

Supporting information

Novel Non-spherical Deltahedra in Trirhenaborane Structures

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Table S1B. Distance table for the lowest-lying Cp₃Re₃B₂H₂ structures.

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Table S8B. Distance table for the lowest-lying Cp₃Re₃B₉H₉ structures.

Table S8C. Energy ranking for all of the Cp₃Re₃B₉H₉ optimized structures.

Complete Gaussian09 Reference (reference 39).

Gaussian 09, Revision A.02,

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

Table S1A. Initial $\text{Cp}_3\text{Re}_3\text{B}_2\text{H}_2$ structures, 3 structures.

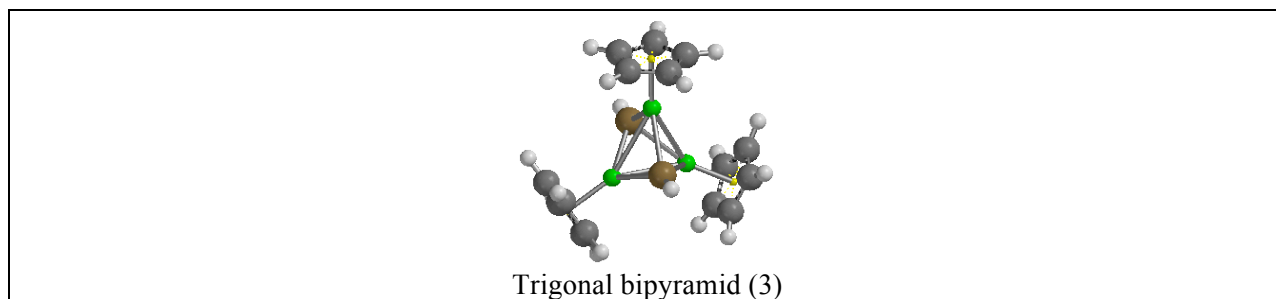


Table S1B. Distance table for the lowest-lying $\text{Cp}_3\text{Re}_3\text{B}_2\text{H}_2$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

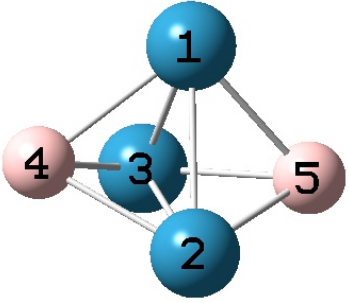
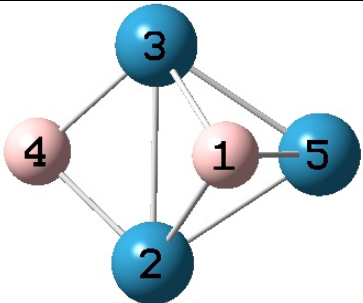
 <p>1. -866.441412 0.0 C_{2v}</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr> <td>1 Re</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 Re</td> <td>2.460308</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 Re</td> <td>2.405719</td> <td>2.826816</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 B</td> <td>2.178413</td> <td>2.190675</td> <td>2.161148</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>2.178156</td> <td>2.191866</td> <td>2.156977</td> <td>3.162801</td> <td>0.000000</td> </tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 Re	2.460308	0.000000				3 Re	2.405719	2.826816	0.000000			4 B	2.178413	2.190675	2.161148	0.000000		5 B	2.178156	2.191866	2.156977	3.162801	0.000000
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Table S2A. Initial $\text{Cp}_3\text{Re}_3\text{B}_3\text{H}_3$ structures, 6 structures.

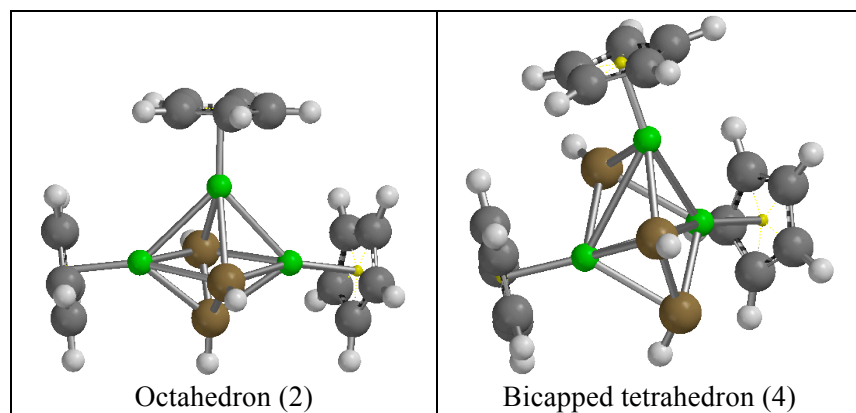


Table S2B. Distance table for the lowest-lying $\text{Cp}_3\text{Re}_3\text{B}_3\text{H}_3$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

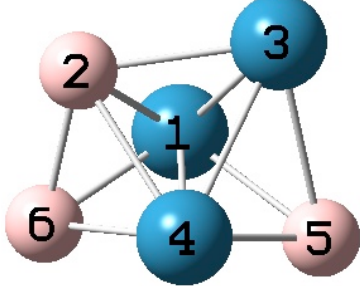
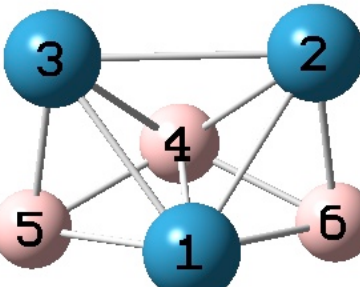
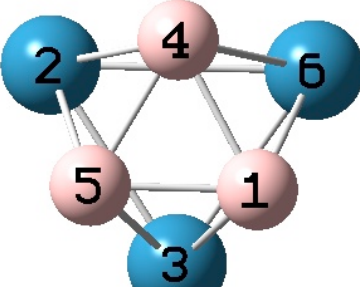
 <p>1. -891.9534200 0.0 (C_s)</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr> <td>1 Re</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 B</td> <td>2.303838</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 Re</td> <td>2.445662</td> <td>2.136284</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 Re</td> <td>2.907780</td> <td>2.221371</td> <td>2.398353</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>2.175838</td> <td>3.219497</td> <td>2.297883</td> <td>2.129146</td> <td>0.000000</td> </tr> <tr> <td>6 B</td> <td>2.087477</td> <td>1.829685</td> <td>3.243648</td> <td>2.124336</td> <td>2.927222</td> </tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 B	2.303838	0.000000				3 Re	2.445662	2.136284	0.000000			4 Re	2.907780	2.221371	2.398353	0.000000		5 B	2.175838	3.219497	2.297883	2.129146	0.000000	6 B	2.087477	1.829685	3.243648	2.124336	2.927222
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No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	06v-02-BicappTd b	-891.7297067	0.00
2	06v-01-Oh a _r-42	-891.7297046	0.00
3	06v-01-Oh a _i-42	-891.7287526	0.60
4	06v-02-BicappTd a	-891.7034819	16.46
5	06v-01-Oh b	-891.6729594	35.61

Table S3A. Initial $\text{Cp}_3\text{Re}_3\text{B}_4\text{H}_4$ structures, 21 structures.

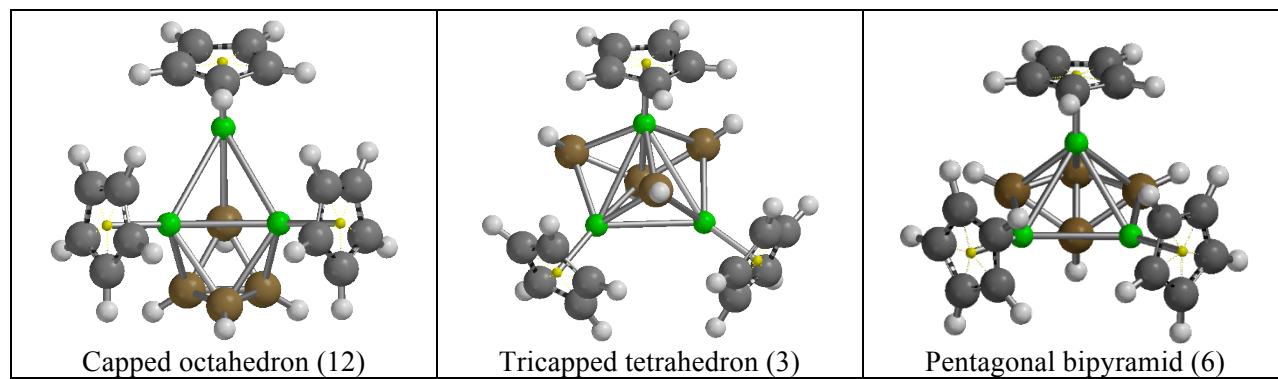
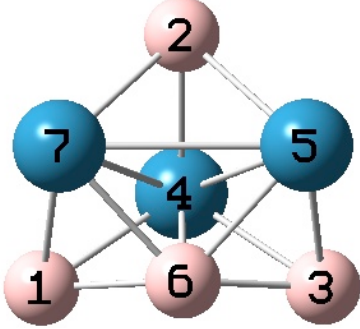
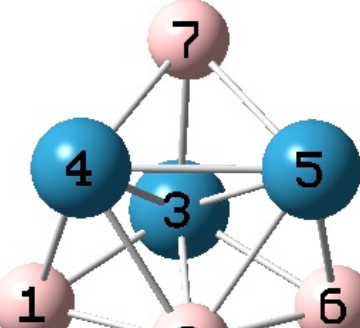
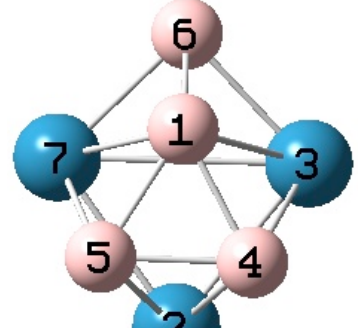


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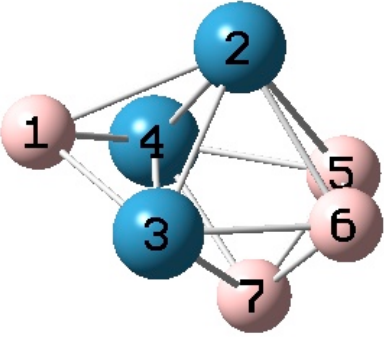
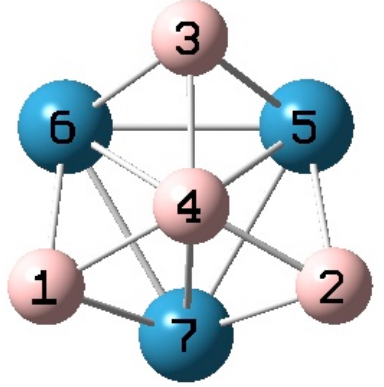
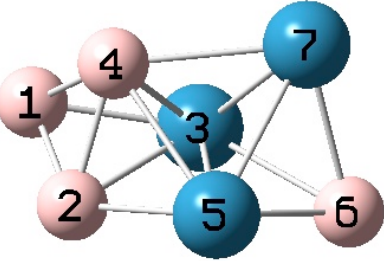
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Table S3C. Energy ranking for all of the Cp₃Re₃B₄H₄ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	07v-01-CapOh d	-917.1960783	0.00
2	07v-02-TricapTd a	-917.1960773	0.00
3	07v-01-CapOh e	-917.1960753	0.00
4	07v-02-TricapTd b	-917.1855134	6.63
5	07v-01-CapOh b	-917.1812464	9.31
6	07v-01-CapOh c _i-20	-917.1799178	10.14
7	07v-03-PentBipyr b	-917.1799043	10.15
8	07v-01-CapOh c _r-20	-917.1797787	10.23
9	07v-02-TricapTd c	-917.1687897	17.12
10	07v-03-PentBipyr c	-917.1687470	17.15
11	07v-03-PentBipyr d _r-31	-917.1685615	17.27
12	07v-03-PentBipyr d _i-31	-917.1681591	17.52
13	07v-01-CapOh j	-917.1553723	25.54
14	07v-01-CapOh l	-917.1517259	27.83
15	07v-01-CapOh h	-917.1517165	27.84
16	07v-01-CapOh k	-917.1467260	30.97
17	07v-03-PentBipyr a	-917.1440511	32.65
18	07v-03-PentBipyr f	-917.1315602	40.49
19	07v-01-CapOh a _r-68	-917.1303480	41.25
20	07v-01-CapOh a _i-68	-917.1277030	42.91
21	07v-01-CapOh f _r-31	-917.1238127	45.35
22	07v-01-CapOh f _i-31	-917.1223875	46.24
23	07v-01-CapOh g	-917.1198923	47.81
24	07v-01-CapOh i	-917.1057128	56.71
25	07v-03-PentBipyr e _i-37	-917.0904312	66.30
26	07v-03-PentBipyr e _r-37	-917.0903893	66.32

Table S4A. Initial $\text{Cp}_3\text{Re}_3\text{B}_5\text{H}_5$ structures, 51 structures.

