

Supporting Information file

Tetracaraboranes: *Nido* Structures Without Bridging Hydrogens

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Table S14. Orbital energies and HOMO/LUMO gaps.

Complete Gaussian09 Reference (reference 40)

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, 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 $C_4B_2H_6$ structures, a total of 22 structures:

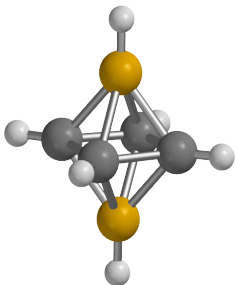
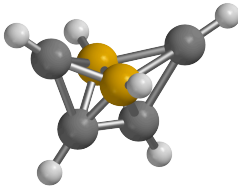
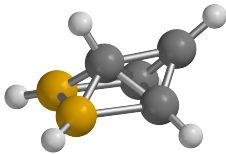
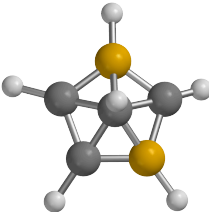
 Octahedron (2)	 Bicapped Tetrahedron (7)
 Capped tetragonal pyramid (9)	 Pentagonal pyramid (4)

Table S1B. Distance table for the lowest-lying C₄B₂H₆ structures. For clarity, only the polyhedral framework is presented.

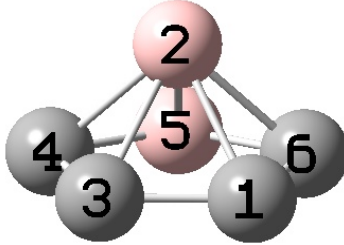
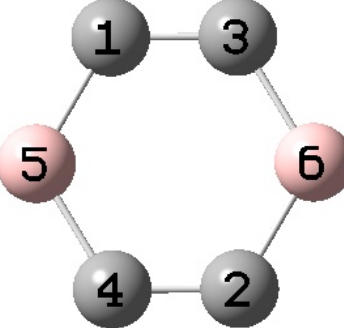
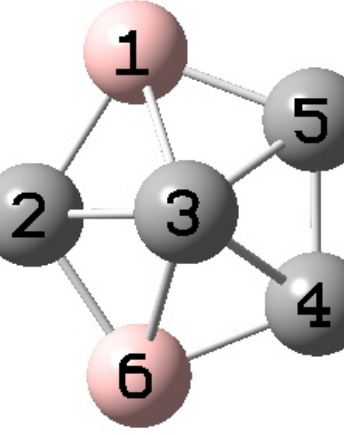
 1. -205.5702897 Cs	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.704697</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.416863</td><td>1.704680</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.326130</td><td>1.710111</td><td>1.436378</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.428576</td><td>1.838743</td><td>2.428620</td><td>1.528286</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.436153</td><td>1.710113</td><td>2.325896</td><td>2.362599</td><td>1.528156</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.704697	0.000000				3 C	1.416863	1.704680	0.000000			4 C	2.326130	1.710111	1.436378	0.000000		5 B	2.428576	1.838743	2.428620	1.528286	0.000000	6 C	1.436153	1.710113	2.325896	2.362599	1.528156
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 2. -205.5159433 D_{2h}	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>3.023049</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.340838</td><td>2.709424</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.709424</td><td>1.340838</td><td>3.023049</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.568542</td><td>2.525540</td><td>2.525540</td><td>1.568542</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.525540</td><td>1.568542</td><td>1.568542</td><td>2.525540</td><td>2.922076</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 C	3.023049	0.000000				3 C	1.340838	2.709424	0.000000			4 C	2.709424	1.340838	3.023049	0.000000		5 B	1.568542	2.525540	2.525540	1.568542	0.000000	6 B	2.525540	1.568542	1.568542	2.525540	2.922076
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 3. -205.5142851 Cs	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>1.538656</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.767511</td><td>1.614669</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.472381</td><td>2.367940</td><td>1.594592</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>1.528670</td><td>2.367968</td><td>1.594582</td><td>1.465713</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.576167</td><td>1.538636</td><td>1.767565</td><td>1.528676</td><td>2.472418</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 C	1.538656	0.000000				3 C	1.767511	1.614669	0.000000			4 C	2.472381	2.367940	1.594592	0.000000		5 C	1.528670	2.367968	1.594582	1.465713	0.000000	6 B	2.576167	1.538636	1.767565	1.528676	2.472418
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Table S1C. Energy ranking for all of the C₄B₂H₆ structures.

1	03-CapTetrPyr-b----c4	-205.6312351	0.00
2	02-BicappTd-d----c4	-205.6312301	0.00
3	01-Oh-a----c4	-205.6312300	0.00
4	02-BicappTd-g----c4	-205.6312290	0.00
5	04-PentPyr-a----c4	-205.6312280	0.00
6	03-CapTetrPyr-a----c4	-205.6312254	0.01
7	02-BicappTd-b----c4	-205.6004328	19.33
8	03-CapTetrPyr-f----c4	-205.6004261	19.33
9	02-BicappTd-e----c4	-205.5740950	35.86
10	03-CapTetrPyr-i----c4	-205.5740945	35.86
11	04-PentPyr-c----c4	-205.5740914	35.86
12	03-CapTetrPyr-h----c4	-205.5740912	35.86
13	03-CapTetrPyr-e----c4	-205.5740846	35.86
14	02-BicappTd-f----c4	-205.5740837	35.86
15	03-CapTetrPyr-d----c4	-205.5740837	35.86
16	03-CapTetrPyr-g----c4	-205.5740837	35.86
17	03-CapTetrPyr-c----c4	-205.5740830	35.86
18	02-BicappTd-a----c4	-205.5396415	57.48
19	04-PentPyr-b----c4	-205.5396323	57.48
20	01-Oh-b----c4_i-84	-205.5225453	68.21
21	01-Oh-b----c4_r-84	-205.5223546	68.32
22	02-BicappTd-c----c4	-205.5204978	69.49

Table S2A. Initial $C_4B_3H_7$ structures, a total of 51 structures:

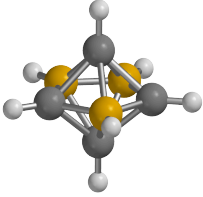
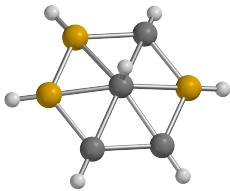
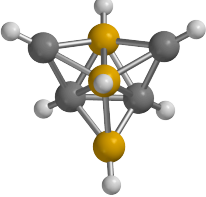
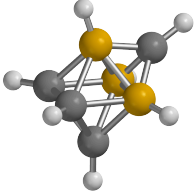
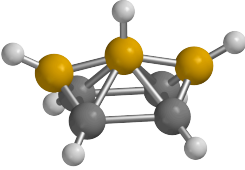
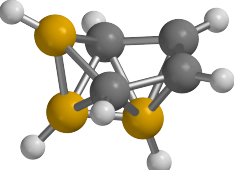
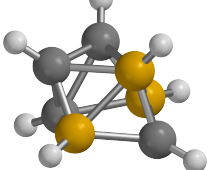
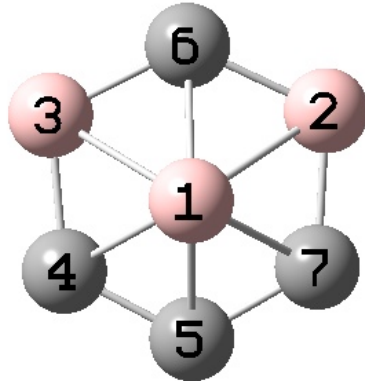
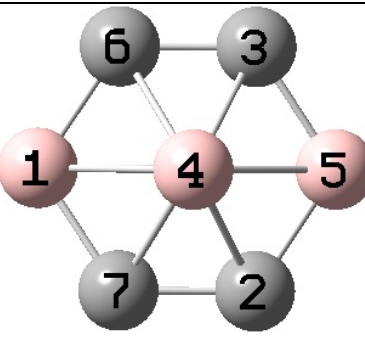
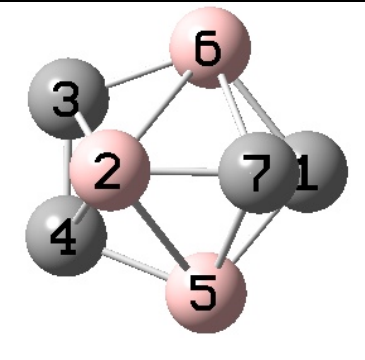
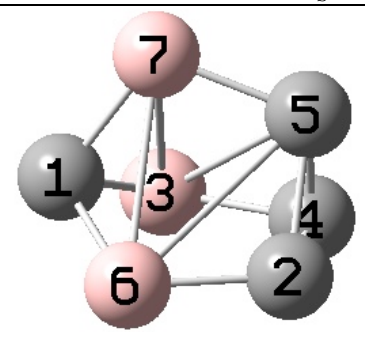
Initial	structures	 Pentagonal bipyramid (5)
 Hexagonal pyramid (6)	 Tricapped tetrahedron (12)	 Capped octahedron (8)
 Dicapped tetragonal pyr (11)	 Bisdisphenoid-1vxA (6)	 Bisdisphenoid-1vxAB (3)

