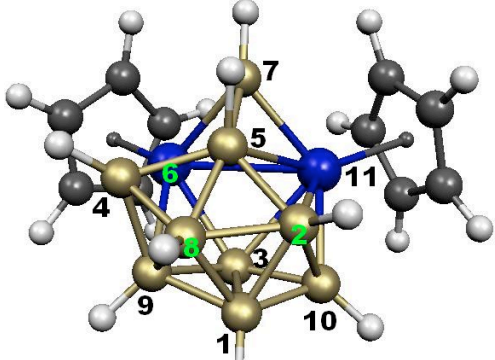
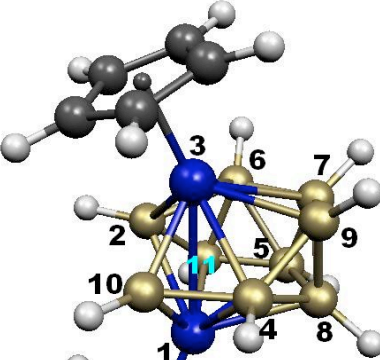
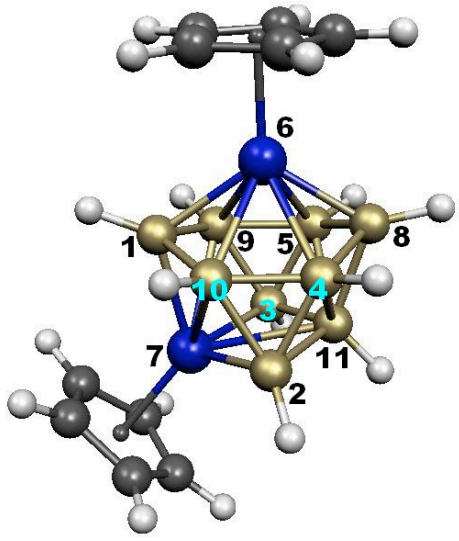
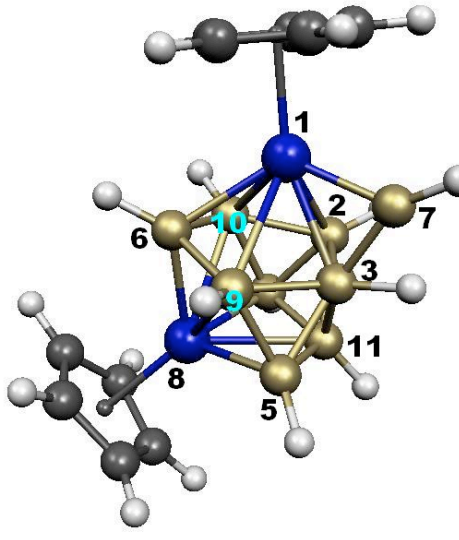
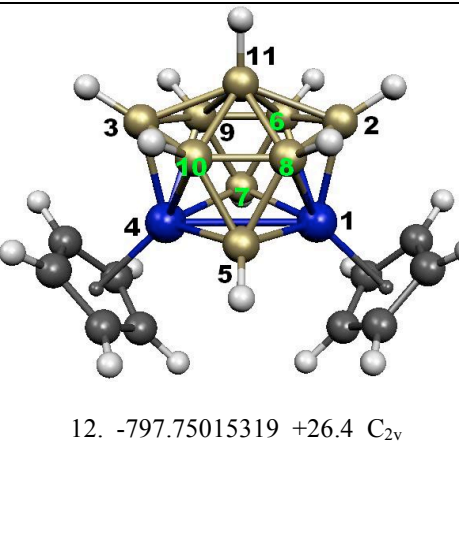
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 <p data-bbox="154 1423 787 1455">3. Octahedron fused to pentagonal bipyramid 24 structures</p>	 <p data-bbox="852 1375 1445 1438">4. Edge-coalesced icosahedrons (icosahedron without a vertex) 20 structures</p>