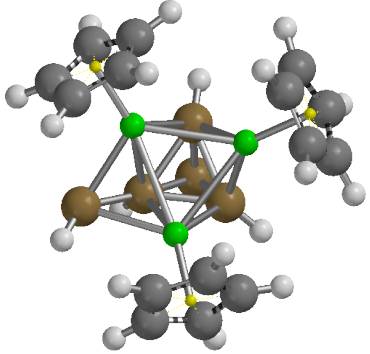
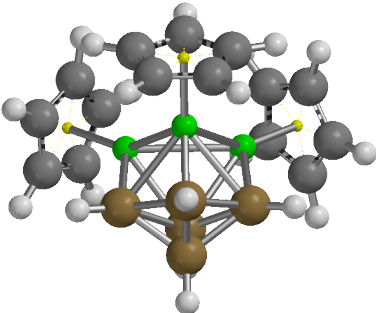
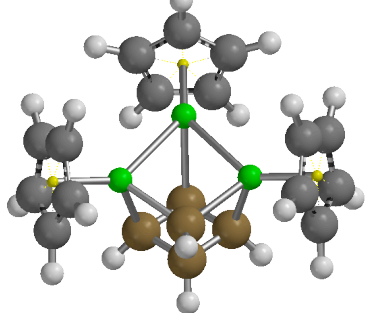
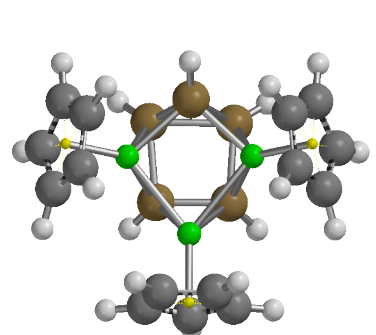
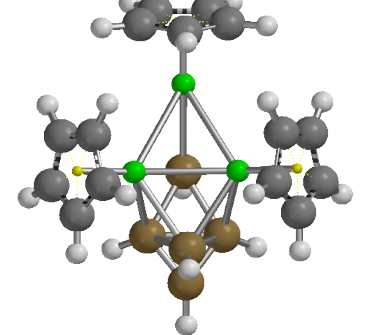
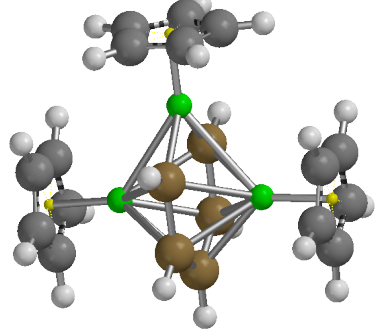
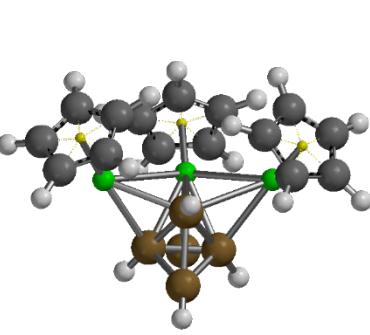
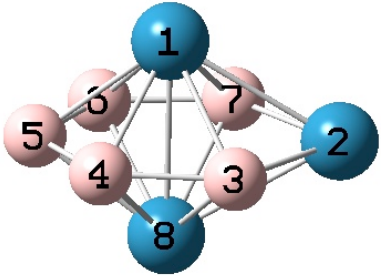
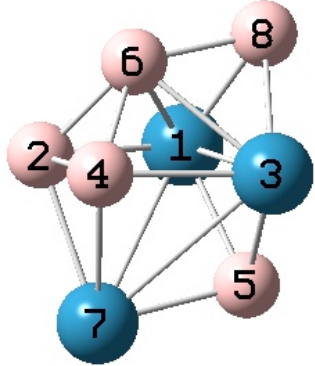
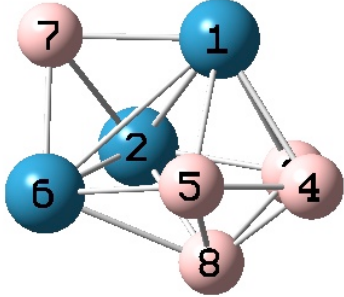
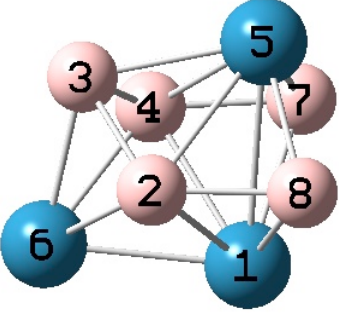
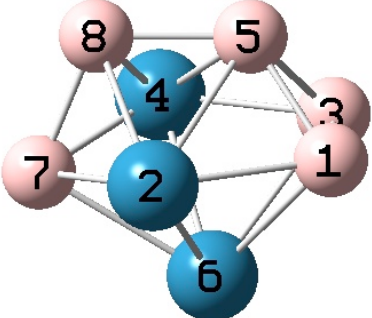
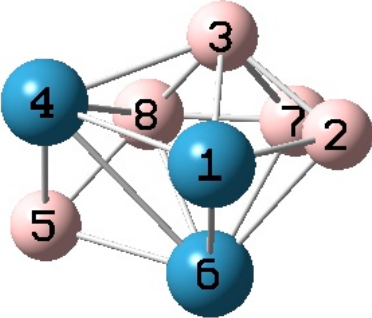
<p>Initial structures</p>	 <p>Dicapped octahedron (11)</p>
 <p>Bisdisphenoid (9)</p>	 <p>Cube (4)</p>
 <p>Antiprism (4)</p>	 <p>Trigonal antiprism (8)</p>
 <p>Hexagonal bipyramid (7)</p>	 <p>All capped tetrahedron (8)</p>

Table S4B. Distance table for the lowest-lying Cp₃Re₃B₅H₅ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

 <p>1. -942.9328102 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 Re</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>2 Re</td> <td>2.606689</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>3 B</td> <td>2.266248</td> <td>2.127726</td> <td>0.000000</td> <td></td> <td></td> </tr> <tr> <td>4 B</td> <td>2.182033</td> <td>3.462758</td> <td>1.760184</td> <td>0.000000</td> <td></td> </tr> <tr> <td>5 B</td> <td>2.192598</td> <td>3.979775</td> <td>3.068192</td> <td>1.706789</td> <td>0.000000</td> </tr> <tr> <td>6 B</td> <td>2.184915</td> <td>3.460037</td> <td>3.562323</td> <td>2.959055</td> <td>1.706354</td> </tr> <tr> <td>7 B</td> <td>2.267974</td> <td>2.124583</td> <td>3.241625</td> <td>3.561145</td> <td>3.065814</td> </tr> <tr> <td>8 Re</td> <td>2.667326</td> <td>2.604968</td> <td>2.270887</td> <td>2.179516</td> <td>2.193784</td> </tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td></td> <td></td> </tr> <tr> <td>6 B</td> <td>0.000000</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>7 B</td> <td>1.757660</td> <td>0.000000</td> <td></td> <td></td> <td></td> </tr> <tr> <td>8 Re</td> <td>2.181244</td> <td>2.272207</td> <td>0.000000</td> <td></td> <td></td> </tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 Re	2.606689	0.000000				3 B	2.266248	2.127726	0.000000			4 B	2.182033	3.462758	1.760184	0.000000		5 B	2.192598	3.979775	3.068192	1.706789	0.000000	6 B	2.184915	3.460037	3.562323	2.959055	1.706354	7 B	2.267974	2.124583	3.241625	3.561145	3.065814	8 Re	2.667326	2.604968	2.270887	2.179516	2.193784		6	7	8			6 B	0.000000					7 B	1.757660	0.000000				8 Re	2.181244	2.272207	0.000000		
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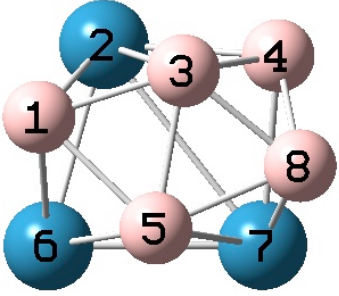
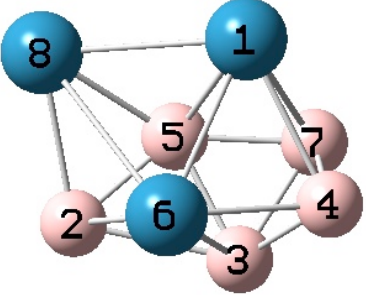
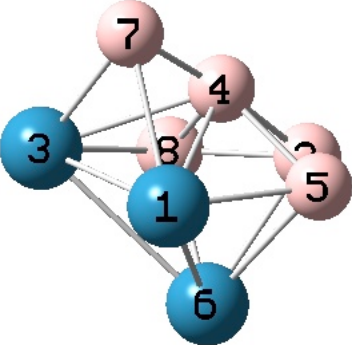
 <p>7. -942.8891070 +27.4 C₁</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Re</td><td>2.129356</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.759035</td><td>2.351836</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.022860</td><td>2.110262</td><td>1.809151</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.855959</td><td>3.011013</td><td>1.822570</td><td>2.773235</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>2.180029</td><td>2.392360</td><td>3.179633</td><td>3.434085</td><td>2.243398</td></tr> <tr><td>7 Re</td><td>3.409481</td><td>2.916940</td><td>3.006224</td><td>2.255639</td><td>2.346763</td></tr> <tr><td>8 B</td><td>3.025344</td><td>3.260118</td><td>1.725618</td><td>1.770188</td><td>1.795387</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td></td> <td></td> </tr> <tr><td>6 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Re</td><td>2.441396</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.464823</td><td>2.103709</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Re	2.129356	0.000000				3 B	1.759035	2.351836	0.000000			4 B	3.022860	2.110262	1.809151	0.000000		5 B	1.855959	3.011013	1.822570	2.773235	0.000000	6 Re	2.180029	2.392360	3.179633	3.434085	2.243398	7 Re	3.409481	2.916940	3.006224	2.255639	2.346763	8 B	3.025344	3.260118	1.725618	1.770188	1.795387		6	7	8			6 Re	0.000000					7 Re	2.441396	0.000000				8 B	3.464823	2.103709	0.000000		
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Table S4C. Energy ranking for all of the Cp₃Re₃B₅H₅ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	08v-06-Bipireex_re a	-942.6499348	0.00
2	08v-06-Bipireex_re c	-942.6392326	6.72
3	08v-02-Bisdisph_re e	-942.6392279	6.72
4	08v-05-AntiprTrig_re e	-942.6392250	6.72
5	08v-03-Cube-re c	-942.6392246	6.72
6	08v-01-DicapOh_re h	-942.6392151	6.73
7	08v-01-DicapOh_re c	-942.6326545	10.84
8	08v-04-Antipr_re d	-942.6324644	10.96
9	08v-02-Bisdisph_re h _i-12	-942.6323409	11.04
10	08v-02-Bisdisph_re h _r-12	-942.6322929	11.07
11	08v-05-AntiprTrig_re g	-942.6299197	12.56
12	08v-03-Cube-re b	-942.6286897	13.33
13	08v-04-Antipr_re b	-942.6283881	13.52
14	08v-04-Antipr_re a	-942.6283877	13.52
15	08v-02-Bisdisph_re c	-942.6283653	13.54
16	08v-07-Tdallcap_re c	-942.6283646	13.54
17	08v-02-Bisdisph_re g _r-22	-942.6278938	13.83
18	08v-02-Bisdisph_re g _i-22	-942.6274290	14.12
19	08v-07-Tdallcap_re h	-942.6259391	15.06
20	08v-07-Tdallcap_re d	-942.6135971	22.80
21	08v-07-Tdallcap_re b	-942.6135960	22.80
22	08v-03-Cube-re a	-942.6135933	22.81
23	08v-01-DicapOh_re g	-942.6135902	22.81
24	08v-06-Bipireex_re f	-942.6119385	23.84
25	08v-01-DicapOh_re b _i-34	-942.6110809	24.38
26	08v-01-DicapOh_re b _r-34	-942.6108209	24.54
27	08v-03-Cube-re d	-942.6072503	26.79
28	08v-05-AntiprTrig_re f	-942.6072503	26.79
29	08v-06-Bipireex_re d	-942.6072117	26.81
30	08v-01-DicapOh_re e	-942.6063000	27.38
31	08v-02-Bisdisph_re b	-942.6033783	29.22
32	08v-04-Antipr_re c	-942.6033122	29.26
33	08v-07-Tdallcap_re f	-942.6001414	31.25
34	08v-07-Tdallcap_re a	-942.5933278	35.52
35	08v-05-AntiprTrig_re b	-942.5917148	36.53
36	08v-07-Tdallcap_re g	-942.5911659	36.88
37	08v-02-Bisdisph_re a	-942.5909139	37.04

38	08v-01-DicapOh_re i	-942.5896298	37.84
39	08v-02-Bisdisph_re d	-942.5891803	38.12
40	08v-01-DicapOh_re k	-942.5863539	39.90
41	08v-06-Bipireex_re e	-942.5794550	44.23
42	08v-05-AntiprTrig_re a	-942.5794512	44.23
43	08v-02-Bisdisph_re f	-942.5786788	44.71
44	08v-02-Bisdisph_re i	-942.5706050	49.78
45	08v-06-Bipireex_re b	-942.5693774	50.55
46	08v-01-DicapOh_re d	-942.5669221	52.09
47	08v-01-DicapOh_re a	-942.5655155	52.97
48	08v-01-DicapOh_re f	-942.5622852	55.00
49	08v-07-Tdallcap_re e	-942.5471122	64.52
50	08v-05-AntiprTrig_re h	-942.5458102	65.34
51	08v-01-DicapOh_re j	-942.5334574	73.09
52	08v-05-AntiprTrig_re c	-942.5265850	77.40
53	08v-05-AntiprTrig_re d	-942.5265849	77.40

Table S5A. Initial $\text{Cp}_3\text{Re}_3\text{B}_6\text{H}_6$ structures, 55 structures.