Table S2B. Distance table for the lowest-lying C₄B₃H₇ structures. For clarity, only the polyhedral framework is presented.

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 2. -230.9851526 C_{2v}	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>2.579615</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.579344</td><td>2.517527</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.933895</td><td>1.792467</td><td>1.792857</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.084767</td><td>1.514484</td><td>1.514526</td><td>1.934307</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.514625</td><td>2.887360</td><td>1.413230</td><td>1.792966</td><td>2.579503</td></tr><tr><td>7 C</td><td>1.514554</td><td>1.413600</td><td>2.887147</td><td>1.792010</td><td>2.579607</td></tr><tr><th></th><th>6</th><th>7</th><th></th><th></th><th></th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.517744</td><td>0.000000</td><td></td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 C	2.579615	0.000000				3 C	2.579344	2.517527	0.000000			4 B	1.933895	1.792467	1.792857	0.000000		5 B	3.084767	1.514484	1.514526	1.934307	0.000000	6 C	1.514625	2.887360	1.413230	1.792966	2.579503	7 C	1.514554	1.413600	2.887147	1.792010	2.579607		6	7				6 C	0.000000					7 C	2.517744	0.000000			
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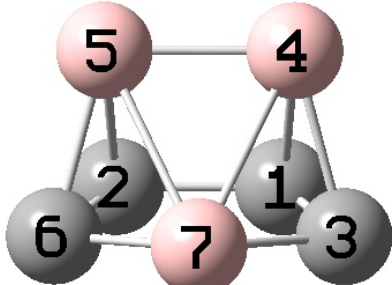
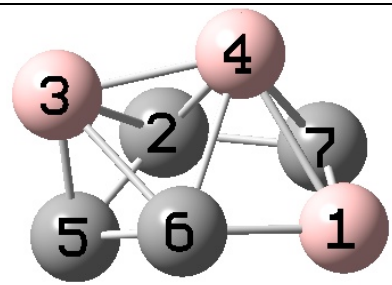
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Table S2C. Energy ranking for all of the C₄B₃H₇ structures.

		E w zpc	delta E w zpc
1	02-HexPyr-a2----c4	-231.0723292	0.00
2	03-TricapTd-e1----c4	-231.0723273	0.00
3	04-CapOh-b4----c4	-231.0723273	0.00
4	04-CapOh-a3----c4	-231.0723261	0.00
5	04-CapOh-b3----c4	-231.0723241	0.00
6	03-TricapTd-a5----c4	-231.0723190	0.01
7	03-TricapTd-b2----c4	-231.0687987	2.22
8	01-PentBipyr-a1----c4	-231.0687878	2.22
9	06-BisdisphA-a3----c4	-231.0687869	2.22
10	01-PentBipyr-a3----c4	-231.0541111	11.43
11	05-DicapTetrPyr-e3----c4	-231.0541111	11.43
12	03-TricapTd-e3----c4	-231.0541068	11.43
13	06-BisdisphA-b1----c4_i-53	-231.0484817	14.96
14	01-PentBipyr-c1----c4_i-58	-231.0484739	14.97
15	04-CapOh-e1----c4_i-70	-231.0484196	15.00
16	01-PentBipyr-c1----c4_r-58	-231.0482851	15.09
17	04-CapOh-e1----c4_r-70	-231.0482851	15.09
18	06-BisdisphA-b1----c4_r-53	-231.0482840	15.09
19	04-CapOh-f2----c4	-231.0441723	17.67
20	05-DicapTetrPyr-e1----c4	-231.0441708	17.67
21	04-CapOh-k1----c4	-231.0441698	17.67
22	04-CapOh-e3----c4	-231.0441688	17.67
23	03-TricapTd-e4----c4	-231.0441686	17.67
24	03-TricapTd-a1----c4	-231.0441685	17.67
25	04-CapOh-c2----c4	-231.0441684	17.67
26	01-PentBipyr-a2----c4	-231.0441667	17.67
27	04-CapOh-e2----c4	-231.0441667	17.67
28	07-BisdisphB-a1----c4	-231.0441650	17.67
29	03-TricapTd-b1----c4	-231.0214103	31.95
30	02-HexPyr-a3----c4_r-64	-231.0126973	37.42
31	03-TricapTd-a2----c4	-231.0126962	37.42
32	02-HexPyr-a3----c4_i-64	-231.0126595	37.44
33	04-CapOh-h1----c4	-231.0086182	39.98
34	04-CapOh-c1----c4	-231.0086064	39.99
35	05-DicapTetrPyr-a3----c4	-231.0044271	42.61
36	03-TricapTd-a3----c4	-231.0044259	42.61
37	06-BisdisphA-e2----c4	-231.0044239	42.61
38	05-DicapTetrPyr-f1----c4	-231.0036794	43.08
39	04-CapOh-i1----c4	-231.0036771	43.08

40	04-CapOh-a1----c4	-231.0032036	43.38
41	05-DicapTetrPyr-c1----c4	-231.0032030	43.38
42	04-CapOh-b2----c4	-231.0032010	43.38
43	03-TricapTd-a4----c4	-231.0031989	43.38
44	04-CapOh-b1----c4	-231.0031986	43.38
45	05-DicapTetrPyr-a2----c4	-231.0025999	43.76
46	06-BisdisphA-a1----c4	-231.0025980	43.76
47	02-HexPyr-b2----c4	-231.0025971	43.76
48	06-BisdisphA-e1----c4	-231.0025971	43.76
49	07-BisdisphB-a2----c4	-231.0025958	43.76
50	04-CapOh-a2----c4	-231.0025916	43.76
51	05-DicapTetrPyr-b1----c4	-231.0004817	45.09
52	02-HexPyr-c1----c4	-231.0004778	45.09
53	06-BisdisphA-a2----c4	-230.9872054	53.42
54	05-DicapTetrPyr-c3----c4	-230.9590723	71.07
55	05-DicapTetrPyr-c2----c4_r-322	-230.9548732	73.71
56	03-TricapTd-e2----c4	-230.9442163	80.39
57	05-DicapTetrPyr-c2----c4_i-322	-230.9202300	95.45
58	04-CapOh-f1----c4	-230.9033379	106.05
59	04-CapOh-k2----c4	-230.9033376	106.05
60	05-DicapTetrPyr-a1----c4	-230.8995707	108.41

Table S3A. Initial $C_4B_4H_8$ structures, a total of 105 structures:

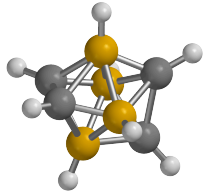
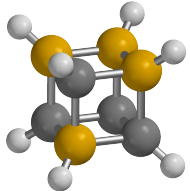
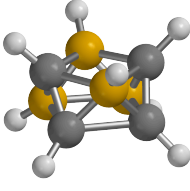
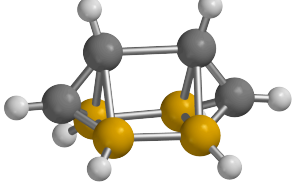
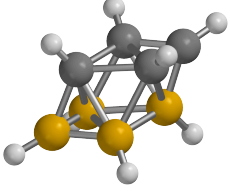
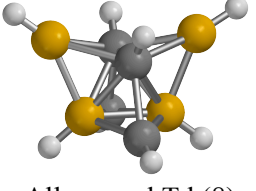
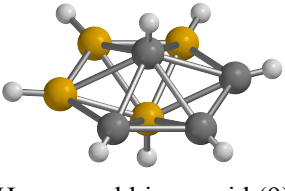
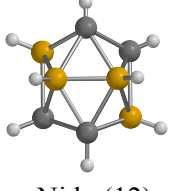
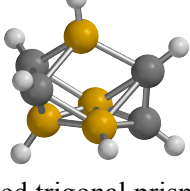
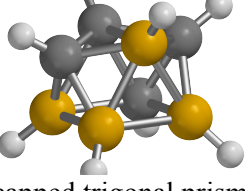
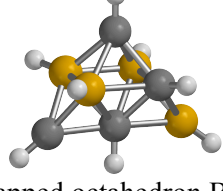
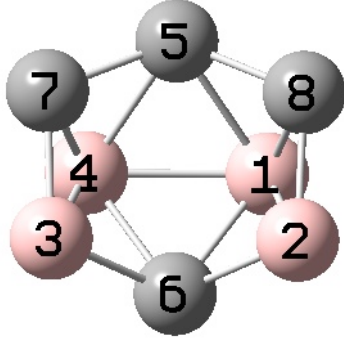
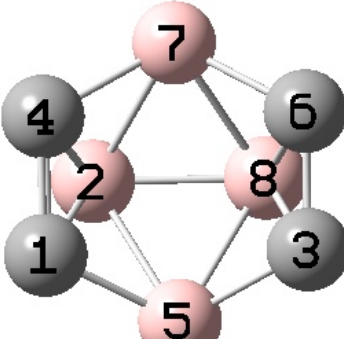
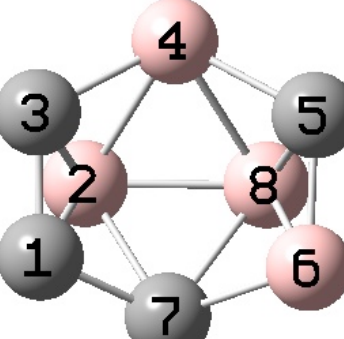
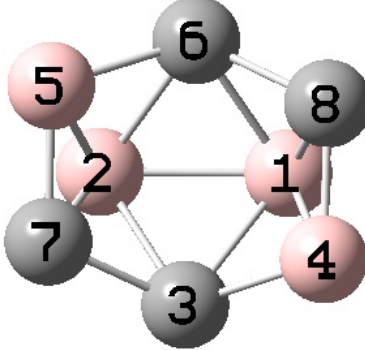
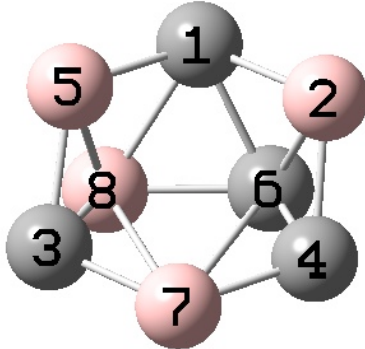
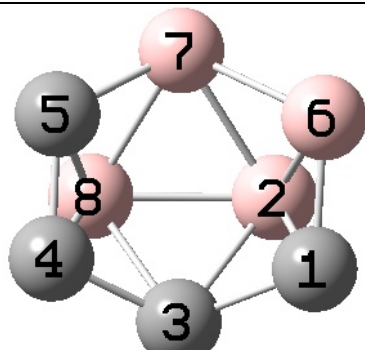
Initial structures	 Bisdiphenoid (21)	 Cube (4)
 Tetragonal antiprism (9)	 Dicapped trigonal prism (10)	 Bicapped octahedron A (8)
 All-capped Td (8)	 Hexagonal bipyramid (9)	 Nido (12)
 Dicapped trigonal prismA (12)	 Dicapped trigonal prismB (6)	 Bicapped octahedron B (6)

Table S3B. Distance table for the lowest-lying C₄B₄H₈ structures. For clarity, only the polyhedral framework is presented.

 1. -256.4387702 C_s	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.802793</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.770966</td><td>2.454307</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.804284</td><td>2.770998</td><td>1.802801</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>1.785343</td><td>2.471889</td><td>2.471878</td><td>1.785383</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.673425</td><td>1.616420</td><td>1.616383</td><td>1.673404</td><td>2.513039</td></tr><tr><td>7 C</td><td>2.704095</td><td>2.916057</td><td>1.492014</td><td>1.642428</td><td>1.491041</td></tr><tr><td>8 C</td><td>1.642404</td><td>1.492042</td><td>2.916079</td><td>2.704155</td><td>1.491056</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.462606</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.462656</td><td>2.557670</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.802793	0.000000				3 B	2.770966	2.454307	0.000000			4 B	1.804284	2.770998	1.802801	0.000000		5 C	1.785343	2.471889	2.471878	1.785383	0.000000	6 C	1.673425	1.616420	1.616383	1.673404	2.513039	7 C	2.704095	2.916057	1.492014	1.642428	1.491041	8 C	1.642404	1.492042	2.916079	2.704155	1.491056		6	7	8			6 C	0.000000					7 C	2.462606	0.000000				8 C	2.462656	2.557670	0.000000		
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 2. -256.4375297 C_{2v}	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.714756</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.601868</td><td>2.719879</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>1.373913</td><td>1.714700</td><td>2.942184</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.585076</td><td>1.867538</td><td>1.585076</td><td>2.510288</td><td>0.000000</td></tr><tr><td>6 C</td><td>2.942184</td><td>2.719734</td><td>1.373913</td><td>2.601518</td><td>2.510288</td></tr><tr><td>7 B</td><td>2.509959</td><td>1.867394</td><td>2.509959</td><td>1.584623</td><td>2.757796</td></tr><tr><td>8 B</td><td>2.719879</td><td>1.713136</td><td>1.714756</td><td>2.719734</td><td>1.867538</td></tr><tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.584623</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.714700</td><td>1.867394</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.714756	0.000000				3 C	2.601868	2.719879	0.000000			4 C	1.373913	1.714700	2.942184	0.000000		5 B	1.585076	1.867538	1.585076	2.510288	0.000000	6 C	2.942184	2.719734	1.373913	2.601518	2.510288	7 B	2.509959	1.867394	2.509959	1.584623	2.757796	8 B	2.719879	1.713136	1.714756	2.719734	1.867538		6	7	8			6 C	0.000000					7 B	1.584623	0.000000				8 B	1.714700	1.867394	0.000000		
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 6. -256.4087744 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.665720</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.502199</td><td>1.787555</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.552238</td><td>2.678017</td><td>1.471161</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.906390</td><td>2.662956</td><td>2.371082</td><td>1.396537</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.469086</td><td>1.790752</td><td>2.494718</td><td>2.973838</td><td>2.586356</td></tr><tr><td>7 B</td><td>2.608080</td><td>1.799359</td><td>2.637353</td><td>2.512671</td><td>1.560530</td></tr><tr><td>8 B</td><td>2.738119</td><td>1.780804</td><td>1.786279</td><td>1.677388</td><td>1.705146</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.772618</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.869325</td><td>1.799313</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.665720	0.000000				3 C	1.502199	1.787555	0.000000			4 C	2.552238	2.678017	1.471161	0.000000		5 C	2.906390	2.662956	2.371082	1.396537	0.000000	6 B	1.469086	1.790752	2.494718	2.973838	2.586356	7 B	2.608080	1.799359	2.637353	2.512671	1.560530	8 B	2.738119	1.780804	1.786279	1.677388	1.705146		6	7	8			6 B	0.000000					7 B	1.772618	0.000000				8 B	2.869325	1.799313	0.000000		
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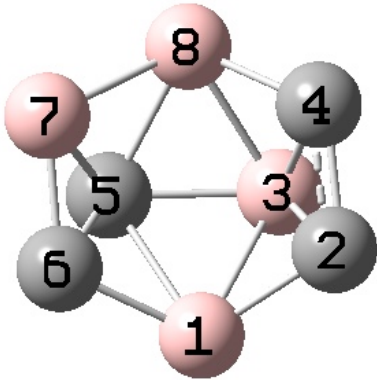
 7. -256.4006732 C₁												
		1	2	3	4	5						
	1 B	0.000000										
	2 C	1.568219	0.000000									
	3 B	1.911567	1.673530	0.000000								
	4 C	2.502870	1.398061	1.699074	0.000000							
	5 C	1.837261	2.570535	1.656765	2.513628	0.000000						
	6 C	1.581163	2.650106	2.737669	2.949385	1.603525						
	7 B	2.630079	3.049246	2.863969	2.622830	1.719275						
	8 B	2.798046	2.526661	1.791464	1.555125	1.690908						
		6	7	8								
	6 C	0.000000										
	7 B	1.469836	0.000000									
	8 B	2.610691	1.774412	0.000000								