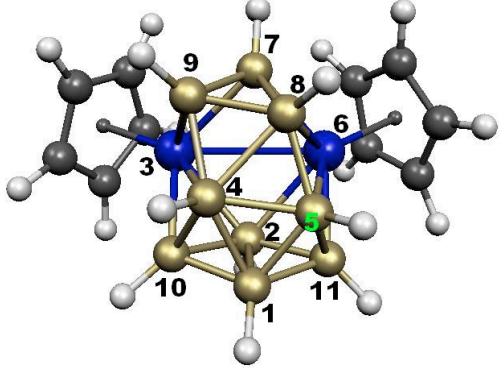
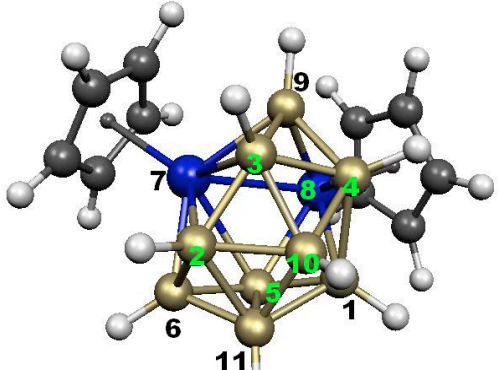
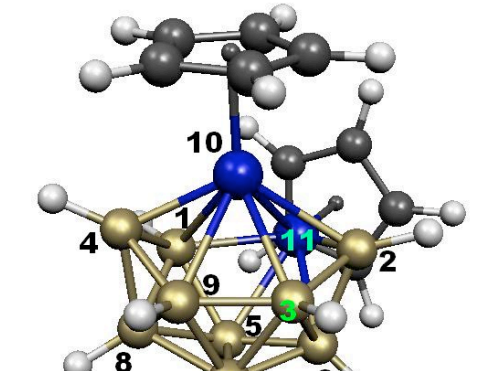
Table S9B. Distance table for the lowest energy $\text{Cp}_2\text{Os}_2\text{B}_9\text{H}_9$ structures