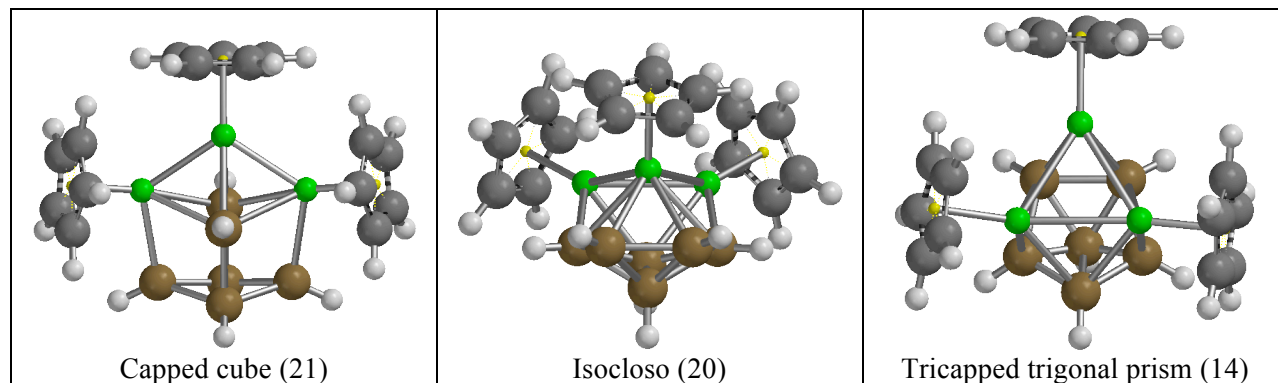
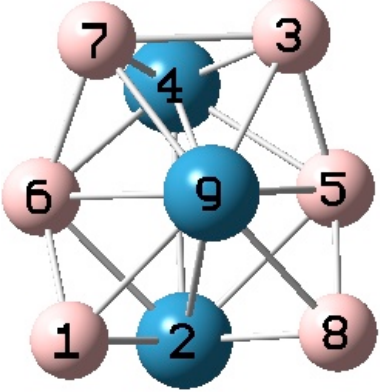
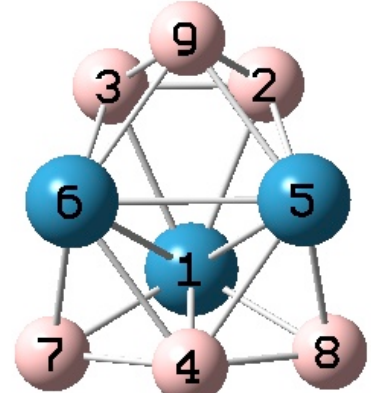
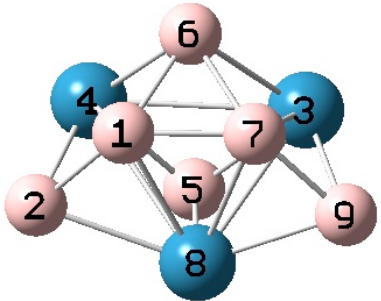
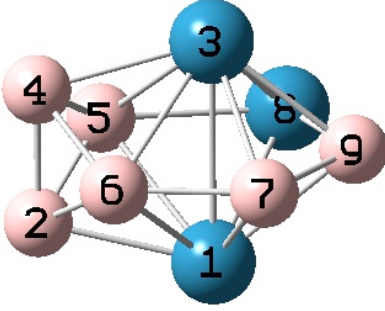
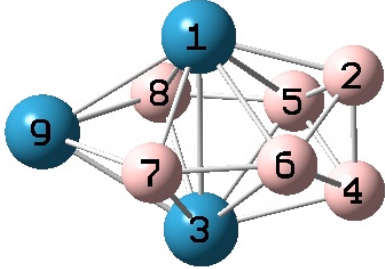
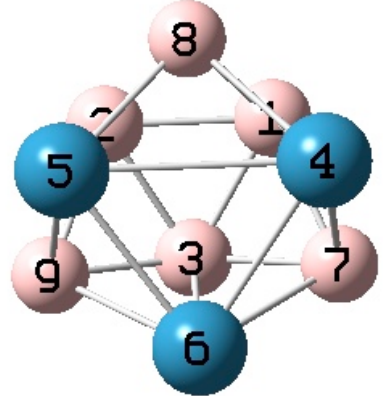


Table S5B. Distance table for the lowest-lying $\text{Cp}_3\text{Re}_3\text{B}_6\text{H}_6$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -968.4254255 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 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Re</td><td>2.043289</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>4.006405</td><td>3.598477</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Re</td><td>3.534431</td><td>2.721175</td><td>2.041483</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.462501</td><td>2.289339</td><td>1.849449</td><td>2.174010</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.742496</td><td>2.292059</td><td>3.149453</td><td>2.177267</td><td>3.129007</td></tr> <tr><td>7 B</td><td>3.179167</td><td>3.597802</td><td>2.068096</td><td>2.043022</td><td>3.142641</td></tr> <tr><td>8 B</td><td>2.855023</td><td>2.040420</td><td>3.178102</td><td>3.532505</td><td>1.745050</td></tr> <tr><td>9 Re</td><td>2.244180</td><td>2.776954</td><td>2.190301</td><td>2.927234</td><td>2.307667</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>7 B</td><td>1.852740</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>3.458224</td><td>3.995617</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Re</td><td>2.306336</td><td>2.182123</td><td>2.238682</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Re	2.043289	0.000000				3 B	4.006405	3.598477	0.000000			4 Re	3.534431	2.721175	2.041483	0.000000		5 B	3.462501	2.289339	1.849449	2.174010	0.000000	6 B	1.742496	2.292059	3.149453	2.177267	3.129007	7 B	3.179167	3.597802	2.068096	2.043022	3.142641	8 B	2.855023	2.040420	3.178102	3.532505	1.745050	9 Re	2.244180	2.776954	2.190301	2.927234	2.307667		6	7	8	9		7 B	1.852740	0.000000				8 B	3.458224	3.995617	0.000000			9 Re	2.306336	2.182123	2.238682	0.000000	
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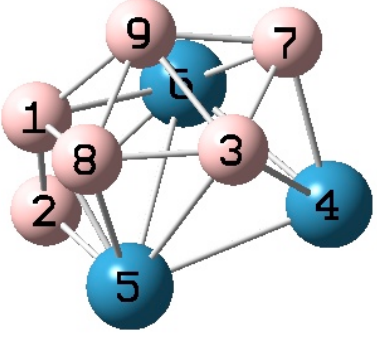
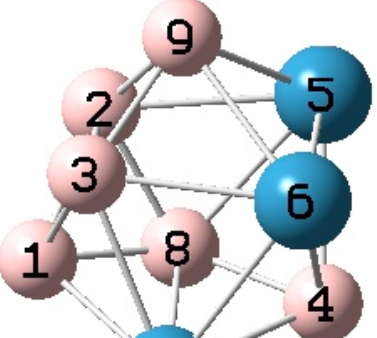
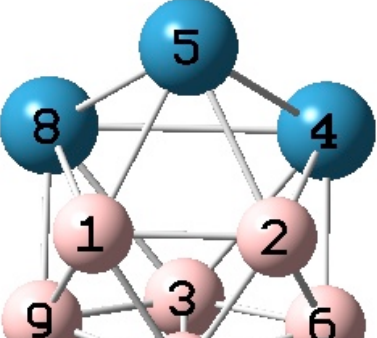
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Table S5C. Energy ranking for all of the $\text{Cp}_3\text{Re}_3\text{B}_6\text{H}_6$ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	09v-01-PressCapCube__Re l	-968.1326974	0.00
2	09v-03-TricTrPrism__Re m __r-103	-968.1325838	0.07
3	09v-03-TricTrPrism__Re j __r-15	-968.1222372	6.56
4	09v-03-TricTrPrism__Re j __i-15	-968.1220467	6.68
5	09v-03-TricTrPrism__Re h	-968.1116228	13.22
6	09v-02-Tl99__Re n __r-44	-968.1114761	13.32
7	09v-02-Tl99__Re n __i-44	-968.1107054	13.80
8	09v-01-PressCapCube__Re p	-968.1079784	15.51
9	09v-03-TricTrPrism__Re e	-968.1079748	15.51
10	09v-01-PressCapCube__Re c __i-17	-968.0969311	22.44
11	09v-01-PressCapCube__Re c __r-17	-968.0968813	22.48
12	09v-01-PressCapCube__Re o	-968.0964124	22.77
13	09v-01-PressCapCube__Re t __r-135	-968.0952157	23.52
14	09v-01-PressCapCube__Re m __r-145	-968.0932564	24.75
15	09v-01-PressCapCube__Re s	-968.0908309	26.27
16	09v-02-Tl99__Re l	-968.0908308	26.27
17	09v-03-TricTrPrism__Re a	-968.0908281	26.27
18	09v-01-PressCapCube__Re d __r-234	-968.0906137	26.41
19	09v-03-TricTrPrism__Re i	-968.0905839	26.43
20	09v-02-Tl99__Re d	-968.0905552	26.45
21	09v-03-TricTrPrism__Re c	-968.0905533	26.45
22	09v-02-Tl99__Re e	-968.0905489	26.45
23	09v-03-TricTrPrism__Re g	-968.0905461	26.45
24	09v-03-TricTrPrism__Re n __r-102	-968.0879266	28.09
25	09v-03-TricTrPrism__Re k	-968.0869033	28.74
26	09v-02-Tl99__Re i	-968.0868927	28.74
27	09v-02-Tl99__Re c __r-803	-968.0822852	31.63
28	09v-01-PressCapCube__Re m __i-145	-968.0812718	32.27
29	09v-03-TricTrPrism__Re m __i-103	-968.0810267	32.42
30	09v-02-Tl99__Re p	-968.0790288	33.68
31	09v-01-PressCapCube__Re f __r-39	-968.0779306	34.37
32	09v-01-PressCapCube__Re i	-968.0778837	34.40
33	09v-02-Tl99__Re g	-968.0767224	35.13
34	09v-02-Tl99__Re q	-968.0766388	35.18
35	09v-02-Tl99__Re r	-968.0766388	35.18
36	09v-02-Tl99__Re j	-968.0766289	35.18
37	09v-01-PressCapCube__Re f __i-39	-968.0763818	35.34

38	09v-02-TI99__Re t _r-13	-968.0760767	35.53
39	09v-02-TI99__Re t _i-13	-968.0750538	36.17
40	09v-02-TI99__Re b	-968.0730687	37.42
41	09v-02-TI99__Re h	-968.0709351	38.76
42	09v-03-TricTrPrism__Re b	-968.0709351	38.76
43	09v-01-PressCapCube__Re g	-968.0709350	38.76
44	09v-03-TricTrPrism__Re f	-968.0696592	39.56
45	09v-01-PressCapCube__Re e	-968.0684016	40.35
46	09v-01-PressCapCube__Re n _r-92	-968.0662932	41.67
47	09v-03-TricTrPrism__Re d	-968.0658488	41.95
48	09v-01-PressCapCube__Re u	-968.0641340	43.02
49	09v-02-TI99__Re f	-968.0599202	45.67
50	09v-03-TricTrPrism__Re l	-968.0564982	47.82
51	09v-01-PressCapCube__Re q	-968.0562819	47.95
52	09v-02-TI99__Re s	-968.0543996	49.13
53	09v-02-TI99__Re k	-968.0518574	50.73
54	09v-01-PressCapCube__Re b	-968.0511942	51.14
55	09v-01-PressCapCube__Re n _i-92	-968.0488493	52.62
56	09v-03-TricTrPrism__Re n _i-102	-968.0484218	52.88
57	09v-01-PressCapCube__Re j	-968.0465537	54.06
58	09v-02-TI99__Re o	-968.0463664	54.17
59	09v-01-PressCapCube__Re t _i-135	-968.0361032	60.61
60	09v-02-TI99__Re c _i-803	-968.0320657	63.15
61	09v-01-PressCapCube__Re k	-968.0304216	64.18
62	09v-02-TI99__Re m	-968.0274668	66.03
63	09v-02-TI99__Re a	-968.0251573	67.48
64	09v-01-PressCapCube__Re r _r-26	-968.0027440	81.55
65	09v-01-PressCapCube__Re r _i-26	-968.0017691	82.16
66	09v-01-PressCapCube__Re a _r-77	-967.9951146	86.34
67	09v-01-PressCapCube__Re h	-967.9851315	92.60
68	09v-01-PressCapCube__Re a _i-77	-967.9837385	93.47
69	09v-01-PressCapCube__Re d _i-234	-967.9735126	99.89

Table S6A. Initial $\text{Cp}_3\text{Re}_3\text{B}_7\text{H}_7$ structures, 110 structures.

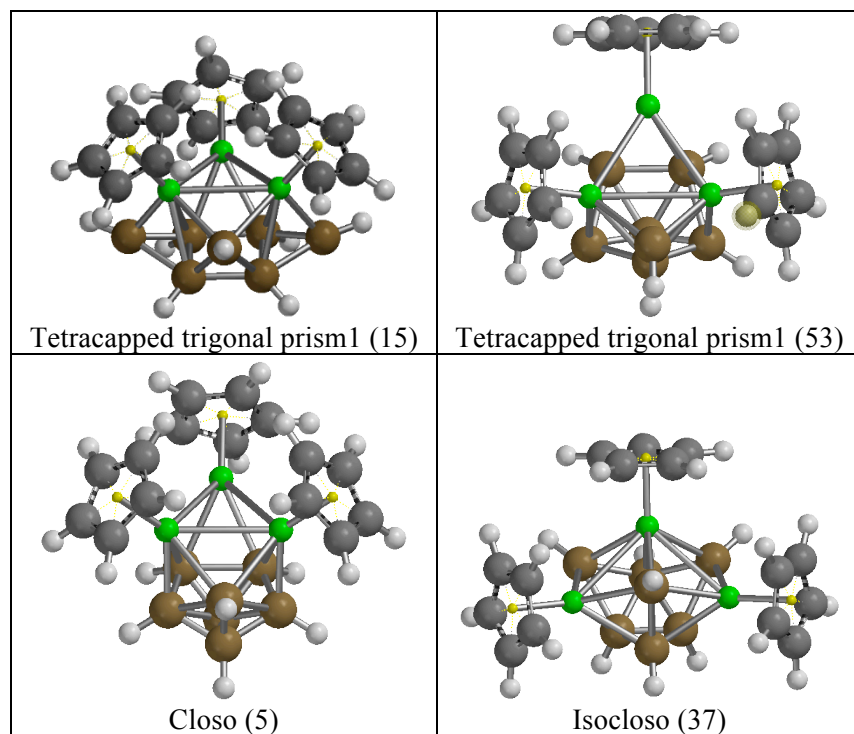
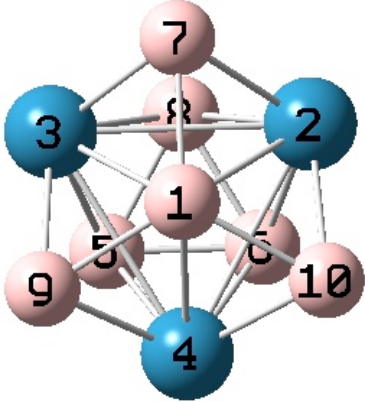
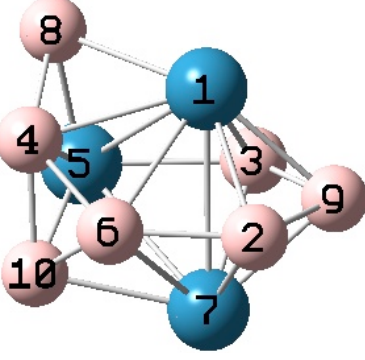
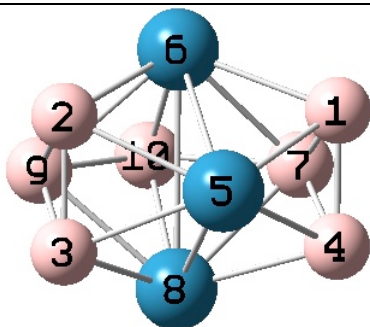