Table S3C. Energy ranking for all of the C₄B₄H₈ structures.

		E w zpc	delta E w zpc
1	10-DicapTrPrB-a16----c4	-256.5329310	0.00
2	11-DicapOh-a16----c4	-256.5329171	0.01
3	03-Antipr-a21----c4	-256.5329141	0.01
4	11-DicapOh-a11----c4	-256.5259049	4.41
5	06-Tdallcap-a15----c4	-256.5259024	4.41
6	08-Nido-a13----c4	-256.5258973	4.41
7	03-Antipr-a22----c4	-256.5258968	4.41
8	10-DicapTrPrB-a14----c4	-256.5258949	4.42
9	07-Bipirhex-a13----c4	-256.5201936	7.99
10	01-Bisdisph-g21----c4	-256.5201908	7.99
11	04-TrigPyr-a41----c4	-256.5201897	8.00
12	09-DicapTrPrA-a12----c4	-256.5201880	8.00
13	04-TrigPyr-a21----c4	-256.5201870	8.00
14	09-DicapTrPrA-a111----c4	-256.5201861	8.00
15	01-Bisdisph-a11----c4	-256.5201859	8.00
16	05-AntiprTrig-a16----c4	-256.5101254	14.31
17	11-DicapOh-a12----c4	-256.5101247	14.31
18	06-Tdallcap-a16----c4	-256.5101232	14.31
19	07-Bipirhex-a19----c4	-256.5101226	14.31
20	05-AntiprTrig-a13----c4	-256.5101190	14.31
21	09-DicapTrPrA-a18----c4	-256.5101177	14.32
22	04-TrigPyr-a22----c4	-256.5098895	14.46
23	08-Nido-a16----c4	-256.5098871	14.46
24	04-TrigPyr-f21----c4	-256.5098831	14.46
25	08-Nido-a12----c4	-256.5010530	20.00
26	06-Tdallcap-a11----c4	-256.5010497	20.01
27	04-TrigPyr-a11----c4	-256.5010489	20.01
28	09-DicapTrPrA-a13----c4	-256.5010443	20.01
29	03-Antipr-a31----c4	-256.4924092	25.43
30	07-Bipirhex-a11----c4	-256.4901147	26.87
31	08-Nido-a11----c4	-256.4901132	26.87
32	09-DicapTrPrA-a14----c4	-256.4901056	26.87
33	04-TrigPyr-a13----c4	-256.4890353	27.55
34	01-Bisdisph-a31----c4	-256.4853722	29.84
35	03-Antipr-c21----c4	-256.4853583	29.85
36	07-Bipirhex-a16----c4	-256.4853174	29.88
37	08-Nido-a18----c4	-256.4841630	30.60
38	01-Bisdisph-b22----c4	-256.4841411	30.62
39	02-Cube-a21----c4_r-769	-256.4841411	30.62

40	05-AntiprTrig-a18----c4	-256.4841396	30.62
41	09-DicapTrPrA-a15----c4	-256.4841393	30.62
42	06-Tdallcap-a17----c4	-256.4841356	30.62
43	01-Bisdisph-b41----c4	-256.4805136	32.89
44	09-DicapTrPrA-a17----c4	-256.4805100	32.90
45	01-Bisdisph-a13----c4	-256.4805078	32.90
46	09-DicapTrPrA-a110----c4	-256.4805059	32.90
47	08-Nido-a112----c4	-256.4805050	32.90
48	04-TrigPyr-a31----c4	-256.4756296	35.96
49	03-Antipr-a12----c4	-256.4756295	35.96
50	10-DicapTrPrB-a13----c4	-256.4756276	35.96
51	02-Cube-a12----c4_r-486	-256.4756238	35.96
52	05-AntiprTrig-a14----c4	-256.4756173	35.97
53	07-Bipirhex-a17----c4	-256.4756168	35.97
54	01-Bisdisph-a14----c4	-256.4749998	36.35
55	08-Nido-a110----c4	-256.4749948	36.36
56	01-Bisdisph-b21----c4	-256.4749860	36.36
57	08-Nido-a17----c4	-256.4733760	37.37
58	06-Tdallcap-a13----c4	-256.4714326	38.59
59	07-Bipirhex-a12----c4	-256.4695472	39.77
60	08-Nido-a14----c4	-256.4695327	39.78
61	07-Bipirhex-a14----c4	-256.4678059	40.87
62	08-Nido-a19----c4	-256.4648195	42.74
63	01-Bisdisph-f23----c4	-256.4648194	42.74
64	03-Antipr-a32----c4	-256.4648186	42.74
65	01-Bisdisph-a22----c4	-256.4648185	42.74
66	03-Antipr-b11----c4	-256.4648152	42.74
67	01-Bisdisph-b32----c4	-256.4633126	43.69
68	06-Tdallcap-a14----c4	-256.4580106	47.01
69	07-Bipirhex-a18----c4	-256.4574874	47.34
70	10-DicapTrPrB-a15----c4	-256.4568495	47.74
71	05-AntiprTrig-a12----c4	-256.4568475	47.74
72	01-Bisdisph-c41----c4	-256.4568455	47.75
73	11-DicapOh-a14----c4	-256.4568452	47.75
74	10-DicapTrPrB-a12----c4	-256.4568424	47.75
75	03-Antipr-a13----c4	-256.4568422	47.75
76	01-Bisdisph-c42----c4	-256.4568414	47.75
77	01-Bisdisph-b31----c4	-256.4568412	47.75
78	01-Bisdisph-f22----c4	-256.4568412	47.75
79	09-DicapTrPrA-a16----c4	-256.4512141	51.28
80	11-DicapOh-a15----c4	-256.4512120	51.28
81	04-TrigPyr-f11----c4	-256.4398832	58.39