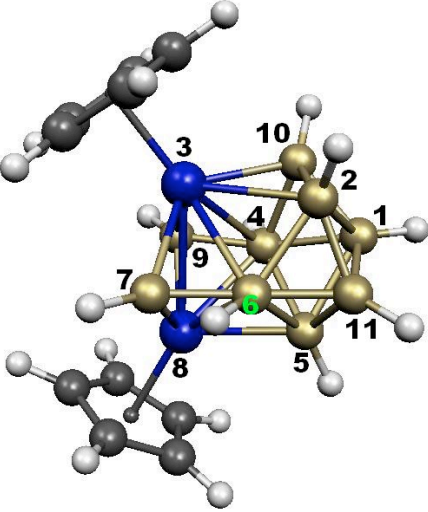
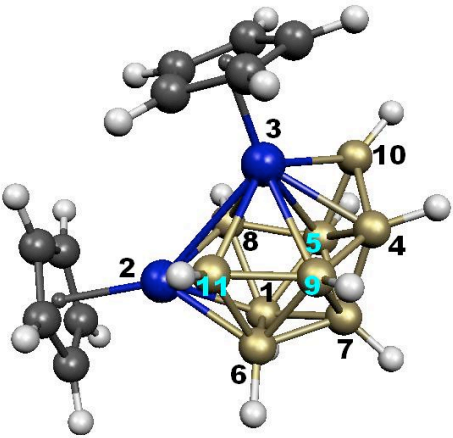
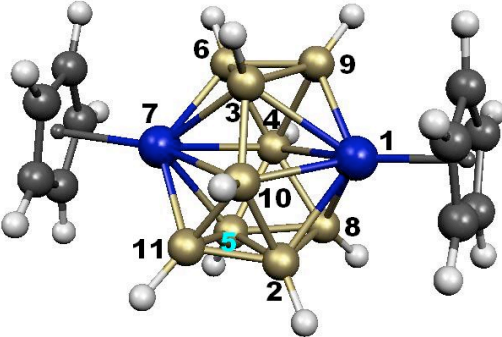
 <p>1. -797.79225403 0.0</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.994072</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.896575</td><td>1.697437</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.796363</td><td>2.918105</td><td>1.822923</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.822460</td><td>3.221450</td><td>3.460962</td><td>2.987464</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.733388</td><td>1.754645</td><td>3.171762</td><td>4.202267</td><td>3.082872</td></tr> <tr><td>7 Os</td><td>3.146540</td><td>2.326175</td><td>2.412248</td><td>3.129331</td><td>2.249189</td></tr> <tr><td>8 B</td><td>1.780856</td><td>3.430883</td><td>2.766440</td><td>1.804429</td><td>1.748637</td></tr> <tr><td>9 B</td><td>2.874722</td><td>3.038196</td><td>1.724546</td><td>1.704058</td><td>3.053342</td></tr> <tr><td>10 B</td><td>1.808029</td><td>1.762310</td><td>1.876235</td><td>1.825598</td><td>3.016609</td></tr> <tr><td>11 Os</td><td>2.255573</td><td>2.184340</td><td>3.332946</td><td>3.455081</td><td>2.114265</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Os</td><td>2.168258</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.983528</td><td>2.401159</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.961334</td><td>2.208387</td><td>1.716429</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.173302</td><td>3.180606</td><td>2.880256</td><td>2.926917</td><td>0.000000</td></tr> <tr><td>11 Os</td><td>2.040719</td><td>2.866035</td><td>3.284380</td><td>3.961704</td><td>2.243622</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.994072	0.000000				3 B	2.896575	1.697437	0.000000			4 B	1.796363	2.918105	1.822923	0.000000		5 B	1.822460	3.221450	3.460962	2.987464	0.000000	6 B	3.733388	1.754645	3.171762	4.202267	3.082872	7 Os	3.146540	2.326175	2.412248	3.129331	2.249189	8 B	1.780856	3.430883	2.766440	1.804429	1.748637	9 B	2.874722	3.038196	1.724546	1.704058	3.053342	10 B	1.808029	1.762310	1.876235	1.825598	3.016609	11 Os	2.255573	2.184340	3.332946	3.455081	2.114265		6	7	8	9	10	6 B	0.000000					7 Os	2.168258	0.000000				8 B	3.983528	2.401159	0.000000			9 B	3.961334	2.208387	1.716429	0.000000		10 B	3.173302	3.180606	2.880256	2.926917	0.000000	11 Os	2.040719	2.866035	3.284380	3.961704	2.243622
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5 B	2.152702	2.861873	3.108959	1.839496	0.000000																																																																																																														
6 B	2.293717	1.759310	2.931247	2.702037	3.522798																																																																																																														
7 B	2.063222	2.987079	2.934000	1.855723	3.108959																																																																																																														
8 B	2.137462	1.745833	3.628660	2.976422	1.821554																																																																																																														
9 B	3.245272	2.865562	1.724552	2.032495	3.615135																																																																																																														
10 Os	3.399400	2.316972	2.063222	2.417730	2.152702																																																																																																														
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4 B	1.867583	2.892458	1.769868	0.000000																																																																																																															
5 B	1.817943	2.744420	3.337910	3.068986	0.000000																																																																																																														
6 B	2.904898	1.759330	3.101254	3.721781	1.747757																																																																																																														
7 Os	3.272226	2.334772	2.365294	3.117160	2.378480																																																																																																														
8 Os	2.276633	3.759787	3.210173	2.328677	2.175148																																																																																																														
9 B	3.105007	3.141683	1.779375	1.808007	3.356191																																																																																																														
10 B	1.777040	1.792209	1.793651	1.753163	2.882032																																																																																																														
11 B	1.796469	1.804560	2.936698	3.007016	1.856744																																																																																																														
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8 Os	3.493736	2.558949	0.000000																																																																																																																
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10 B	2.923409	3.290150	3.400270	3.016202	0.000000																																																																																																														
11 B	1.720247	3.127193	3.487170	3.865590	1.774823																																																																																																														
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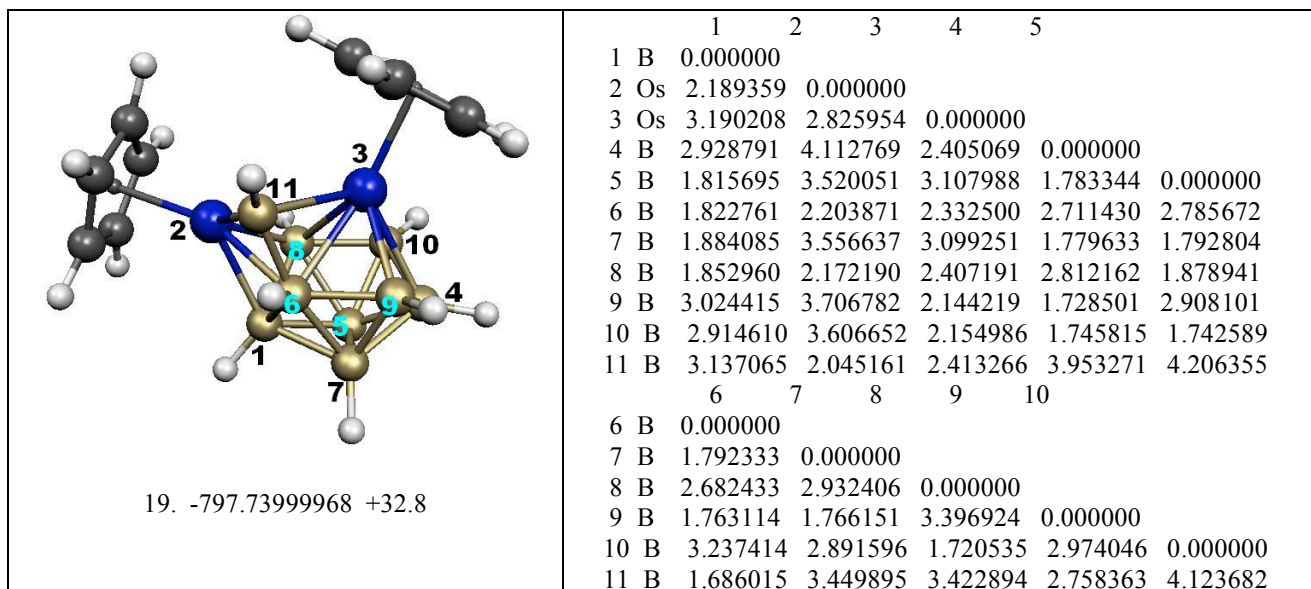