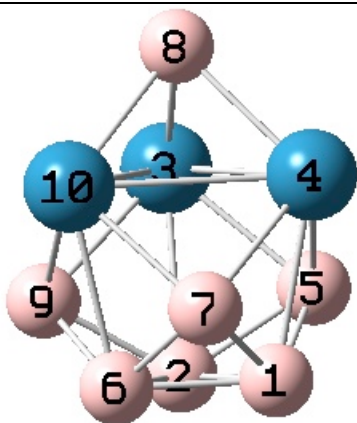
Table S6B. Distance table for the lowest-lying Cp₃Re₃B₇H₇ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -993.92792330 0.0 C_{3v}</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 Re</td><td>2.281709</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.283191</td><td>2.837007</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Re</td><td>2.284783</td><td>2.837747</td><td>2.835439</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.460335</td><td>3.138575</td><td>2.237531</td><td>2.241891</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.459196</td><td>2.242786</td><td>3.135078</td><td>2.238961</td><td>1.699462</td></tr> <tr><td>7 B</td><td>1.836565</td><td>2.090081</td><td>2.090905</td><td>3.630714</td><td>3.797305</td></tr> <tr><td>8 B</td><td>3.457251</td><td>2.239541</td><td>2.239092</td><td>3.135284</td><td>1.698365</td></tr> <tr><td>9 B</td><td>1.838599</td><td>3.631072</td><td>2.090575</td><td>2.092114</td><td>3.027130</td></tr> <tr><td>10 B</td><td>1.835406</td><td>2.092168</td><td>3.629143</td><td>2.090861</td><td>3.800662</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>3.798532</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.698547</td><td>3.023047</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.798823</td><td>3.104824</td><td>3.798553</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.027372</td><td>3.105196</td><td>3.797837</td><td>3.103219</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Re	2.281709	0.000000				3 Re	2.283191	2.837007	0.000000			4 Re	2.284783	2.837747	2.835439	0.000000		5 B	3.460335	3.138575	2.237531	2.241891	0.000000	6 B	3.459196	2.242786	3.135078	2.238961	1.699462	7 B	1.836565	2.090081	2.090905	3.630714	3.797305	8 B	3.457251	2.239541	2.239092	3.135284	1.698365	9 B	1.838599	3.631072	2.090575	2.092114	3.027130	10 B	1.835406	2.092168	3.629143	2.090861	3.800662		6	7	8	9	10	6 B	0.000000					7 B	3.798532	0.000000				8 B	1.698547	3.023047	0.000000			9 B	3.798823	3.104824	3.798553	0.000000		10 B	3.027372	3.105196	3.797837	3.103219	0.000000
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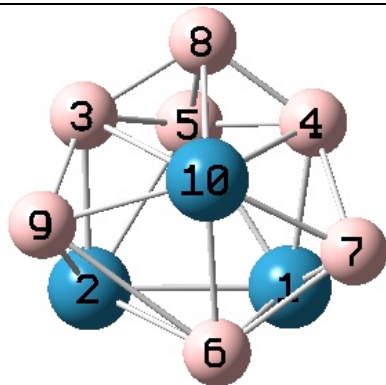
3. -993.90842290 +12.2 C_{2v}

	1	2	3	4	5
1 B	0.000000				
2 B	3.523924	0.000000			
3 B	3.906581	1.689296	0.000000		
4 B	1.692817	3.903757	3.516159	0.000000	
5 Re	2.241583	2.241636	2.229331	2.226142	0.000000
6 Re	2.205721	2.204367	3.163735	3.165105	2.705870
7 B	1.731179	3.852697	3.860508	1.753993	3.102503
8 Re	3.118372	3.117207	2.189609	2.187112	2.661997
9 B	3.852470	1.732784	1.751734	3.856761	3.102897
10 B	3.229763	3.233223	3.265786	3.261799	3.681939
	6	7	8	9	10
6 Re	0.000000				
7 B	2.289063	0.000000			
8 Re	2.981328	2.268117	0.000000		
9 B	2.288046	3.360640	2.265206	0.000000	
10 B	2.063532	1.992234	2.095371	1.996137	0.000000



4. -993.88085070 +29.5 C_{3v}

	1	2	3	4	5
1 B	0.000000				
2 B	1.793707	0.000000			
3 Re	3.221556	2.341923	0.000000		
4 Re	2.342133	3.215569	2.717327	0.000000	
5 B	1.776851	1.773096	2.158090	2.152787	0.000000
6 B	1.793603	1.793252	3.217611	3.219244	2.929103
7 B	1.773972	2.927410	3.585357	2.154740	3.025912
8 B	3.877370	3.873749	2.137068	2.142288	3.320499
9 B	2.931183	1.778174	2.154953	3.587891	3.029617
10 Re	3.220894	3.220093	2.715968	2.719532	3.589238
	6	7	8	9	10
6 B	0.000000				
7 B	1.775690	0.000000			
8 B	3.874689	3.317216	0.000000		
9 B	1.773822	3.025222	3.316749	0.000000	
10 Re	2.344486	2.154879	2.136173	2.154722	0.000000



5. -993.87042250 +36.1 C₁

	1	2	3	4	5	
1 Re	0.000000					
2 Re	2.472832	0.000000				
3 B	3.431158	2.208461	0.000000			
4 B	2.181211	3.425231	2.813181	0.000000		
5 B	2.336855	2.408517	1.808981	1.835773	0.000000	
6 B	2.160325	2.254794	3.392447	3.185677	3.445644	
7 B	2.029525	3.569007	3.769104	1.920972	3.250948	
8 B	3.380750	3.404630	1.718506	1.707148	1.725448	
9 B	3.803032	2.053567	1.815572	3.785434	3.233280	
10 Re	3.094324	2.978010	2.312201	2.320267	2.921227	
	6	7	8	9	10	
6 B	0.000000					
7 B	2.075904	0.000000				
8 B	3.839656	3.215830	0.000000			
9 B	2.666481	3.836105	3.136553	0.000000		
10 Re	2.256303	2.145840	2.220320	2.131146	0.000000	

Table S6C. Energy ranking for all of the Cp₃Re₃B₇H₇ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	10v-02-TetrTriPri2__Re ag r-37	-993.62352740	0.00
2	10v-02-TetrTriPri2__Re ak r-37	-993.62352700	0.00
3	10v-03-Isocloso 27_r-31	-993.62337180	0.10
4	10v-02-TetrTriPri2__Re ag i-37	-993.62234100	0.74
5	10v-02-TetrTriPri2__Re ak i-37	-993.62234100	0.74
6	10v-03-Isocloso 27_i-31	-993.62051640	1.89
7	10v-01-TetrTriPri1__Re f	-993.60521370	11.49
8	10v-03-Isocloso 17_r-13	-993.59311400	19.09
9	10v-03-Isocloso 17_i-13	-993.59273950	19.32
10	10v-03-Isocloso 28_r-33	-993.57917620	27.83
11	10v-02-TetrTriPri2__Re af r-22	-993.57894220	27.98
12	10v-02-TetrTriPri2__Re af i-22	-993.57853550	28.23
13	10v-03-Isocloso 28_i-33	-993.57750480	28.88
14	10v-03-Isocloso 3_r-31	-993.56638030	35.86
15	10v-03-Isocloso 10_r-31	-993.56638000	35.86
16	10v-03-Isocloso 21_r-42	-993.56620920	35.97
17	10v-03-Isocloso 22_r-42	-993.56620920	35.97
18	10v-03-Isocloso 3_i-31	-993.56620870	35.97
19	10v-03-Isocloso 10_i-31	-993.56620770	35.97
20	10v-02-TetrTriPri2__Re as	-993.56610260	36.04
21	10v-02-TetrTriPri2__Re i	-993.56610260	36.04
22	10v-03-Isocloso 1	-993.56609870	36.04
23	10v-03-Isocloso 36	-993.56609580	36.04
24	10v-03-Isocloso 21_i-42	-993.56483350	36.83
25	10v-03-Isocloso 22_i-42	-993.56483350	36.83
26	10v-03-Isocloso 14_r-37	-993.56455990	37.00
27	10v-02-TetrTriPri2__Re l	-993.56443350	37.08
28	10v-02-TetrTriPri2__Re ae	-993.56440390	37.10
29	10v-02-TetrTriPri2__Re ar	-993.56440300	37.10
30	10v-03-Isocloso 7_i-23	-993.56343700	37.71
31	10v-03-Isocloso 6	-993.56332810	37.78
32	10v-03-Isocloso 7_r-23	-993.56322510	37.84
33	10v-02-TetrTriPri2__Re b	-993.56320550	37.85
34	10v-02-TetrTriPri2__Re aa	-993.56320450	37.85
35	10v-02-TetrTriPri2__Re ai i-12	-993.56167730	38.81
36	10v-03-Isocloso 30	-993.56164140	38.83
37	10v-03-Isocloso 2	-993.56161060	38.85

38	10v-02-TetrcTriPri2__Re ai r-12	-993.56155710	38.89
39	10v-02-TetrcTriPri2__Re y	-993.55515410	42.91
40	10v-03-Isocloso 12	-993.55514740	42.91
41	10v-01-TetrcTriPri1__Re c	-993.55378760	43.76
42	10v-02-TetrcTriPri2__Re ac	-993.55234560	44.67
43	10v-02-TetrcTriPri2__Re v	-993.55234560	44.67
44	10v-03-Isocloso 15	-993.55230550	44.69
45	10v-03-Isocloso 16	-993.55230360	44.69
46	10v-01-TetrcTriPri1__Re a	-993.55076750	45.66
47	10v-03-Isocloso 8	-993.55076590	45.66
48	10v-03-Isocloso 9	-993.55076360	45.66
49	10v-03-Isocloso 11	-993.55076180	45.66
50	10v-03-Isocloso 5	-993.55076170	45.66
51	10v-03-Isocloso 4	-993.55076130	45.66
52	10v-03-Isocloso 29	-993.55075900	45.66
53	10v-01-TetrcTriPri1__Re b	-993.55075560	45.67
54	10v-01-TetrcTriPri1__Re h	-993.54957190	46.41
55	10v-01-TetrcTriPri1__Re n	-993.54850460	47.08
56	10v-02-TetrcTriPri2__Re am	-993.54570580	48.83
57	10v-02-TetrcTriPri2__Re ax	-993.54570580	48.83
58	10v-02-TetrcTriPri2__Re e	-993.54570580	48.83
59	10v-01-TetrcTriPri1__Re j	-993.54226390	50.99
60	10v-04-closo c Re	-993.54106830	51.74
61	10v-02-TetrcTriPri2__Re u	-993.53778670	53.80
62	10v-02-TetrcTriPri2__Re ab	-993.53778380	53.81
63	10v-01-TetrcTriPri1__Re m	-993.53642890	54.66
64	10v-01-TetrcTriPri1__Re i	-993.53640900	54.67
65	10v-02-TetrcTriPri2__Re a r-17	-993.53515460	55.46
66	10v-02-TetrcTriPri2__Re a i-17	-993.53513990	55.46
67	10v-01-TetrcTriPri1__Re g	-993.53452930	55.85
68	10v-02-TetrcTriPri2__Re al r-25	-993.53341960	56.54
69	10v-02-TetrcTriPri2__Re aj r-25	-993.53341950	56.54
70	10v-02-TetrcTriPri2__Re al i-25	-993.53330760	56.61
71	10v-02-TetrcTriPri2__Re aj i-25	-993.53330380	56.62
72	10v-03-Isocloso 13_i-13	-993.53181220	57.55
73	10v-03-Isocloso 13_r-13	-993.53173220	57.60
74	10v-01-TetrcTriPri1__Re d	-993.53004740	58.66
75	10v-02-TetrcTriPri2__Re h	-993.52984810	58.79
76	10v-02-TetrcTriPri2__Re ah	-993.52984710	58.79
77	10v-02-TetrcTriPri2__Re at	-993.52984340	58.79
78	10v-02-TetrcTriPri2__Re ba r-178	-993.52704050	60.55

79	10v-02-TetrTriPri2__Re k r-178	-993.52703670	60.55
80	10v-03-Isocloso 31	-993.52637050	60.97
81	10v-02-TetrTriPri2__Re c r-80	-993.52584320	61.30
82	10v-04-closo a Re	-993.52566780	61.41
83	10v-02-TetrTriPri2__Re g r-25	-993.52557160	61.47
84	10v-03-Isocloso 23_r-25	-993.52556790	61.47
85	10v-02-TetrTriPri2__Re az r-25	-993.52553700	61.49
86	10v-03-Isocloso 23_i-25	-993.52531360	61.63
87	10v-02-TetrTriPri2__Re az i-25	-993.52531150	61.63
88	10v-02-TetrTriPri2__Re g i-25	-993.52530870	61.63
89	10v-02-TetrTriPri2__Re av	-993.52464080	62.05
90	10v-02-TetrTriPri2__Re j	-993.52464080	62.05
91	10v-02-TetrTriPri2__Re r	-993.52464080	62.05
92	10v-03-Isocloso 24	-993.52448350	62.15
93	10v-03-Isocloso 18_r-16	-993.52420610	62.33
94	10v-02-TetrTriPri2__Re q	-993.52364970	62.68
95	10v-03-Isocloso 18_i-16	-993.52315180	62.99
96	10v-03-Isocloso 19	-993.52028750	64.79
97	10v-02-TetrTriPri2__Re z	-993.51962510	65.20
98	10v-02-TetrTriPri2__Re ad	-993.51718000	66.74
99	10v-03-Isocloso 33	-993.51716030	66.75
100	10v-03-Isocloso 34	-993.51715840	66.75
101	10v-02-TetrTriPri2__Re ay	-993.51627780	67.30
102	10v-02-TetrTriPri2__Re f	-993.51627470	67.30
103	10v-01-TetrTriPri1__Re k i-20	-993.51600340	67.47
104	10v-01-TetrTriPri1__Re k r-20	-993.51589020	67.54
105	10v-02-TetrTriPri2__Re k i-178	-993.51534170	67.89
106	10v-02-TetrTriPri2__Re ba i-178	-993.51534160	67.89
107	10v-02-TetrTriPri2__Re d	-993.51307910	69.31
108	10v-02-TetrTriPri2__Re an r-10	-993.51263510	69.59
109	10v-01-TetrTriPri1__Re e	-993.50878800	72.00
110	10v-02-TetrTriPri2__Re w	-993.50844970	72.21
111	10v-02-TetrTriPri2__Re an i-10	-993.50551250	74.06
112	10v-03-Isocloso 32_r-263	-993.50359840	75.26
113	10v-04-closo e Re	-993.49814990	78.68
114	10v-03-Isocloso 35	-993.49717510	79.29
115	10v-03-Isocloso 37	-993.49701120	79.39
116	10v-03-Isocloso 14_i-37	-993.49696670	79.42
117	10v-03-Isocloso 25	-993.49465740	80.87
118	10v-04-closo d Re	-993.49465440	80.87
119	10v-02-TetrTriPri2__Re ao	-993.49271760	82.09