82	04-TrigPyr-f22----c4	-256.4370440	60.17
83	02-Cube-a12----c4_i-486	-256.4355588	61.10
84	11-DicapOh-a13----c4	-256.4331015	62.65
85	08-Nido-a15----c4	-256.4292682	65.05
86	05-AntiprTrig-a15----c4	-256.4292672	65.05
87	03-Antipr-a11----c4	-256.4270994	66.41
88	08-Nido-a111----c4	-256.4270981	66.41
89	09-DicapTrPrA-a112----c4	-256.4270980	66.41
90	06-Tdallcap-a12----c4	-256.4270977	66.41
91	01-Bisdisph-a12----c4	-256.4270971	66.41
92	01-Bisdisph-b33----c4	-256.4244159	68.10
93	06-Tdallcap-a18----c4	-256.4244153	68.10
94	10-DicapTrPrB-a11----c4_r-201	-256.4232778	68.81
95	09-DicapTrPrA-a11----c4	-256.4231629	68.88
96	04-TrigPyr-a12----c4	-256.4202375	70.72
97	05-AntiprTrig-a11----c4	-256.3967030	85.49
98	09-DicapTrPrA-a19----c4	-256.3772627	97.68
99	10-DicapTrPrB-a11----c4_i-201	-256.3714278	101.35
100	02-Cube-a21----c4_i-769	-256.3710045	101.61

Table S4A. Initial $C_4B_5H_9$ structures, a total of 76 structures:

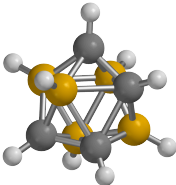
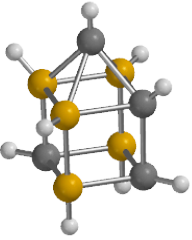
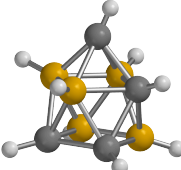
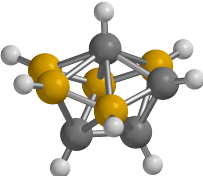
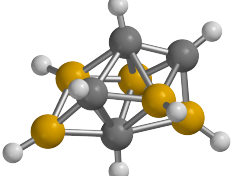
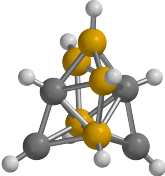
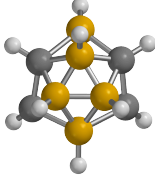
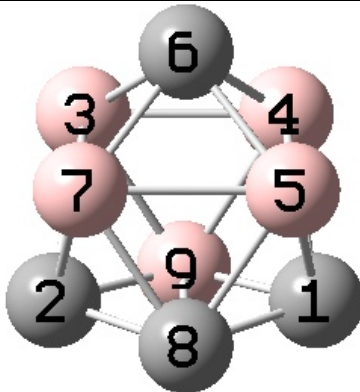
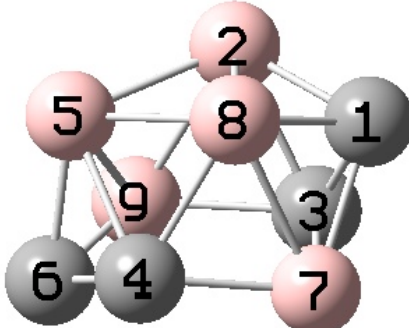
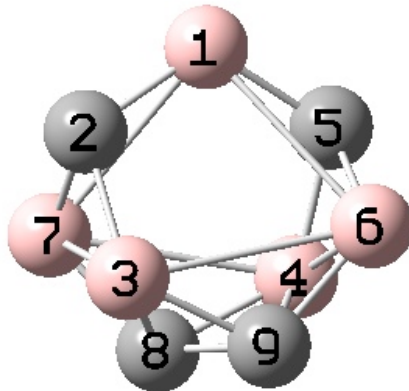
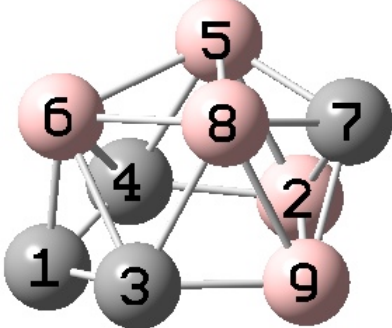
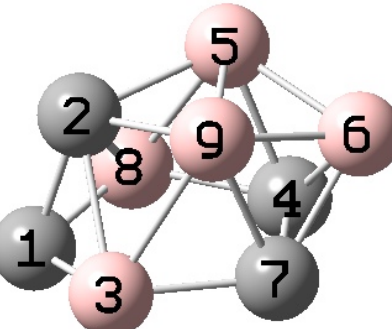
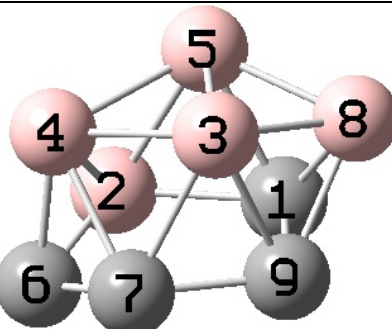
Initial	structures	 Tricapped trigonal prism (8)
 Capped cube (14)	 Capped square antiprism (10)	 Isocloso (10)
 Capped bisdisphenoid (12)	 Bicapped pentag bipy (12)	 10vx-Isocloso-1vx (10)

Table S4B. Distance table for the lowest-lying C₄B₅H₉ structures. For clarity, only the polyhedral framework is presented.

 1. -281.8774395 C_s	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>2.299118</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.642396</td><td>1.703655</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.703410</td><td>2.642534</td><td>1.774854</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.663465</td><td>2.653130</td><td>2.622407</td><td>1.892119</td><td>0.000000</td></tr><tr><td>6 C</td><td>2.588098</td><td>2.588425</td><td>1.631962</td><td>1.631976</td><td>1.604848</td></tr><tr><td>7 B</td><td>2.652819</td><td>1.663652</td><td>1.892026</td><td>2.622366</td><td>1.857602</td></tr><tr><td>8 C</td><td>1.538914</td><td>1.538792</td><td>2.602340</td><td>2.602416</td><td>1.692893</td></tr><tr><td>9 B</td><td>1.646104</td><td>1.645950</td><td>1.762986</td><td>1.762999</td><td>2.737647</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th></th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.604903</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.565730</td><td>1.692655</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>2.728210</td><td>2.737487</td><td>2.194313</td><td>0.000000</td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 C	2.299118	0.000000				3 B	2.642396	1.703655	0.000000			4 B	1.703410	2.642534	1.774854	0.000000		5 B	1.663465	2.653130	2.622407	1.892119	0.000000	6 C	2.588098	2.588425	1.631962	1.631976	1.604848	7 B	2.652819	1.663652	1.892026	2.622366	1.857602	8 C	1.538914	1.538792	2.602340	2.602416	1.692893	9 B	1.646104	1.645950	1.762986	1.762999	2.737647		6	7	8	9		6 C	0.000000					7 B	1.604903	0.000000				8 C	2.565730	1.692655	0.000000			9 B	2.728210	2.737487	2.194313	0.000000	
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 2. -281.8678784 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.598980</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.541391</td><td>1.743826</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.625485</td><td>2.701051</td><td>2.546384</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.730351</td><td>1.799347</td><td>2.698112</td><td>1.751168</td><td>0.000000</td></tr><tr><td>6 C</td><td>3.308390</td><td>2.740031</td><td>2.595788</td><td>1.474452</td><td>1.626402</td></tr><tr><td>7 B</td><td>1.639483</td><td>2.558168</td><td>1.620977</td><td>1.666143</td><td>2.765966</td></tr><tr><td>8 B</td><td>1.572655</td><td>1.870202</td><td>2.467643</td><td>1.728483</td><td>1.801004</td></tr><tr><td>9 B</td><td>2.782213</td><td>1.901581</td><td>1.700713</td><td>2.396649</td><td>1.910073</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th></th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.558005</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.730085</td><td>1.886377</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>1.508260</td><td>2.615960</td><td>2.872163</td><td>0.000000</td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.598980	0.000000				3 C	1.541391	1.743826	0.000000			4 C	2.625485	2.701051	2.546384	0.000000		5 B	2.730351	1.799347	2.698112	1.751168	0.000000	6 C	3.308390	2.740031	2.595788	1.474452	1.626402	7 B	1.639483	2.558168	1.620977	1.666143	2.765966	8 B	1.572655	1.870202	2.467643	1.728483	1.801004	9 B	2.782213	1.901581	1.700713	2.396649	1.910073		6	7	8	9		6 C	0.000000					7 B	2.558005	0.000000				8 B	2.730085	1.886377	0.000000			9 B	1.508260	2.615960	2.872163	0.000000	
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7 B	2.478099	1.549206	1.895569	2.516130	2.974842																																																																																						
8 C	3.066074	2.507492	1.813878	1.630608	2.780241																																																																																						
9 C	3.065847	2.780371	1.630572	1.813823	2.507473																																																																																						
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7 B	3.393952	0.000000																																																																																									
8 C	2.692304	1.558957	0.000000																																																																																								
9 C	1.558958	2.692325	1.573992	0.000000																																																																																							

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Table S4C. Energy ranking for all of the C₄B₅H₉ structures.