Table S9C. Energy ranking of the $\text{Cp}_2\text{Os}_2\text{B}_9\text{H}_9$ structures

1	1-Os-global minimum	-797.79225403	0.00
2	1-Os-PentaCapTrPr-d	-797.77348532	11.78
3	1-Os-PentaCapTrPr-f	-797.77348532	11.78
4	2-Os-TricapCubeA-b	-797.76702255	15.83
5	2-Os-TricapCubeB-j	-797.76701582	15.84
6	2-Os-TricapCubeA-k	-797.76649440	16.16
7	2-Os-TricapCubeA-q	-797.76649440	16.16
8	2-Os-TricapCubeB-g	-797.76649435	16.16
9	4-Os-lcos-1vx-d	-797.76644029	16.20
10	3-Os-OhfusettoPentBipyr-o	-797.76643994	16.20
11	4-Os-lcos-1vx-n	-797.76383872	17.83
12	1-Os-PentaCapTrPr-k	-797.76383871	17.83
13	2-Os-TricapCubeB-p	-797.76361798	17.97
14	2-Os-TricapCubeA-j	-797.76346454	18.07
15	1-Os-PentaCapTrPr-h	-797.75788726	21.57
16	2-Os-TricapCubeB-b	-797.75788726	21.57
17	2-Os-TricapCubeB-f	-797.75788726	21.57
18	2-Os-TricapCubeB-o	-797.75788726	21.57
19	1-Os-PentaCapTrPr-j	-797.75788724	21.57
20	1-Os-PentaCapTrPr-b	-797.75647286	22.45
21	4-Os-lcos-1vx-l	-797.75015319	26.42
22	2-Os-TricapCubeA-m	-797.74945369	26.86
23	2-Os-TricapCubeB-a	-797.74945369	26.86
24	2-Os-TricapCubeA-r	-797.74918738	27.02
25	4-Os-lcos-1vx-c	-797.74918738	27.02
26	4-Os-lcos-1vx-j	-797.74918738	27.02
27	4-Os-lcos-1vx-o	-797.74918737	27.02
28	2-Os-TricapCubeA-c	-797.74554496	29.31
29	2-Os-TricapCubeA-a	-797.74554492	29.31
30	1-Os-PentaCapTrPr-i	-797.74554491	29.31
31	2-Os-TricapCubeB-n	-797.74554491	29.31
32	2-Os-TricapCubeA-o	-797.74485961	29.74
33	4-Os-lcos-1vx-h_r-25-114	-797.74415287	30.18
34	4-Os-lcos-1vx-h_r-104	-797.74415286	30.18
35	2-Os-TricapCubeB-d	-797.74251580	31.21
36	2-Os-TricapCubeA-n	-797.74251574	31.21
37	4-Os-lcos-1vx-h_r-171-83	-797.73999968	32.79
38	4-Os-lcos-1vx-h_r-27-53	-797.73999968	32.79
39	4-Os-lcos-1vx-i	-797.73999967	32.79
40	1-Os-PentaCapTrPr-e	-797.73814905	33.95
41	4-Os-lcos-1vx-k	-797.73579475	35.43
42	2-Os-TricapCubeB-i	-797.73579474	35.43
43	4-Os-lcos-1vx-m	-797.73579474	35.43