120	10v-02-TetrTriPri2__Re x	-993.49271760	82.09
121	10v-01-TetrTriPri1__Re o	-993.48966300	84.00
122	10v-03-Isocloso 20	-993.48887240	84.50
123	10v-04-closo b Re __r-996	-993.48642850	86.03
124	10v-03-Isocloso 26	-993.48642480	86.03
125	10v-02-TetrTriPri2__Re au	-993.48517720	86.82
126	10v-02-TetrTriPri2__Re m	-993.48517560	86.82
127	10v-01-TetrTriPri1__Re l	-993.47194060	95.12
128	10v-02-TetrTriPri2__Re o	-993.46317500	100.62
129	10v-04-closo b Re __i-996	-993.46268830	100.93
130	10v-03-Isocloso 32_i-263	-993.46201020	101.36
131	10v-02-TetrTriPri2__Re s	-993.45740510	104.25
132	10v-02-TetrTriPri2__Re n	-993.45740020	104.25
133	10v-02-TetrTriPri2__Re aq	-993.45740010	104.25
134	10v-02-TetrTriPri2__Re c i-80	-993.45023150	108.75
135	10v-02-TetrTriPri2__Re p	-993.44435130	112.44
136	10v-02-TetrTriPri2__Re ap	-993.44434830	112.44
137	10v-02-TetrTriPri2__Re aw	-993.44120950	114.41
138	10v-02-TetrTriPri2__Re t	-993.43644150	117.40

Table S7A. Initial $\text{Cp}_3\text{Re}_3\text{B}_8\text{H}_8$ structures, 215 structures.

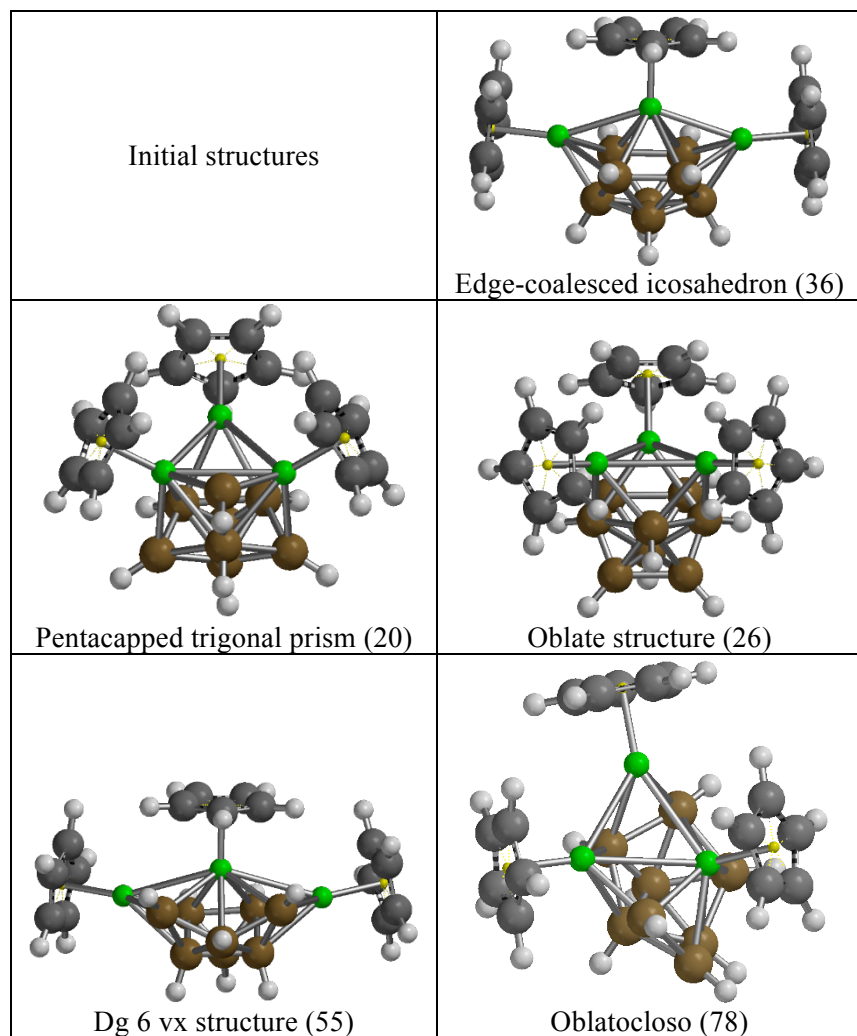
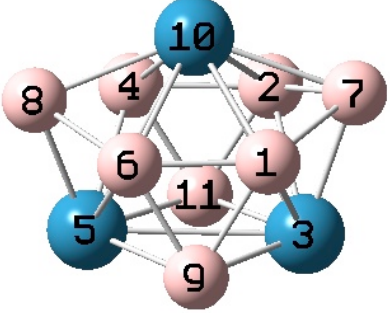
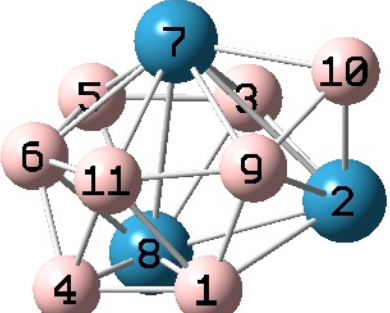
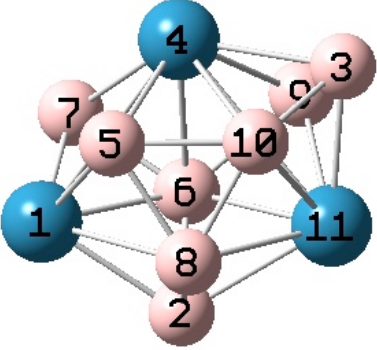
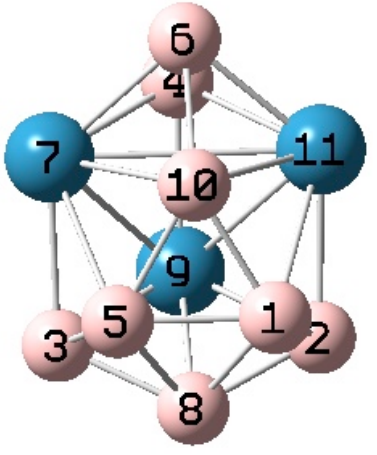
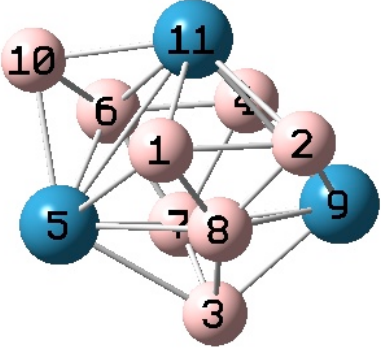
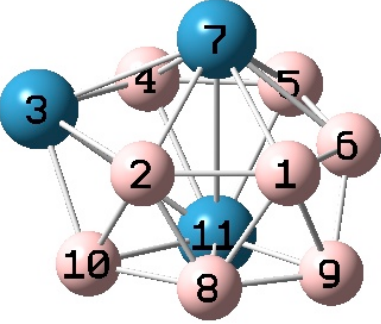
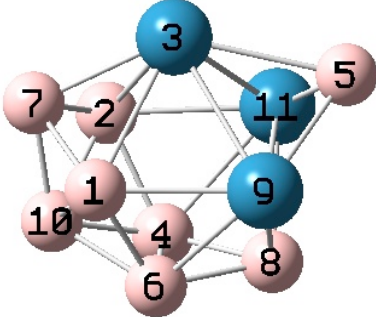
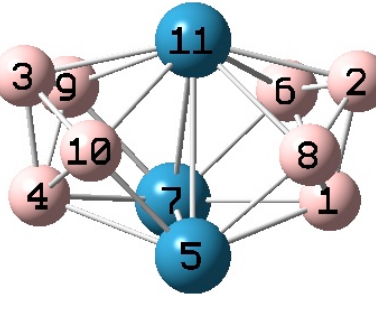


Table S7B. Distance table for the lowest-lying $\text{Cp}_3\text{Re}_3\text{B}_8\text{H}_8$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -1019.4058055 0.0 C1</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>3.344371</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.262667</td><td>2.263315</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.809771</td><td>1.773018</td><td>3.151387</td><td>0.000000</td><td></td></tr> <tr><td>5 Re</td><td>3.171308</td><td>3.191434</td><td>2.763621</td><td>2.280155</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.756380</td><td>3.850220</td><td>3.161560</td><td>3.455151</td><td>2.288624</td></tr> <tr><td>7 B</td><td>1.961448</td><td>2.119578</td><td>2.004692</td><td>3.401889</td><td>3.865314</td></tr> <tr><td>8 B</td><td>3.244271</td><td>3.688570</td><td>3.944897</td><td>2.514043</td><td>2.012229</td></tr> <tr><td>9 B</td><td>1.773125</td><td>3.819351</td><td>2.186034</td><td>3.829998</td><td>2.201044</td></tr> <tr><td>10 Re</td><td>2.245429</td><td>2.255283</td><td>2.973524</td><td>2.224461</td><td>2.903772</td></tr> <tr><td>11 B</td><td>3.817648</td><td>1.716184</td><td>2.200495</td><td>1.696105</td><td>2.257094</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>3.317290</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.840261</td><td>4.073648</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.721151</td><td>3.229441</td><td>3.113344</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>2.257571</td><td>2.162708</td><td>2.191676</td><td>3.179743</td><td>0.000000</td></tr> <tr><td>11 B</td><td>3.874002</td><td>3.303085</td><td>3.574782</td><td>3.450022</td><td>3.151471</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.344371	0.000000				3 Re	2.262667	2.263315	0.000000			4 B	3.809771	1.773018	3.151387	0.000000		5 Re	3.171308	3.191434	2.763621	2.280155	0.000000	6 B	1.756380	3.850220	3.161560	3.455151	2.288624	7 B	1.961448	2.119578	2.004692	3.401889	3.865314	8 B	3.244271	3.688570	3.944897	2.514043	2.012229	9 B	1.773125	3.819351	2.186034	3.829998	2.201044	10 Re	2.245429	2.255283	2.973524	2.224461	2.903772	11 B	3.817648	1.716184	2.200495	1.696105	2.257094		6	7	8	9	10	6 B	0.000000					7 B	3.317290	0.000000				8 B	1.840261	4.073648	0.000000			9 B	1.721151	3.229441	3.113344	0.000000		10 Re	2.257571	2.162708	2.191676	3.179743	0.000000	11 B	3.874002	3.303085	3.574782	3.450022	3.151471
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8 B	2.339049	1.770882	3.202525	3.060685	1.783142																																																																																																														
9 B	3.838589	3.268803	1.969074	2.156825	3.834196																																																																																																														
10 B	3.329600	3.067369	1.821050	2.286832	1.796000																																																																																																														
11 Re	3.621332	2.181369	2.083361	3.006480	3.381026																																																																																																														
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7 B	1.755844	0.000000																																																																																																																	
8 B	2.801834	3.701240	0.000000																																																																																																																
9 B	1.879923	2.898415	3.656016	0.000000																																																																																																															
10 B	3.189358	3.956291	1.753695	3.101754	0.000000																																																																																																														
11 Re	2.251926	3.832900	2.306490	2.100081	2.235355																																																																																																														
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 <p>7. -1019.3537842 +32.6 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>2.669325</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.349440</td><td>2.338087</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.826881</td><td>1.783632</td><td>3.335014</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.737384</td><td>3.721387</td><td>2.357412</td><td>3.796113</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.782482</td><td>2.826298</td><td>3.335961</td><td>1.802087</td><td>3.799758</td></tr> <tr><td>7 B</td><td>1.746865</td><td>1.745207</td><td>2.118707</td><td>2.925478</td><td>4.209654</td></tr> <tr><td>8 B</td><td>3.059743</td><td>3.056618</td><td>3.451448</td><td>1.756322</td><td>2.877008</td></tr> <tr><td>9 Re</td><td>2.280151</td><td>3.614475</td><td>2.516543</td><td>3.252738</td><td>2.096954</td></tr> <tr><td>10 B</td><td>1.797491</td><td>1.801477</td><td>3.132859</td><td>1.777120</td><td>4.501503</td></tr> <tr><td>11 Re</td><td>3.632735</td><td>2.282639</td><td>2.531512</td><td>2.288522</td><td>2.090789</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>2.926356</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.754926</td><td>3.876164</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Re</td><td>2.288827</td><td>3.547293</td><td>2.198591</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.778008</td><td>1.705411</td><td>2.989154</td><td>3.462230</td><td>0.000000</td></tr> <tr><td>11 Re</td><td>3.255369</td><td>3.560741</td><td>2.194340</td><td>2.969295</td><td>3.469400</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.669325	0.000000				3 Re	2.349440	2.338087	0.000000			4 B	2.826881	1.783632	3.335014	0.000000		5 B	3.737384	3.721387	2.357412	3.796113	0.000000	6 B	1.782482	2.826298	3.335961	1.802087	3.799758	7 B	1.746865	1.745207	2.118707	2.925478	4.209654	8 B	3.059743	3.056618	3.451448	1.756322	2.877008	9 Re	2.280151	3.614475	2.516543	3.252738	2.096954	10 B	1.797491	1.801477	3.132859	1.777120	4.501503	11 Re	3.632735	2.282639	2.531512	2.288522	2.090789		6	7	8	9	10	6 B	0.000000					7 B	2.926356	0.000000				8 B	1.754926	3.876164	0.000000			9 Re	2.288827	3.547293	2.198591	0.000000		10 B	1.778008	1.705411	2.989154	3.462230	0.000000	11 Re	3.255369	3.560741	2.194340	2.969295	3.469400
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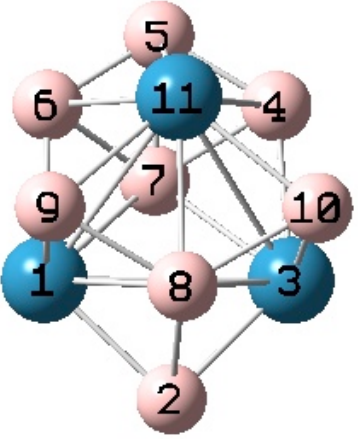
 <p>9. -1019.3466271 +37.1 CS</p>	1	2	3	4	5
	1 Re	0.000000			
2 B	2.074378	0.000000			
3 Re	2.919683	2.072740	0.000000		
4 B	3.544798	3.877258	2.165937	0.000000	
5 B	3.387330	4.531334	3.392231	1.625377	0.000000
6 B	2.166164	3.882747	3.554199	2.708253	1.625392
7 B	2.375231	3.216173	2.389981	1.800850	1.753968
8 B	2.281309	1.854593	2.280543	3.501870	4.063519
9 B	2.062842	3.099337	3.674939	4.071470	3.885387
10 B	3.673977	3.097989	2.063934	2.834826	3.889809
11 Re	2.881357	3.637100	2.880419	2.352819	2.399342
	6	7	8	9	10
6 B	0.000000				
7 B	1.797124	0.000000			
8 B	3.502669	3.456102	0.000000		
9 B	2.826636	3.710522	1.840067	0.000000	
10 B	4.074115	3.720900	1.837642	3.166121	0.000000
11 Re	2.352728	2.884664	2.281371	2.142981	2.140192