		E w zpc	delta E w zpc
1	06-BicapPentBipyr-a15----c4	-281.9732255	0.00
2	05-CapBisdisph-a18----c4	-281.9732243	0.00
3	07-Isocloso-6vx-a17----c4	-281.9732239	0.00
4	03-CapSqAntPr-a17----c4	-281.9677489	3.44
5	01-TricTrPrism-a14----c4	-281.9677454	3.44
6	03-CapSqAntPr-a15----c4	-281.9677446	3.44
7	01-TricTrPrism-a18----c4	-281.9677413	3.44
8	03-CapSqAntPr-a14----c4	-281.9677374	3.44
9	01-TricTrPrism-a15----c4	-281.9664347	4.26
10	04-Tl99-a11----c4	-281.9664253	4.27
11	04-Tl99-a19----c4	-281.9555246	11.11
12	07-Isocloso-6vx-a11----c4	-281.9545095	11.74
13	02-CapCube-a112----c4	-281.9545040	11.75
14	02-CapCube-a12----c4	-281.9508248	14.06
15	04-Tl99-a15----c4	-281.9508219	14.06
16	01-TricTrPrism-a12----c4	-281.9508185	14.06
17	01-TricTrPrism-a13----c4	-281.9495236	14.87
18	07-Isocloso-6vx-a14----c4	-281.9475223	16.13
19	03-CapSqAntPr-a16----c4	-281.9475175	16.13
20	02-CapCube-a17----c4	-281.9470816	16.41
21	05-CapBisdisph-a17----c4	-281.9470775	16.41
22	04-Tl99-a110----c4	-281.9444248	18.07
23	07-Isocloso-6vx-a15----c4	-281.9436750	18.54
24	06-BicapPentBipyr-a17----c4	-281.9436694	18.55
25	07-Isocloso-6vx-a18----c4	-281.9416138	19.84
26	02-CapCube-a111----c4	-281.9416129	19.84
27	02-CapCube-a114----c4	-281.9416129	19.84
28	07-Isocloso-6vx-a12----c4	-281.9416081	19.84
29	05-CapBisdisph-a16----c4	-281.9414886	19.92
30	06-BicapPentBipyr-a12----c4	-281.9384946	21.79
31	02-CapCube-a13----c4	-281.9371333	22.65
32	05-CapBisdisph-a15----c4	-281.9338617	24.70
33	06-BicapPentBipyr-a11----c4	-281.9338602	24.70
34	06-BicapPentBipyr-a110----c4	-281.9328152	25.36
35	05-CapBisdisph-a14----c4	-281.9323091	25.68
36	04-Tl99-a12----c4	-281.9323023	25.68
37	07-Isocloso-6vx-a16----c4	-281.9314344	26.22
38	01-TricTrPrism-a17----c4	-281.9301296	27.04
39	06-BicapPentBipyr-a18----c4	-281.9297099	27.31

40	02-CapCube-a14----c4_r-238	-281.9279732	28.40
41	05-CapBisdisph-a112----c4	-281.9256564	29.85
42	07-Isocloso-6vx-a110----c4	-281.9250476	30.23
43	01-TricTrPrism-a16----c4	-281.9237381	31.05
44	06-BicapPentBipyr-a14----c4	-281.9237344	31.06
45	03-CapSqAntPr-a12----c4	-281.9224050	31.89
46	06-BicapPentBipyr-a13----c4	-281.9223983	31.90
47	06-BicapPentBipyr-a16----c4	-281.9223398	31.93
48	03-CapSqAntPr-a110----c4	-281.9223213	31.94
49	02-CapCube-a110----c4_r-467	-281.9222971	31.96
50	02-CapCube-a14----c4_i-238	-281.9177820	34.79
51	06-BicapPentBipyr-a112----c4	-281.9114123	38.79
52	02-CapCube-a18----c4_r-222	-281.9114118	38.79
53	05-CapBisdisph-a11----c4	-281.9114115	38.79
54	05-CapBisdisph-a19----c4	-281.9114110	38.79
55	03-CapSqAntPr-a19----c4	-281.9109977	39.05
56	06-BicapPentBipyr-a19----c4	-281.9109967	39.05
57	05-CapBisdisph-a110----c4	-281.9068725	41.64
58	03-CapSqAntPr-a11----c4	-281.9023809	44.46
59	01-TricTrPrism-a11----c4	-281.9023805	44.46
60	02-CapCube-a19----c4_r-300	-281.9004009	45.70
61	07-Isocloso-6vx-a13----c4	-281.9003984	45.70
62	05-CapBisdisph-a111----c4_r-188	-281.9003976	45.70
63	04-Tl99-a14----c4	-281.9003885	45.71
64	06-BicapPentBipyr-a111----c4	-281.9003885	45.71
65	04-Tl99-a16----c4	-281.9002461	45.80
66	04-Tl99-a13----c4	-281.9002439	45.80
67	05-CapBisdisph-a111----c4_i-188	-281.8980452	47.18
68	03-CapSqAntPr-a13----c4	-281.8930218	50.33
69	04-Tl99-a17----c4	-281.8924444	50.69
70	02-CapCube-a18----c4_i-222	-281.8890303	52.83
71	07-Isocloso-6vx-a19----c4_r-170	-281.8888529	52.95
72	02-CapCube-a19----c4_i-300	-281.8863298	54.53
73	02-CapCube-a15----c4_r-665	-281.8825630	56.89
74	05-CapBisdisph-a13----c4	-281.8821433	57.16
75	07-Isocloso-6vx-a19----c4_i-170	-281.8818448	57.34
76	03-CapSqAntPr-a18----c4	-281.8731887	62.78
77	02-CapCube-a16----c4_r-684	-281.8703121	64.58
78	02-CapCube-a11----c4_r-198	-281.8682647	65.87
79	04-Tl99-a18----c4	-281.8661241	67.21
80	02-CapCube-a113----c4_r-751	-281.8586764	71.88
81	02-CapCube-a11----c4_i-198	-281.8502160	77.19

82	05-CapBisdisph-a12----c4	-281.8411743	82.86
83	02-CapCube-a110----c4_i-467	-281.8360489	86.08
84	02-CapCube-a15----c4_i-665	-281.8113133	101.60
85	02-CapCube-a16----c4_i-684	-281.7560349	136.29
86	02-CapCube-a113----c4_i-751	-281.7294247	152.99

Table S5A. Initial $C_4B_6H_{10}$ structures, a total of 164 structures.