44	4-Os-Icos-1vx-r_r-15	-797.73579474	35.43
45	2-Os-TricapCubeA-p	-797.73579473	35.43
46	4-Os-Icos-1vx-r	-797.73575348	35.45
47	2-Os-TricapCubeB-h	-797.73265890	37.40
48	2-Os-TricapCubeA-e	-797.73150479	38.12
49	2-Os-TricapCubeB-m	-797.73135717	38.21
50	4-Os-Icos-1vx-b	-797.73135717	38.21
51	4-Os-Icos-1vx-p	-797.72934693	39.47
52	1-Os-PentaCapTrPr-g	-797.72728152	40.77
53	2-Os-TricapCubeA-i	-797.72570405	41.76
54	2-Os-TricapCubeA-d	-797.72566344	41.79
55	3-Os-OhfusettoPentBipyr-f_r-221	-797.72546600	41.91
56	3-Os-OhfusettoPentBipyr-h	-797.72500230	42.20
57	2-Os-TricapCubeB-l	-797.72248552	43.78
58	2-Os-TricapCubeB-e	-797.72047481	45.04
59	2-Os-TricapCubeB-k	-797.72047481	45.04
60	4-Os-Icos-1vx-a_r-38	-797.72047477	45.04
61	2-Os-TricapCubeA-g	-797.72030684	45.15
62	4-Os-Icos-1vx-a i-38	-797.71801451	46.59
63	3-Os-OhfusettoPentBipyr-j	-797.71461946	48.72
64	4-Os-Structure-3	-797.71386890	49.19
65	2-Os-TricapCubeB-c	-797.71313785	49.65
66	4-Os-Icos-1vx-h_r-27 i-53	-797.70963552	51.84
67	4-Os-Icos-1vx-h_r-171 i-83	-797.70963551	51.84
68	4-Os-Icos-1vx-h_r-25 i-114	-797.70913033	52.16
69	4-Os-Icos-1vx-s	-797.70368766	55.58
70	2-Os-TricapCubeA-f	-797.70364589	55.60
71	4-Os-Icos-1vx-q_r-42	-797.70359846	55.63
72	4-Os-Icos-1vx-q_r-39	-797.70328211	55.83
73	4-Os-Icos-1vx-q imag	-797.70251060	56.31
74	2-Os-TricapCubeA-h	-797.69979393	58.02
75	4-Os-Icos-1vx-e	-797.69845591	58.86
76	3-Os-OhfusettoPentBipyr-g	-797.69534226	60.81
77	3-Os-OhfusettoPentBipyr-m	-797.69342467	62.02
78	3-Os-OhfusettoPentBipyr-s	-797.68977677	64.30
79	4-Os-Icos-1vx-g_r-19	-797.68509192	67.24
80	4-Os-Icos-1vx-g i-19	-797.68484987	67.40
81	3-Os-OhfusettoPentBipyr-b	-797.68188447	69.26
82	2-Os-TricapCubeA-l	-797.68139945	69.56
83	4-Os-Icos-1vx-f	-797.67557911	73.21
84	3-Os-OhfusettoPentBipyr-v	-797.67450008	73.89
85	4-Os-Icos-1vx-t	-797.67444797	73.92
86	3-Os-OhfusettoPentBipyr-l	-797.67404227	74.18
87	3-Os-OhfusettoPentBipyr-a	-797.67260028	75.08
88	3-Os-OhfusettoPentBipyr-w	-797.66301722	81.10

89	3-Os-OhfusetopentBipyr-n	-797.65641648	85.24
90	3-Os-OhfusetopentBipyr-k_r-81-394	-797.65595974	85.52
91	3-Os-OhfusetopentBipyr-k_r-422	-797.65595972	85.52
92	3-Os-OhfusetopentBipyr-k_r-83	-797.65595970	85.52
93	3-Os-OhfusetopentBipyr-q	-797.65539357	85.88
94	3-Os-OhfusetopentBipyr-p	-797.65119773	88.51
95	3-Os-OhfusetopentBipyr-c	-797.65113961	88.55
96	3-Os-OhfusetopentBipyr-i	-797.65037231	89.03
97	3-Os-OhfusetopentBipyr-d	-797.64952222	89.56
98	1-Os-PentaCapTrPr-a	-797.64842652	90.25
99	3-Os-OhfusetopentBipyr-u	-797.64708141	91.10
100	3-Os-OhfusetopentBipyr-t	-797.64486377	92.49
101	3-Os-OhfusetopentBipyr-kr-81 i-394	-797.64372732	93.20
102	3-Os-OhfusetopentBipyr-e	-797.64317968	93.54
103	3-Os-OhfusetopentBipyr-x_r-78	-797.64227446	94.11
104	3-Os-OhfusetopentBipyr-f i-221	-797.64084225	95.01
105	3-Os-OhfusetopentBipyr-x i-78	-797.63379641	99.43
106	3-Os-OhfusetopentBipyr-r	-797.63141627	100.93
107	3-Os-OhfusetopentBipyr-k imag	-797.63122908	101.04
108	4-Os-Icos-1vx-h imag	-797.60340532	118.50
109	4-Os-Bipyr-nonag	-797.58393876	130.72

The 12-vertex $\text{Cp}_2\text{Os}_2\text{B}_{10}\text{H}_{10}$ Structures

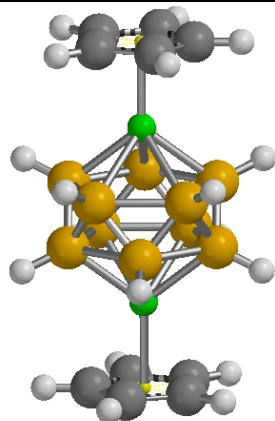
Table S10A. Initial structures

Table S10B. Distances in the lowest energy structures.