Table S7C. Energy ranking for all of the Cp₃Re₃B₈H₈ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	11v-02-PentaCapTriPri__i	-1019.0739663	0.00
2	11v-03-TriFlatPentaCapTrigPrism__g	-1019.0526858	13.35
3	11v-05-Oblatocloso__e Re	-1019.0524875	13.48
4	11v-04-ThatStructure__ax	-1019.0524671	13.49
5	11v-05-Oblatocloso__bl Re	-1019.0522699	13.61
6	11v-03-TriFlatPentaCapTrigPrism__w_i-13	-1019.0521615	13.68
7	11v-03-TriFlatPentaCapTrigPrism__w_r-13	-1019.0520194	13.77
8	11v-04-ThatStructure__p	-1019.0497043	15.22
9	11v-05-Oblatocloso__s Re	-1019.0495533	15.32
10	11v-05-Oblatocloso__bt Re	-1019.0493408	15.45
11	11v-01-Icos-1vx__g	-1019.0457161	17.73
12	11v-02-PentaCapTriPri__s1	-1019.0417323	20.23
13	11v-01-Icos-1vx__e	-1019.0417121	20.24
14	11v-03-TriFlatPentaCapTrigPrism__i	-1019.0294896	27.91
15	11v-02-PentaCapTriPri__a	-1019.0294507	27.93
16	11v-01-Icos-1vx__j	-1019.0290407	28.19
17	11v-05-Oblatocloso__m Re	-1019.0263371	29.89
18	11v-02-PentaCapTriPri__d_i-10	-1019.0254701	30.43
19	11v-02-PentaCapTriPri__d_r-10	-1019.0254446	30.45

20	11v-02-PentaCapTriPri__o1	-1019.0253082	30.53
21	11v-02-PentaCapTriPri__l1	-1019.0252172	30.59
22	11v-05-Oblatocloso__l Re	-1019.0242456	31.20
23	11v-04-ThatStructure__n	-1019.0240258	31.34
24	11v-03-TriFlatPentaCapTrigPrism__p	-1019.0234996	31.67
25	11v-03-TriFlatPentaCapTrigPrism__q	-1019.0234707	31.69
26	11v-02-PentaCapTriPri__r1	-1019.0227410	32.14
27	11v-02-PentaCapTriPri__f	-1019.0223060	32.42
28	11v-04-ThatStructure__af	-1019.0219994	32.61
29	11v-01-Icos-1vx__y	-1019.0196774	34.07
30	11v-05-Oblatocloso__an Re	-1019.0194530	34.21
31	11v-01-Icos-1vx__f	-1019.0194080	34.24
32	11v-05-Oblatocloso__bz Re	-1019.0190137	34.48
33	11v-05-Oblatocloso__r Re	-1019.0184523	34.84
34	11v-05-Oblatocloso__ak Re	-1019.0183234	34.92
35	11v-04-ThatStructure__t	-1019.0173730	35.51
36	11v-05-Oblatocloso__ad Re	-1019.0160643	36.33
37	11v-01-Icos-1vx__o	-1019.0160368	36.35
38	11v-05-Oblatocloso__bu Re	-1019.0158951	36.44
39	11v-05-Oblatocloso__bw Re	-1019.0158058	36.50
40	11v-05-Oblatocloso__bv Re	-1019.0157897	36.51
41	11v-05-Oblatocloso__y Re	-1019.0157719	36.52
42	11v-01-Icos-1vx__n	-1019.0156665	36.58
43	11v-03-TriFlatPentaCapTrigPrism__t	-1019.0156216	36.61
44	11v-02-PentaCapTriPri__j	-1019.0130906	38.20
45	11v-03-TriFlatPentaCapTrigPrism__h	-1019.0118218	39.00
46	11v-01-Icos-1vx__x	-1019.0117573	39.04
47	11v-05-Oblatocloso__v Re	-1019.0115073	39.19
48	11v-04-ThatStructure__s	-1019.0113954	39.26
49	11v-02-PentaCapTriPri__b	-1019.0110878	39.46
50	11v-05-Oblatocloso__h Re	-1019.0077966	41.52
51	11v-05-Oblatocloso__j Re	-1019.0069498	42.05
52	11v-05-Oblatocloso__br Re	-1019.0066193	42.26
53	11v-01-Icos-1vx__d	-1019.0065645	42.30
54	11v-05-Oblatocloso__am Re	-1019.0065571	42.30
55	11v-03-TriFlatPentaCapTrigPrism__d	-1019.0063395	42.44
56	11v-01-Icos-1vx__ac	-1019.0057226	42.82
57	11v-05-Oblatocloso__av Re	-1019.0044984	43.59
58	11v-01-Icos-1vx__h	-1019.0026935	44.73
59	11v-05-Oblatocloso__bb Re	-1019.0016368	45.39
60	11v-01-Icos-1vx__ad	-1019.0002587	46.25

61	11v-05-Oblatocloso__p Re	-1019.0000179	46.40
62	11v-04-ThatStructure__k	-1018.9997452	46.58
63	11v-04-ThatStructure__al	-1018.9996689	46.62
64	11v-04-ThatStructure__q	-1018.9996559	46.63
65	11v-03-TriFlatPentaCapTrigPrism__u	-1018.9988743	47.12
66	11v-05-Oblatocloso__bo Re	-1018.9987710	47.19
67	11v-03-TriFlatPentaCapTrigPrism__b	-1018.9987115	47.22
68	11v-05-Oblatocloso__bn Re	-1018.9987068	47.23
69	11v-03-TriFlatPentaCapTrigPrism__v	-1018.9987057	47.23
70	11v-01-Icos-1vx__ab	-1018.9986415	47.27
71	11v-04-ThatStructure__bc	-1018.9984899	47.36
72	11v-04-ThatStructure__av	-1018.9975053	47.98
73	11v-03-TriFlatPentaCapTrigPrism__r	-1018.9974174	48.04
74	11v-03-TriFlatPentaCapTrigPrism__f	-1018.9955997	49.18
75	11v-01-Icos-1vx__af	-1018.9955353	49.22
76	11v-04-ThatStructure__m	-1018.9949728	49.57
77	11v-04-ThatStructure__j	-1018.9942512	50.02
78	11v-04-ThatStructure__i	-1018.9941952	50.06
79	11v-04-ThatStructure__bb	-1018.9935947	50.43
80	11v-05-Oblatocloso__at Re	-1018.9925939	51.06
81	11v-04-ThatStructure__am	-1018.9925426	51.10
82	11v-01-Icos-1vx__t	-1018.9925121	51.11
83	11v-04-ThatStructure__au	-1018.9922286	51.29
84	11v-04-ThatStructure__c	-1018.9905597	52.34
85	11v-05-Oblatocloso__bf Re	-1018.9905363	52.35
86	11v-04-ThatStructure__z	-1018.9904973	52.38
87	11v-01-Icos-1vx__a	-1018.9904741	52.39
88	11v-01-Icos-1vx__r	-1018.9904388	52.42
89	11v-04-ThatStructure__w	-1018.9903700	52.46
90	11v-01-Icos-1vx__b	-1018.9903432	52.48
91	11v-01-Icos-1vx__i	-1018.9903105	52.50
92	11v-01-Icos-1vx__v	-1018.9902711	52.52
93	11v-05-Oblatocloso__ay Re	-1018.9901748	52.58
94	11v-05-Oblatocloso__o Re	-1018.9899154	52.74
95	11v-05-Oblatocloso__u Re	-1018.9895116	53.00
96	11v-04-ThatStructure__f	-1018.9893004	53.13
97	11v-05-Oblatocloso__q Re	-1018.9891581	53.22
98	11v-05-Oblatocloso__n Re	-1018.9889384	53.36
99	11v-05-Oblatocloso__as Re	-1018.9888820	53.39
100	11v-05-Oblatocloso__ac Re	-1018.9888314	53.42
101	11v-05-Oblatocloso__t Re	-1018.9883053	53.75

102	11v-05-Oblatocloso__k Re	-1018.9881873	53.83
103	11v-03-TriFlatPentaCapTrigPrism__x	-1018.9880563	53.91
104	11v-03-TriFlatPentaCapTrigPrism__s	-1018.9879772	53.96
105	11v-04-ThatStructure__ai	-1018.9879667	53.97
106	11v-04-ThatStructure__ba	-1018.9878687	54.03
107	11v-04-ThatStructure__as	-1018.9878680	54.03
108	11v-01-Icos-1vx__ae	-1018.9875906	54.20
109	11v-03-TriFlatPentaCapTrigPrism__z	-1018.9871729	54.46
110	11v-04-ThatStructure__u	-1018.9869966	54.58
111	11v-03-TriFlatPentaCapTrigPrism__a	-1018.9867184	54.75
112	11v-05-Oblatocloso__f Re	-1018.9860699	55.16
113	11v-04-ThatStructure__ak	-1018.9855762	55.47
114	11v-05-Oblatocloso__aw Re	-1018.9847739	55.97
115	11v-04-ThatStructure__r	-1018.9835506	56.74
116	11v-03-TriFlatPentaCapTrigPrism__m	-1018.9815562	57.99
117	11v-03-TriFlatPentaCapTrigPrism__j	-1018.9810619	58.30
118	11v-05-Oblatocloso__ba Re	-1018.9810480	58.31
119	11v-05-Oblatocloso__d Re	-1018.9810450	58.31
120	11v-03-TriFlatPentaCapTrigPrism__e	-1018.9809862	58.35
121	11v-05-Oblatocloso__bs Re	-1018.9809292	58.38
122	11v-04-ThatStructure__h	-1018.9791757	59.48
123	11v-05-Oblatocloso__ah Re	-1018.9788526	59.69
124	11v-02-PentaCapTriPri__m1	-1018.9780375	60.20
125	11v-05-Oblatocloso__ae Re	-1018.9775960	60.47
126	11v-04-ThatStructure__ao	-1018.9770366	60.83
127	11v-04-ThatStructure__d	-1018.9766885	61.04
128	11v-02-PentaCapTriPri__h	-1018.9765709	61.12
129	11v-05-Oblatocloso__be Re	-1018.9751412	62.01
130	11v-05-Oblatocloso__aa Re	-1018.9747602	62.25
131	11v-03-TriFlatPentaCapTrigPrism__y	-1018.9745277	62.40
132	11v-01-Icos-1vx__ag	-1018.9744179	62.47
133	11v-03-TriFlatPentaCapTrigPrism__k	-1018.9742208	62.59
134	11v-05-Oblatocloso__ar Re	-1018.9741689	62.62
135	11v-04-ThatStructure__a	-1018.9740665	62.69
136	11v-02-PentaCapTriPri__k1	-1018.9738702	62.81
137	11v-01-Icos-1vx__aj	-1018.9737482	62.89
138	11v-01-Icos-1vx__aa	-1018.9725047	63.67
139	11v-05-Oblatocloso__ao Re	-1018.9723600	63.76
140	11v-05-Oblatocloso__ap Re	-1018.9722144	63.85
141	11v-01-Icos-1vx__w_i-26	-1018.9717142	64.17
142	11v-04-ThatStructure__aw	-1018.9716028	64.24