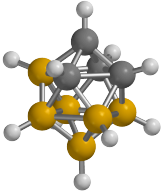
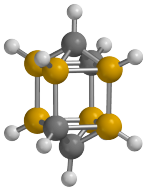
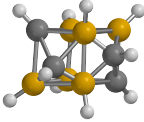
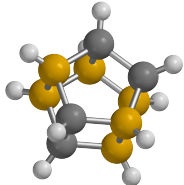
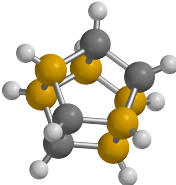
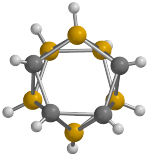
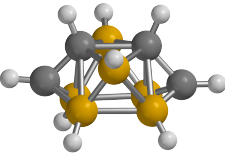
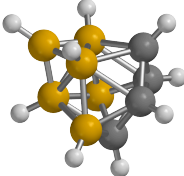
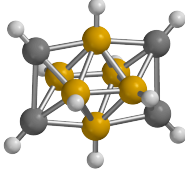
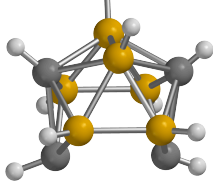
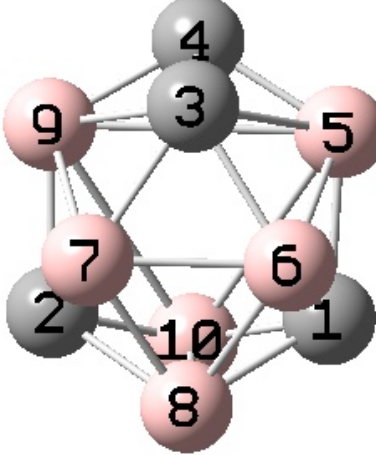
Initial structures	 Bicapped square antiprism (20)	 Bicapped cube A (8)
 Bicapped cube B (15)	 Pentagonal prism (8)	 Pentagonal antiprism (6)
 Tetracapped trig prism A (15)	 Tetracapped trig prism B (28)	 Isocloso (25)
 Tetracapped octahedron (14)	 Bisdisphenoid-like (15)	 Edge-coalesc icos -1vx (10)

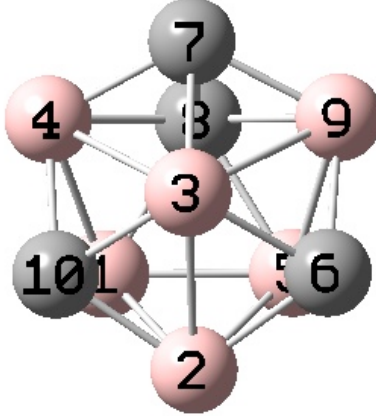
Table S5B. Distance table for the lowest-lying C₄B₆H₁₀ structures. For clarity, only the polyhedral framework is presented.

framework is presented.



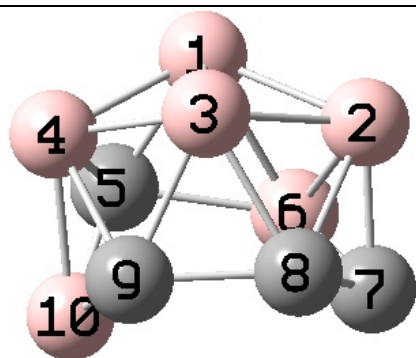
1. -307.3362576 C_s

	1	2	3	4	5
1 C	0.000000				
2 C	2.474947	0.000000			
3 C	2.651070	2.651086	0.000000		
4 C	2.749147	2.749205	1.577814	0.000000	
5 B	1.683292	3.043045	1.816937	1.528827	0.000000
6 B	1.665280	2.691395	1.671856	2.711617	1.891027
7 B	2.691382	1.665245	1.671881	2.711646	2.875114
8 B	1.686645	1.686645	2.754466	3.380691	2.882354
9 B	3.042945	1.683317	1.816888	1.528795	2.596542
10 B	1.555346	1.555354	3.129830	2.809881	2.535132
	6	7	8	9	10
6 B	0.000000				
7 B	1.806291	0.000000			
8 B	1.745180	1.745167	0.000000		
9 B	2.875049	1.891027	2.882330	0.000000	
10 B	2.726504	2.726478	1.821611	2.535072	0.000000



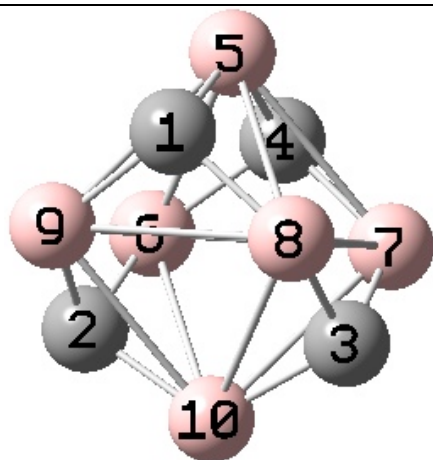
2. -307.3313874 C_s

	1	2	3	4	5
1 B	0.000000				
2 B	1.800056	0.000000			
3 B	2.641507	1.996235	0.000000		
4 B	1.856510	2.753978	2.044364	0.000000	
5 B	1.773984	1.799896	2.641522	2.888023	0.000000
6 C	2.709564	1.613145	1.683191	3.101890	1.659766
7 C	2.699515	3.099498	1.781956	1.583934	2.699068
8 C	1.704470	2.730900	2.560022	1.782149	1.704759
9 B	2.889132	2.754170	2.044131	2.759577	1.857484
10 C	1.659389	1.613136	1.683053	1.577332	2.709142
	6	7	8	9	10
6 C	0.000000				
7 C	2.564373	0.000000			
8 C	2.588599	1.583055	0.000000		
9 B	1.577139	1.583178	1.783983	0.000000	
10 C	2.585365	2.564832	2.587941	3.102040	0.000000



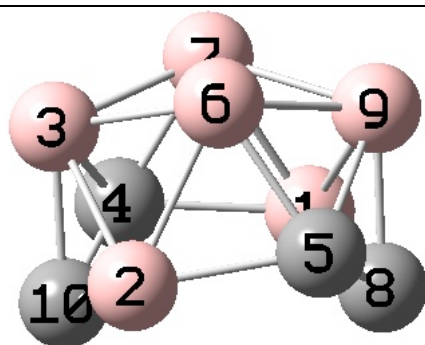
3. -307.3260557 C_1

	1	2	3	4	5
1 B	0.000000				
2 B	1.792398	0.000000			
3 B	1.801679	1.788034	0.000000		
4 B	1.747633	2.909508	1.729324	0.000000	
5 C	1.663872	2.827649	2.691598	1.671560	0.000000
6 B	1.909963	1.907130	2.857978	2.864080	1.707882
7 C	2.714222	1.624595	2.681461	3.343372	2.779949
8 C	2.703151	1.740634	1.724800	2.740463	2.965608
9 C	2.697172	2.773772	1.719770	1.724620	2.445532
10 B	2.739259	3.348038	2.781705	1.821948	1.533053
	6	7	8	9	10
6 B	0.000000				
7 C	1.517714	0.000000			
8 C	2.464669	1.456637	0.000000		
9 C	2.925750	2.605196	1.581082	0.000000	
10 B	2.506043	2.832747	2.591648	1.564322	0.000000



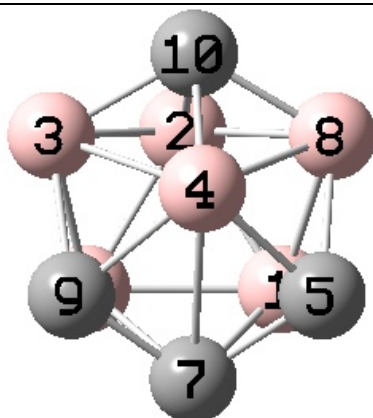
4. -307.3258471 $C_{3v}S_4$

	1	2	3	4	5
1 C	0.000000				
2 C	2.709448	0.000000			
3 C	2.709694	2.709428	0.000000		
4 C	2.709273	2.709181	2.709461	0.000000	
5 B	1.569592	3.028049	3.027265	1.568483	0.000000
6 B	3.026406	1.568898	3.029055	1.569241	2.473414
7 B	3.027390	3.027338	1.569174	1.568875	2.473249
8 B	1.568703	3.027320	1.569864	3.027890	2.474265
9 B	1.569368	1.568932	3.026973	3.028224	2.476308
10 B	3.028978	1.569290	1.569028	3.026454	3.499502
	6	7	8	9	10
6 B	0.000000				
7 B	2.475837	0.000000			
8 B	3.499539	2.475020	0.000000		
9 B	2.473700	3.499138	2.473069	0.000000	
10 B	2.474709	2.473103	2.475759	2.474914	0.000000