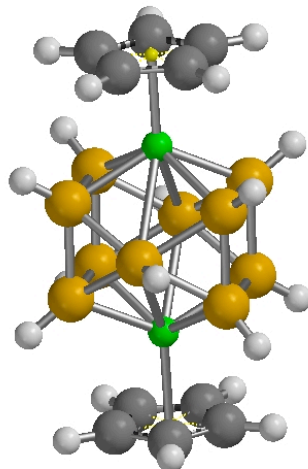
Table S10C. Global ranking of all structures

Table S10A. Initial $\text{Cp}_2\text{Os}_2\text{B}_{10}\text{H}_{10}$ structures (one example from each family); 22 structures in total

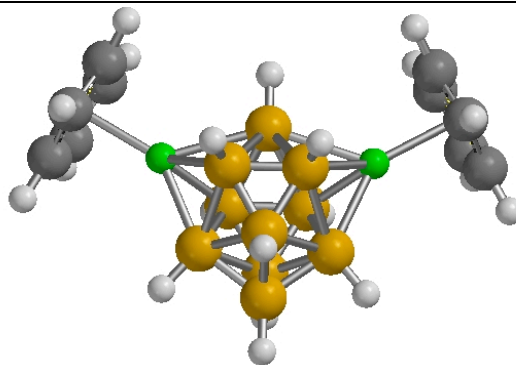
Initial structures



1. Icosahedron 3 structures

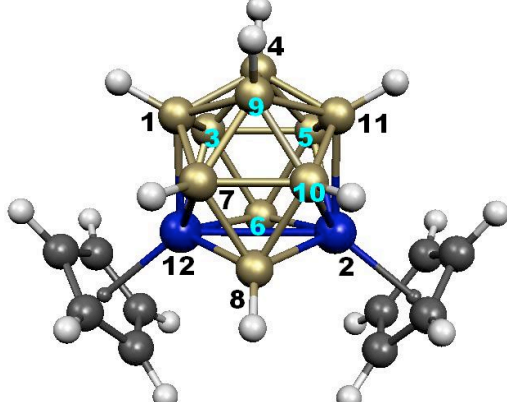
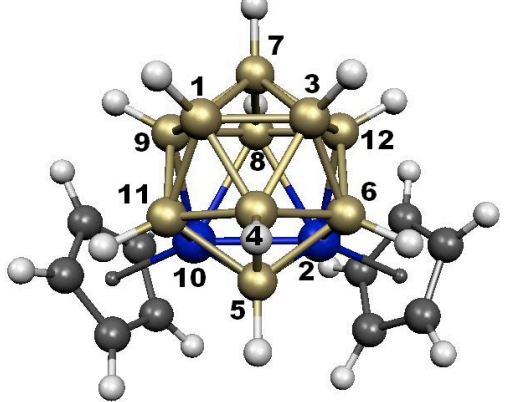


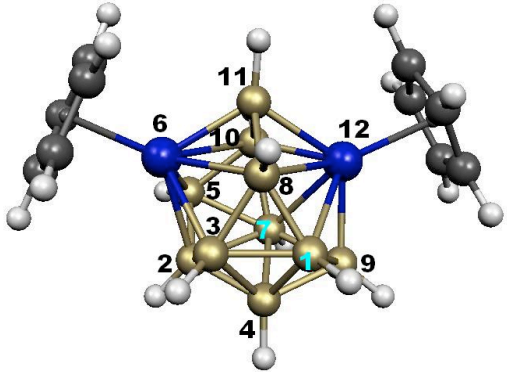
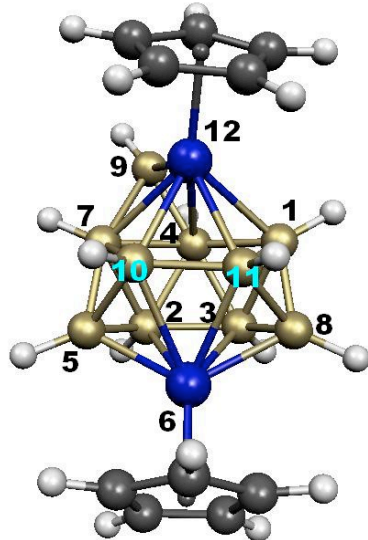
2. Cubeoctahedron 9 structures