143	11v-01-Icos-1vx__z	-1018.9715868	64.25
144	11v-01-Icos-1vx__w_r-26	-1018.9714564	64.33
145	11v-05-Oblatocloso__bp Re	-1018.9714531	64.33
146	11v-05-Oblatocloso__bk Re	-1018.9695244	65.54
147	11v-02-PentaCapTriPri__q1	-1018.9689575	65.90
148	11v-05-Oblatocloso__by Re	-1018.9685426	66.16
149	11v-03-TriFlatPentaCapTrigPrism__c	-1018.9684809	66.19
150	11v-04-ThatStructure__e	-1018.9684762	66.20
151	11v-01-Icos-1vx__m	-1018.9671559	67.03
152	11v-05-Oblatocloso__b Re	-1018.9657733	67.89
153	11v-01-Icos-1vx__q	-1018.9651400	68.29
154	11v-03-TriFlatPentaCapTrigPrism__l	-1018.9647017	68.57
155	11v-01-Icos-1vx__k	-1018.9645445	68.66
156	11v-01-Icos-1vx__s	-1018.9645107	68.69
157	11v-04-ThatStructure__v	-1018.9641169	68.93
158	11v-04-ThatStructure__aj	-1018.9629220	69.68
159	11v-05-Oblatocloso__bq Re	-1018.9626905	69.83
160	11v-05-Oblatocloso__x Re	-1018.9620636	70.22
161	11v-05-Oblatocloso__bg Re	-1018.9620312	70.24
162	11v-01-Icos-1vx__c	-1018.9616652	70.47
163	11v-05-Oblatocloso__bx Re	-1018.9616015	70.51
164	11v-04-ThatStructure__ad	-1018.9615224	70.56
165	11v-04-ThatStructure__ah	-1018.9612416	70.74
166	11v-04-ThatStructure__ar	-1018.9604713	71.22
167	11v-04-ThatStructure__az	-1018.9597391	71.68
168	11v-04-ThatStructure__l	-1018.9597340	71.68
169	11v-01-Icos-1vx__l	-1018.9589260	72.19
170	11v-02-PentaCapTriPri__e	-1018.9578749	72.85
171	11v-02-PentaCapTriPri__p1	-1018.9566955	73.59
172	11v-05-Oblatocloso__i Re	-1018.9566867	73.60
173	11v-04-ThatStructure__ac	-1018.9552424	74.50
174	11v-01-Icos-1vx__ah	-1018.9548747	74.73
175	11v-01-Icos-1vx__p	-1018.9548611	74.74
176	11v-02-PentaCapTriPri__t1	-1018.9544630	74.99
177	11v-04-ThatStructure__at	-1018.9536885	75.48
178	11v-04-ThatStructure__an	-1018.9536509	75.50
179	11v-05-Oblatocloso__bj Re	-1018.9518536	76.63
180	11v-02-PentaCapTriPri__c	-1018.9515189	76.84
181	11v-05-Oblatocloso__w Re	-1018.9514747	76.87
182	11v-01-Icos-1vx__u	-1018.9511253	77.09
183	11v-04-ThatStructure__aa	-1018.9509904	77.17

184	11v-05-Oblatocloso__bc Re	-1018.9508957	77.23
185	11v-01-Icos-1vx__ai	-1018.9508364	77.27
186	11v-05-Oblatocloso__af Re	-1018.9500874	77.74
187	11v-05-Oblatocloso__bi Re	-1018.9482005	78.92
188	11v-04-ThatStructure__g	-1018.9466132	79.92
189	11v-04-ThatStructure__ab	-1018.9451450	80.84
190	11v-05-Oblatocloso__au Re	-1018.9444786	81.26
191	11v-02-PentaCapTriPri__g_i-10	-1018.9419671	82.83
192	11v-02-PentaCapTriPri__g_r-10	-1018.9419252	82.86
193	11v-05-Oblatocloso__az Re	-1018.9414983	83.13
194	11v-04-ThatStructure__x	-1018.9399236	84.11
195	11v-05-Oblatocloso__bm Re	-1018.9384392	85.05
196	11v-05-Oblatocloso__ab Re	-1018.9363594	86.35
197	11v-04-ThatStructure__y	-1018.9360330	86.56
198	11v-04-ThatStructure__aq	-1018.9358839	86.65
199	11v-04-ThatStructure__ay	-1018.9345385	87.49
200	11v-04-ThatStructure__ae	-1018.9344187	87.57
201	11v-05-Oblatocloso__a Re	-1018.9312239	89.57
202	11v-05-Oblatocloso__ag Re	-1018.9292532	90.81
203	11v-04-ThatStructure__b_r-21	-1018.9280669	91.55
204	11v-05-Oblatocloso__g Re	-1018.9279954	91.60
205	11v-04-ThatStructure__b_i-21	-1018.9278830	91.67
206	11v-05-Oblatocloso__z Re	-1018.9232950	94.55
207	11v-05-Oblatocloso__ax Re	-1018.9215374	95.65
208	11v-04-ThatStructure__ag	-1018.9212290	95.85
209	11v-04-ThatStructure__ap	-1018.9195274	96.91
210	11v-03-TriFlatPentaCapTrigPrism__o	-1018.9162718	98.96
211	11v-03-TriFlatPentaCapTrigPrism__n	-1018.9162074	99.00
212	11v-05-Oblatocloso__aq Re	-1018.9135071	100.69
213	11v-05-Oblatocloso__bd Re	-1018.9124797	101.34
214	11v-05-Oblatocloso__ai Re	-1018.9118580	101.73
215	11v-05-Oblatocloso__c Re	-1018.9087008	103.71
216	11v-04-ThatStructure__o	-1018.9082756	103.97
217	11v-05-Oblatocloso__bh Re	-1018.9052634	105.86
218	11v-05-Oblatocloso__al Re_i-20	-1018.8994694	109.50
219	11v-05-Oblatocloso__al Re_r-20	-1018.8992934	109.61
220	11v-02-PentaCapTriPri__n1	-1018.8990890	109.74
221	11v-05-Oblatocloso__aj Re	-1018.8949259	112.35

Table S8A. Initial $\text{Cp}_3\text{Re}_3\text{B}_9\text{H}_9$ structures, 39 structures.

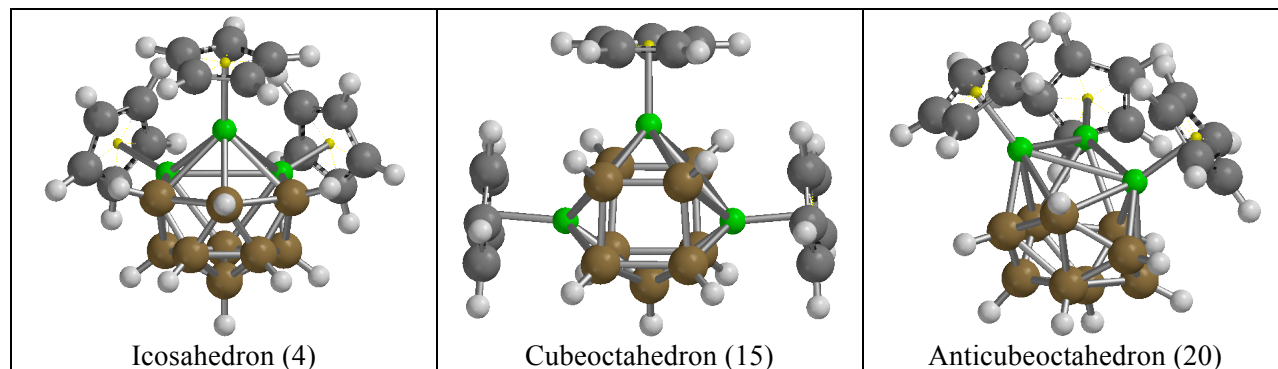
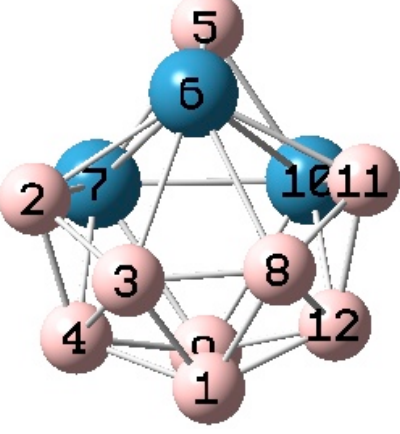
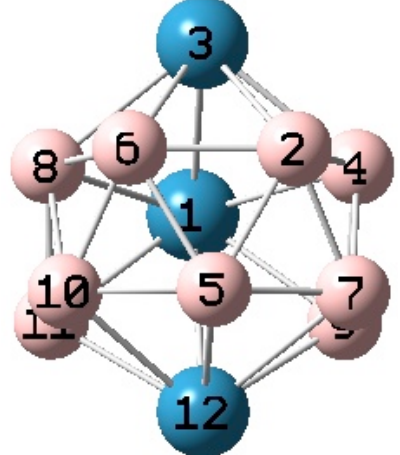
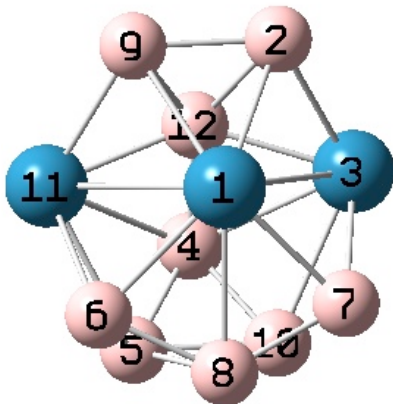


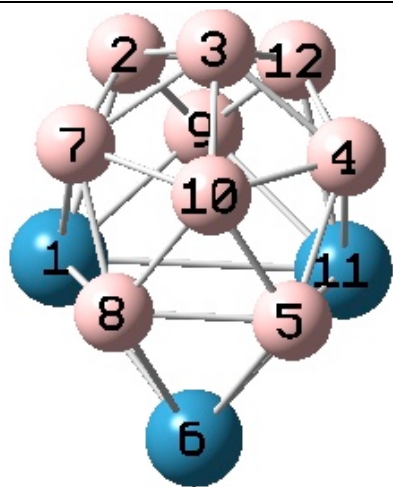
Table S8B. Distance table for the lowest-lying $\text{Cp}_3\text{Re}_3\text{B}_9\text{H}_9$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

 <p>1. -1044.82987860 0.0 $C_1(C_s)$</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>2.932523</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.764245</td><td>1.714594</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.757907</td><td>1.761977</td><td>1.803338</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>4.480038</td><td>3.256602</td><td>4.028497</td><td>3.993841</td><td>0.000000</td></tr> <tr><td>6 Re</td><td>3.369834</td><td>2.196196</td><td>2.369217</td><td>3.214706</td><td>2.104350</td></tr> <tr><td>7 Re</td><td>3.394769</td><td>2.163923</td><td>3.215648</td><td>2.270474</td><td>2.217661</td></tr> <tr><td>8 B</td><td>1.774816</td><td>3.047991</td><td>1.729315</td><td>2.878307</td><td>3.887050</td></tr> <tr><td>9 B</td><td>1.753452</td><td>3.074358</td><td>2.845494</td><td>1.794207</td><td>3.694911</td></tr> <tr><td>10 Re</td><td>3.485035</td><td>3.844132</td><td>3.951709</td><td>3.585767</td><td>2.162996</td></tr> <tr><td>11 B</td><td>2.959477</td><td>3.767864</td><td>3.111075</td><td>3.773572</td><td>2.962347</td></tr> <tr><td>12 B</td><td>1.771090</td><td>3.775357</td><td>2.904679</td><td>2.956071</td><td>3.836852</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>7 Re</td><td>2.756239</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.330273</td><td>3.740215</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.496535</td><td>2.312634</td><td>2.823850</td><td>0.000000</td><td></td></tr> <tr><td>10 Re</td><td>2.972088</td><td>2.440717</td><td>3.292651</td><td>2.355315</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.216951</td><td>3.610670</td><td>1.731855</td><td>3.055753</td><td>2.183199</td></tr> <tr><td>12 B</td><td>3.229801</td><td>3.447460</td><td>1.802655</td><td>1.789209</td><td>2.277051</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>12 B</td><td>1.764894</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	2.932523	0.000000				3 B	1.764245	1.714594	0.000000			4 B	1.757907	1.761977	1.803338	0.000000		5 B	4.480038	3.256602	4.028497	3.993841	0.000000	6 Re	3.369834	2.196196	2.369217	3.214706	2.104350	7 Re	3.394769	2.163923	3.215648	2.270474	2.217661	8 B	1.774816	3.047991	1.729315	2.878307	3.887050	9 B	1.753452	3.074358	2.845494	1.794207	3.694911	10 Re	3.485035	3.844132	3.951709	3.585767	2.162996	11 B	2.959477	3.767864	3.111075	3.773572	2.962347	12 B	1.771090	3.775357	2.904679	2.956071	3.836852		6	7	8	9	10	7 Re	2.756239	0.000000				8 B	2.330273	3.740215	0.000000			9 B	3.496535	2.312634	2.823850	0.000000		10 Re	2.972088	2.440717	3.292651	2.355315	0.000000	11 B	2.216951	3.610670	1.731855	3.055753	2.183199	12 B	3.229801	3.447460	1.802655	1.789209	2.277051		11	12				12 B	1.764894	0.000000			
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 <p>2. -1044.82902040 +0.5 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 Re</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.287891</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Re</td><td>2.386660</td><td>2.194941</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.326971</td><td>1.787435</td><td>2.187673</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.557460</td><td>1.843914</td><td>3.379342</td><td>2.944086</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.287879</td><td>1.824829</td><td>2.194133</td><td>3.071794</td><td>1.841493</td></tr> <tr><td>7 B</td><td>3.205958</td><td>1.772394</td><td>3.392606</td><td>1.812722</td><td>1.786329</td></tr> <tr><td>8 B</td><td>2.325723</td><td>3.070273</td><td>2.187407</td><td>3.418625</td><td>2.937971</td></tr> <tr><td>9 B</td><td>2.192863</td><td>2.993545</td><td>3.524897</td><td>1.819109</td><td>3.068768</td></tr> <tr><td>10 B</td><td>3.205796</td><td>2.995214</td><td>3.394759</td><td>3.765645</td><td>1.786455</td></tr> <tr><td>11 B</td><td>2.193672</td><td>3.859607</td><td>3.527153</td><td>3.796450</td><td>3.067018</td></tr> <tr><td>12 Re</td><td>2.803486</td><td>3.310844</td><td>4.080608</td><td>3.212269</td><td>2.164153</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>7 B</td><td>2.990251</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.786272</td><td>3.759564</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.857723</td><td>1.798991</td><td>3.792697</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.777344</td><td>3.181832</td><td>1.809277</td><td>3.681980</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.996676</td><td>3.680824</td><td>1.820064</td><td>3.243379</td><td>1.797026</td></tr> <tr><td>12 Re</td><td>3.311694</td><td>2.245543</td><td>3.209894</td><td>2.097119</td><td>2.246907</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>12 Re</td><td>2.097215</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Re	0.000000					2 B	3.287891	0.000000				3 Re	2.386660	2.194941	0.000000			4 B	2.326971	1.787435	2.187673	0.000000		5 B	3.557460	1.843914	3.379342	2.944086	0.000000	6 B	3.287879	1.824829	2.194133	3.071794	1.841493	7 B	3.205958	1.772394	3.392606	1.812722	1.786329	8 B	2.325723	3.070273	2.187407	3.418625	2.937971	9 B	2.192863	2.993545	3.524897	1.819109	3.068768	10 B	3.205796	2.995214	3.394759	3.765645	1.786455	11 B	2.193672	3.859607	3.527153	3.796450	3.067018	12 Re	2.803486	3.310844	4.080608	3.212269	2.164153		6	7	8	9	10	7 B	2.990251	0.000000				8 B	1.786272	3.759564	0.000000			9 B	3.857723	1.798991	3.792697	0.000000		10 B	1.777344	3.181832	1.809277	3.681980	0.000000	11 B	2.996676	3.680824	1.820064	3.243379	1.797026	12 Re	3.311694	2.245543	3.209894	2.097119	2.246907		11	12				12 Re	2.097215	0.000000			
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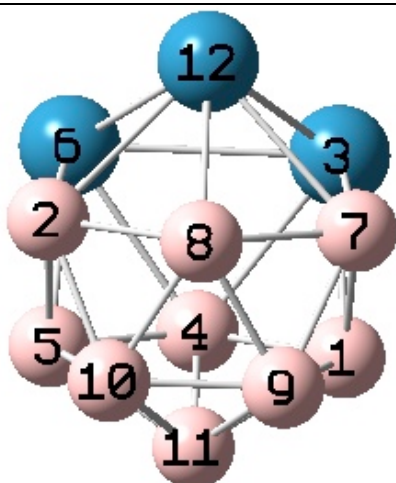
3. -1044.80921500 +13.0 C_s

	1	2	3	4	5
1 Re	0.000000				
2 B	2.248722	0.000000			
3 Re	2.794091	2.196339	0.000000		
4 B	3.209418	3.385197	2.346718	0.000000	
5 B	3.111275	4.323610	3.488695	1.765132	0.000000
6 B	2.255266	4.106047	4.038535	2.993773	1.751842
7 B	2.254035	3.362706	2.139257	2.996633	2.932073
8 B	2.392680	4.167688	3.318882	2.852393	1.783002
9 B	2.252155	1.809683	3.424527	3.384099	3.930357
10 B	3.107767	3.929187	2.307999	1.765094	1.791832
11 Re	2.800279	3.427947	3.821172	2.351336	2.312137
12 B	2.391614	1.834905	2.034889	1.720014	2.868728
	6	7	8	9	10
7 B	3.078774	0.000000			
8 B	1.725362	1.724124	0.000000		
9 B	3.361013	4.109475	4.168857	0.000000	
10 B	2.928189	1.751886	1.780042	4.321795	0.000000
11 Re	2.138668	4.045936	3.323832	2.196383	3.492223
12 B	3.163791	3.169996	3.406149	1.830494	2.869636
	11	12			
12 B	2.032989	0.000000			
Bridge B2-H-B9 B2-H 1.3329 B9-H 1.3281					



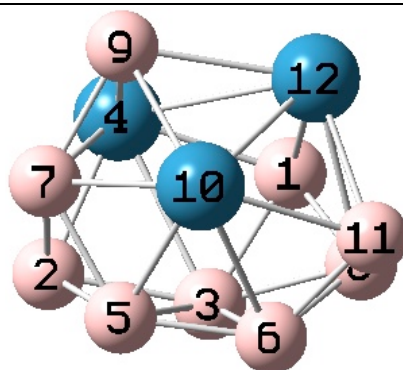
4. -1044.80693440 +14.4 C_s

	1	2	3	4	5
1 Re	0.000000				
2 B	2.298677	0.000000			
3 B	3.387305	1.744452	0.000000		
4 B	3.664112	2.835084	1.768784	0.000000	
5 B	3.275470	3.616424	2.938121	1.814509	0.000000
6 Re	2.414418	4.059030	4.312945	3.565531	2.215251
7 B	2.265189	1.754548	1.771314	2.822289	2.912242
8 B	2.298923	3.136733	2.945355	2.925555	1.854636
9 B	2.181169	1.779022	2.981499	3.076424	3.668555
10 B	3.375071	2.919144	1.764622	1.808865	1.749517
11 Re	2.967309	3.253331	3.411100	2.286884	2.343163
12 B	3.248608	1.766552	1.747840	1.760711	3.151148
	6	7	8	9	10
6 Re	0.000000				
7 B	3.571776	0.000000			
8 B	2.223809	1.810799	0.000000		
9 B	3.507090	3.074485	3.667770	0.000000	
10 B	3.455605	1.801131	1.756366	3.810609	0.000000
11 Re	2.434584	3.699133	3.324517	2.188422	3.415269
12 B	4.071837	2.848147	3.639051	1.790946	2.933054
	11	12			
12 B	2.317433	0.000000			



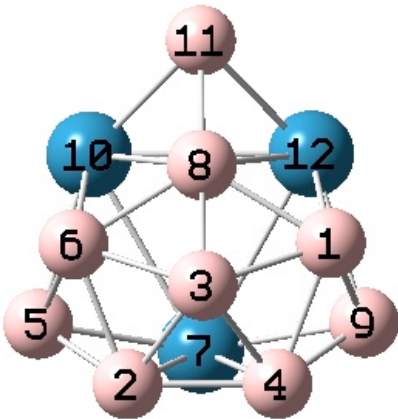
5. -1044.80573880 +15.2 C_s

	1	2	3	4	5
1 B	0.000000				
2 B	3.528217	0.000000			
3 Re	2.200849	3.689331	0.000000		
4 B	1.850500	3.045372	2.282399	0.000000	
5 B	2.951830	1.817845	3.582477	1.850823	0.000000
6 Re	3.582198	2.287113	2.706110	2.282245	2.201498
7 B	1.818215	3.097817	2.286069	3.045489	3.528542
8 B	2.891131	1.814598	3.489051	3.444915	2.890653
9 B	1.781312	2.924577	3.464693	2.926640	2.886911
10 B	2.887064	1.771373	4.091354	2.926654	1.780992
11 B	1.781160	2.911786	3.463365	1.787785	1.781140
12 Re	3.399516	2.286897	2.412388	3.388626	3.398385
	6	7	8	9	10
6 Re	0.000000				
7 B	3.689430	0.000000			
8 B	3.489290	1.815498	0.000000		
9 B	4.091385	1.771532	1.776025	0.000000	
10 B	3.465481	2.925394	1.776199	1.748811	0.000000
11 B	3.463558	2.912225	2.855895	1.758844	1.758593
12 Re	2.411093	2.288519	2.227739	3.434874	3.434660
	11	12			
12 Re	3.938225	0.000000			



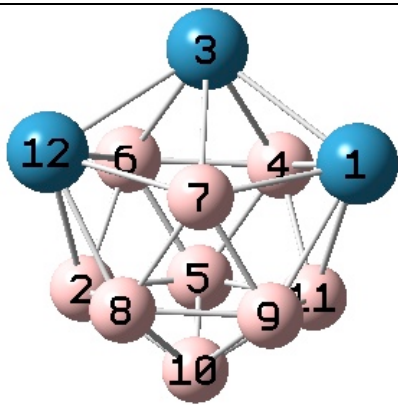
6. -1044.80530810 +15.4 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	3.098658	0.000000			
3 B	1.865100	1.884464	0.000000		
4 Re	2.094423	2.032625	2.412730	0.000000	
5 B	3.399759	1.762671	1.923732	3.031592	0.000000
6 B	2.971054	3.055059	1.850140	3.677193	1.737830
7 B	3.607924	1.823948	2.863459	2.279601	1.783012
8 B	1.767983	3.605275	1.877693	3.376938	3.015924
9 B	3.301848	3.108225	3.512186	2.134801	3.100791
10 Re	3.758269	3.476958	3.278649	3.557752	2.225965
11 B	3.123786	4.287894	3.028096	4.147110	3.089602
12 Re	2.221242	3.957731	3.131954	2.824441	3.548956
	6	7	8	9	10
6 B	0.000000				
7 B	3.144771	0.000000			
8 B	1.732864	3.893815	0.000000		
9 B	3.739444	1.777347	3.851229	0.000000	
10 Re	2.320177	2.237030	3.174660	2.281101	0.000000
11 B	1.733225	3.852552	1.739233	3.656491	2.173835
12 Re	3.033456	3.333078	2.309694	2.269201	2.478308
	11	12			
12 Re	2.166354	0.000000			



7. -1044.80314790 +16.8 C_s

	1	2	3	4	5
1 B	0.000000				
2 B	2.938977	0.000000			
3 B	1.795090	1.790845	0.000000		
4 B	1.791464	1.778934	1.790868	0.000000	
5 B	3.853769	1.733947	2.974429	3.144996	0.000000
6 B	3.052143	1.788395	1.795580	2.937554	1.740867
7 Re	3.049322	2.307770	3.215847	2.309279	2.159692
8 B	1.793019	2.737993	1.717184	2.738120	2.971154
9 B	1.740375	3.141237	2.969977	1.731276	3.865934
10 Re	3.662595	3.301032	3.508966	3.947928	2.189450
11 B	3.006414	4.223136	3.401356	4.222397	3.886676
12 Re	2.319104	3.945344	3.507981	3.300796	3.867919
	6	7	8	9	10
7 Re	3.044951	0.000000			
8 B	1.794896	3.080039	0.000000		
9 B	3.847954	2.160798	2.966282	0.000000	
10 Re	2.317515	2.678446	2.315416	3.867908	0.000000
11 B	3.010641	3.897065	1.686834	3.880424	2.166456
12 Re	3.659680	2.677261	2.313786	2.187998	2.630736
	11	12			
12 Re	2.162081	0.000000			
bridge B8-H-B11	B8-H	1.2645	B11-H1	4.367	



8. -1044.78351300 +29.1 C_s

	1	2	3	4	5
1 Re	0.000000				
2 B	4.026449	0.000000			
3 Re	2.433273	3.469282	0.000000		
4 B	2.266861	2.946967	2.232055	0.000000	
5 B	3.479236	1.777871	3.422512	1.782529	0.000000
6 B	3.526544	1.806481	2.232016	1.892239	1.782499
7 B	2.162783	2.955580	2.344481	3.073618	3.477824
8 B	3.448800	1.761092	3.515846	3.486409	2.887020
9 B	2.193355	2.891884	3.515796	2.946068	2.886977
10 B	3.454228	1.759241	4.037761	2.918526	1.794545
11 B	2.272228	2.864966	3.469335	1.806471	1.777872
12 Re	3.856819	2.272137	2.433330	3.526623	3.479221
	6	7	8	9	10
6 B	0.000000				
7 B	3.073608	0.000000			
8 B	2.946158	1.824172	0.000000		
9 B	3.486342	1.824163	1.836570	0.000000	
10 B	2.918542	2.908640	1.761227	1.761192	0.000000
11 B	2.946947	2.955629	2.891921	1.761060	1.759184
12 Re	2.266910	2.162806	2.193381	3.448789	3.454235
	11	12			
12 Re	4.026493	0.000000			

Table S8C. Energy ranking for all of the Cp₃Re₃B₉H₉ optimized structures after B3LYP/6-31G(d) optimizations:

No.	Structure	Final energy (a.u.)	ΔE (kcal/mol)
1	12v-03-AnticubeOh 18	-1044.5079970	0.00
2	12v-03-AnticubeOh 6_r-113	-1044.5078636	0.08
3	12v-03-AnticubeOh 5	-1044.5006400	4.62
4	12v-02-CubeOh 2	-1044.4904192	11.03
5	12v-01-Icos 1	-1044.4904184	11.03
6	12v-01-Icos 3	-1044.4898355	11.40
7	12v-01-Icos 2	-1044.4898272	11.40
8	12v-03-AnticubeOh 3_r-72	-1044.4897114	11.47
9	12v-03-AnticubeOh 14	-1044.4711818	23.10
10	12v-03-AnticubeOh 2	-1044.4709453	23.25
11	12v-03-AnticubeOh 17	-1044.4645688	27.25
12	12v-03-AnticubeOh 4	-1044.4640333	27.59
13	12v-02-CubeOh 12	-1044.4590480	30.72
14	12v-02-CubeOh 3	-1044.4590467	30.72
15	12v-02-CubeOh 11	-1044.4590449	30.72
16	12v-01-Icos 4	-1044.4531745	34.40
17	12v-02-CubeOh 14	-1044.4524918	34.83
18	12v-02-CubeOh 1	-1044.4516855	35.34
19	12v-03-AnticubeOh 13	-1044.4496195	36.63
20	12v-03-AnticubeOh 10	-1044.4486319	37.25
21	12v-02-CubeOh 6	-1044.4429776	40.80
22	12v-03-AnticubeOh 15	-1044.4427722	40.93
23	12v-02-CubeOh 9	-1044.4414964	41.73
24	12v-03-AnticubeOh 7	-1044.4414934	41.73
25	12v-02-CubeOh 13	-1044.4392336	43.15
26	12v-02-CubeOh 8	-1044.4392320	43.15
27	12v-02-CubeOh 10	-1044.4392288	43.15
28	12v-03-AnticubeOh 8	-1044.4359102	45.24
29	12v-03-AnticubeOh 6_i-113	-1044.4325566	47.34
30	12v-02-CubeOh 5	-1044.4311657	48.21
31	12v-03-AnticubeOh 11	-1044.4260311	51.44
32	12v-03-AnticubeOh 20_i-14	-1044.4245844	52.34
33	12v-03-AnticubeOh 20_r-14	-1044.4245408	52.37
34	12v-02-CubeOh 4	-1044.4226496	53.56
35	12v-02-CubeOh 7	-1044.4119056	60.30
36	12v-02-CubeOh 15	-1044.4077786	62.89
37	12v-03-AnticubeOh 12_r-918	-1044.3946364	71.14
38	12v-03-AnticubeOh 1	-1044.3919234	72.84
39	12v-03-AnticubeOh 19	-1044.3919224	72.84

40	12v-03-AnticubeOh 16	-1044.3706218	86.21
41	12v-03-AnticubeOh 3_i-72	-1044.3630151	90.98
42	12v-03-AnticubeOh 12_i-918	-1044.3532037	97.14
43	12v-03-AnticubeOh 9	-1044.3017890	129.40