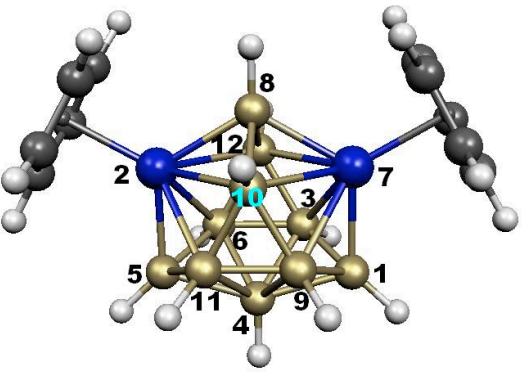
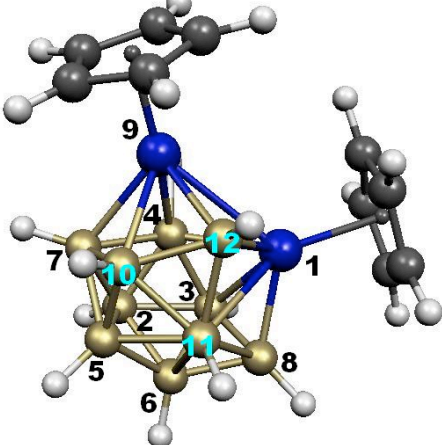


3. Anticubeoctahedron 10 structures

Table S10B.. Distance table for the lowest energy Cp₂Os₂B₁₀H₁₀ structures

 <p>1. -823.25459160 0.0 C_{2v}</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Os</td><td>3.673748</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.750179</td><td>3.241934</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.785502</td><td>3.347174</td><td>1.762035</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.915586</td><td>2.243001</td><td>1.889600</td><td>1.762035</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.130472</td><td>2.122477</td><td>1.862098</td><td>3.013429</td><td>1.862098</td></tr> <tr><td>7 B</td><td>1.757805</td><td>3.257771</td><td>3.046244</td><td>2.933601</td><td>3.619548</td></tr> <tr><td>8 B</td><td>3.263181</td><td>2.077975</td><td>3.631041</td><td>3.919267</td><td>3.631041</td></tr> <tr><td>9 B</td><td>1.825687</td><td>3.316811</td><td>2.955961</td><td>1.836989</td><td>2.955961</td></tr> <tr><td>10 B</td><td>2.984885</td><td>2.179202</td><td>3.619548</td><td>2.933601</td><td>3.046244</td></tr> <tr><td>11 B</td><td>2.877600</td><td>2.269919</td><td>2.915586</td><td>1.785502</td><td>1.750179</td></tr> <tr><td>12 Os</td><td>2.269919</td><td>2.899600</td><td>2.243001</td><td>3.347174</td><td>3.241934</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>3.579029</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.022897</td><td>2.034710</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.815901</td><td>1.746966</td><td>3.121104</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.579029</td><td>2.022400</td><td>2.034710</td><td>1.746966</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.130472</td><td>2.984885</td><td>3.263181</td><td>1.825687</td><td>1.757805</td></tr> <tr><td>12 Os</td><td>2.122477</td><td>2.179202</td><td>2.077975</td><td>3.316811</td><td>3.257771</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Os</td><td>3.673748</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Os	3.673748	0.000000				3 B	1.750179	3.241934	0.000000			4 B	1.785502	3.347174	1.762035	0.000000		5 B	2.915586	2.243001	1.889600	1.762035	0.000000	6 B	3.130472	2.122477	1.862098	3.013429	1.862098	7 B	1.757805	3.257771	3.046244	2.933601	3.619548	8 B	3.263181	2.077975	3.631041	3.919267	3.631041	9 B	1.825687	3.316811	2.955961	1.836989	2.955961	10 B	2.984885	2.179202	3.619548	2.933601	3.046244	11 B	2.877600	2.269919	2.915586	1.785502	1.750179	12 Os	2.269919	2.899600	2.243001	3.347174	3.241934		6	7	8	9	10	6 B	0.000000					7 B	3.579029	0.000000				8 B	3.022897	2.034710	0.000000			9 B	3.815901	1.746966	3.121104	0.000000		10 B	3.579029	2.022400	2.034710	1.746966	0.000000	11 B	3.130472	2.984885	3.263181	1.825687	1.757805	12 Os	2.122477	2.179202	2.077975	3.316811	3.257771		11	12				11 B	0.000000					12 Os	3.673748	0.000000			
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11 B	2.003977	2.925396	1.890831	3.393318	1.904336																																																																																																																																												
12 B	3.602713	3.086959	3.114853	2.226990	1.812175																																																																																																																																												
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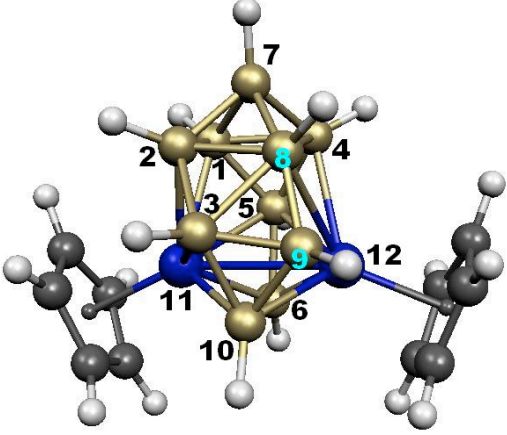
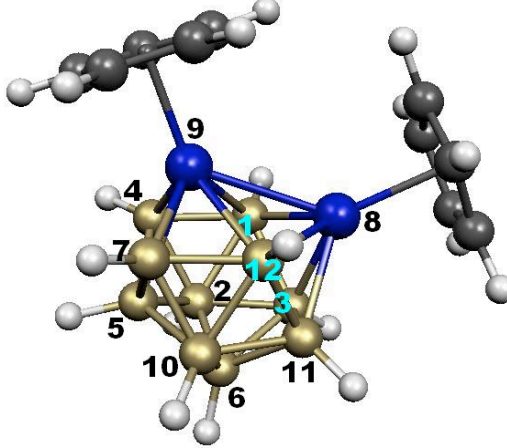
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Table S10C. Energy ranking of the $\text{Cp}_2\text{Os}_2\text{B}_{10}\text{H}_{10}$ structures.

No	Initial structure	Final energy (a.u.)	ΔE kcal/mole
1	2-Os-Cuboctaedru-g_r-103	-823.25459160	0.00
2	2-Os-Cuboctaedru-g_r-19	-823.25459155	0.00
3	2-Os-Cuboctaedru-g imag	-823.25439392	0.12
4	2-Os-Cuboctaedru-e	-823.23117850	14.69
5	1-Os-Icos-a_r-30	-823.23110523	14.74
6	1-Os-Icos-a_r-38	-823.23109728	14.74
7	1-Os-Icos-a imag	-823.23101573	14.79
8	3-Os-Anticuboh-e	-823.22763413	16.92
9	4-Os-new structure-2	-823.22347701	19.52
10	3-Os-Anticuboh-j_r-18	-823.22246461	20.16
11	3-Os-Anticuboh-j_r-959	-823.22246461	20.16
12	3-Os-Anticuboh-j_r-54	-823.22243273	20.18
13	2-Os-Cuboctaedru-h	-823.22156564	20.72
14	3-Os-Anticuboh-i_r-225	-823.22156563	20.72
15	4-Os-new structure-3	-823.22011969	21.63
16	3-Os-Structure-4	-823.21042409	27.72
17	3-Os-Anticuboh-i_r-156-130	-823.20602605	30.47
18	2-Os-Cuboctaedru-b	-823.20360606	31.99
19	3-Os-Anticuboh-h_r-120	-823.20360606	31.99
20	2-Os-Cuboctaedru-a	-823.19774616	35.67
21	3-Os-Anticuboh-a_r-56	-823.19230857	39.08
22	3-Os-Anticuboh-c	-823.19230856	39.08
23	2-Os-Cuboctaedru-d	-823.18673771	42.58
24	1-Os-Icos-b	-823.18451997	43.97
25	2-Os-Cuboctaedru-f	-823.18451997	43.97
26	3-Os-Anticuboh-d	-823.18451997	43.97
27	3-Os-Anticuboh-i_r-130	-823.18363437	44.53
28	2-Os-Cuboctaedru-i_r-32	-823.18276181	45.07
29	2-Os-Cuboctaedru-i_r-37	-823.18262989	45.16
30	1-Os-Icos-c	-823.18257184	45.19
31	2-Os-Cuboctaedru-l i-37 -32	-823.18011745	46.73
32	3-Os-Anticuboh-f	-823.16139508	58.48
33	3-Os-Anticuboh-b	-823.15830848	60.42
34	2-Os-Cuboctaedru-c	-823.15703372	61.22
35	3-Os-Anticuboh-i_r-156 i-130	-823.13045862	77.89
36	3-Os-Anticuboh-a i-56	-823.12334550	82.36
37	3-Os-Anticuboh-j imag	-823.12286861	82.66
38	3-Os-Anticuboh-g	-823.11943075	84.81
39	3-Os-Anticuboh-i_r-337	-823.11941289	84.82
40	3-Os-Anticuboh-h i-120	-823.11088845	90.17
41	3-Os-Bipypr-decag	-823.05921115	122.60
42	3-Os-Anticuboh-l imag	-823.01407361	150.93

Complete Gaussian09 Reference (reference 33)

Gaussian 09, Revision A.02,

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