5. -307.3256633 C_2

	1	2	3	4	5
1 B	0.000000				
2 B	3.096054	0.000000			
3 B	2.956468	1.861248	0.000000		
4 C	1.756580	2.473381	1.706454	0.000000	
5 C	2.473368	1.756469	2.820561	2.944560	0.000000
6 B	2.841764	1.849116	1.768068	2.669284	1.661093
7 B	1.849131	2.841791	1.780726	1.661107	2.669305
8 C	1.502169	2.683113	3.383524	2.706564	1.445947
9 B	1.861210	2.956429	2.957697	2.820602	1.706474
10 C	2.683176	1.502162	1.676195	1.445956	2.706496
	6	7	8	9	10
6 B	0.000000				
7 B	1.829557	0.000000			
8 C	2.648037	2.676098	0.000000		
9 B	1.780714	1.768097	1.676195	0.000000	
10 C	2.676059	2.648057	2.922629	3.383518	0.000000



6. -307.3206890 C_s

	1	2	3	4	5
1 B	0.000000				
2 B	1.781406	0.000000			
3 B	2.856378	1.816164	0.000000		
4 B	2.703002	2.670650	1.987460	0.000000	
5 C	1.665327	2.732712	3.019676	1.716824	0.000000
6 B	1.849875	1.781363	1.793534	2.703082	2.679552
7 C	1.725870	2.758322	2.670519	2.150930	1.502773
8 B	1.793426	1.816059	2.671780	1.987750	1.659889
9 C	2.679552	2.732754	1.659736	1.717151	2.382198
10 C	2.726336	1.694668	1.574023	1.672955	2.604452
	6	7	8	9	10
6 B	0.000000				
7 C	1.725889	0.000000			
8 B	2.856425	2.670716	0.000000		
9 C	1.665278	1.502721	3.020088	0.000000	
10 C	2.726429	3.079886	1.573972	2.604747	0.000000

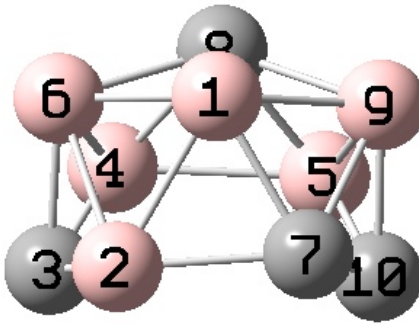
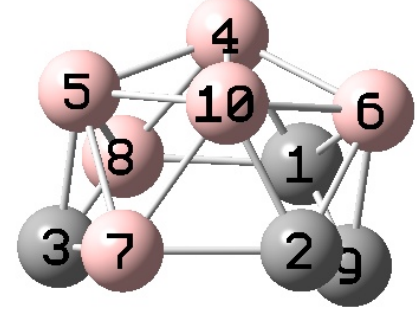
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9 B	2.946910	1.703553	1.713731	0.000000																																																																																																			
10 C	3.375021	1.457981	2.521393	1.656766	0.000000																																																																																																		
	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>2.354463</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.740730</td><td>2.740539</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.679159</td><td>2.677071</td><td>2.711177</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.814597</td><td>2.814448</td><td>1.688155</td><td>1.762268</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.725555</td><td>1.725604</td><td>3.477471</td><td>1.786122</td><td>2.953844</td></tr><tr><td>7 B</td><td>3.047521</td><td>1.799121</td><td>1.509151</td><td>2.839324</td><td>1.819201</td></tr><tr><td>8 B</td><td>1.799446</td><td>3.047521</td><td>1.509189</td><td>1.821372</td><td>1.819163</td></tr><tr><td>9 C</td><td>1.420648</td><td>1.420614</td><td>2.933369</td><td>2.613369</td><td>3.303757</td></tr><tr><td>10 B</td><td>2.677077</td><td>1.679020</td><td>2.711092</td><td>1.846443</td><td>1.762237</td></tr></table> <table><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>2.993673</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.993804</td><td>2.569571</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>1.681778</td><td>2.703520</td><td>2.703720</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>1.786088</td><td>1.821263</td><td>2.839325</td><td>2.613271</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 C	2.354463	0.000000				3 C	2.740730	2.740539	0.000000			4 B	1.679159	2.677071	2.711177	0.000000		5 B	2.814597	2.814448	1.688155	1.762268	0.000000	6 B	1.725555	1.725604	3.477471	1.786122	2.953844	7 B	3.047521	1.799121	1.509151	2.839324	1.819201	8 B	1.799446	3.047521	1.509189	1.821372	1.819163	9 C	1.420648	1.420614	2.933369	2.613369	3.303757	10 B	2.677077	1.679020	2.711092	1.846443	1.762237		6	7	8	9	10	6 B	0.000000					7 B	2.993673	0.000000				8 B	2.993804	2.569571	0.000000			9 C	1.681778	2.703520	2.703720	0.000000		10 B	1.786088	1.821263	2.839325	2.613271	0.000000
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10 B	1.786088	1.821263	2.839325	2.613271	0.000000																																																																																																		

Table S5C. Energy ranking for all of the C₄B₆H₁₀ structures.

		E w zpc	delta E w zpc
1	10-BisDisphenoid-Like-a112----c4_r-807	-307.46219760	0.00
2	02-BicapCubA-a16----c4_r-807	-307.46219120	0.00
3	08-Isocloso-a110----c4	-307.44675270	9.69
4	02-BicapCubA-a14----c4	-307.44675050	9.69
5	11-EdgeCoalsced-1vx-a19----c4	-307.44675040	9.69
6	09-DistTetracapOh-a113----c4	-307.44674860	9.69
7	07-TetrTriPri2-a116----c4	-307.44674760	9.70
8	02-BicapCubA-a13----c4	-307.44310300	11.98
9	02-BicapCubA-a17----c4	-307.44310170	11.98
10	06-TetrTriPri1-a13----c4	-307.44310110	11.98
11	09-DistTetracapOh-a13----c4	-307.44309650	11.99
12	03-BicapCubB-a112----c4	-307.44309400	11.99
13	05-PentAntiPr-a16----c4	-307.43942650	14.29
14	10-BisDisphenoid-Like-a114----c4	-307.43942060	14.29
15	07-TetrTriPri2-a125----c4	-307.43941930	14.29
16	10-BisDisphenoid-Like-a18----c4	-307.43941600	14.30
17	01-BicapSqAntipr-a112----c4	-307.43346330	18.03
18	08-Isocloso-a122----c4	-307.43345560	18.04
19	06-TetrTriPri1-a16----c4	-307.43132100	19.38
20	10-BisDisphenoid-Like-a110----c4	-307.42877740	20.97
21	08-Isocloso-a15----c4	-307.42877330	20.97
22	11-EdgeCoalsced-1vx-a110----c4	-307.42843840	21.18
23	01-BicapSqAntipr-a15----c4	-307.42843770	21.19
24	04-PentagPrism-a18----c4	-307.42843480	21.19
25	06-TetrTriPri1-a17----c4	-307.42736310	21.86
26	08-Isocloso-a18----c4	-307.42709880	22.03
27	09-DistTetracapOh-a19----c4	-307.42560480	22.96
28	08-Isocloso-a123----c4	-307.42431440	23.77
29	08-Isocloso-a121----c4	-307.42342890	24.33
30	07-TetrTriPri2-a112----c4	-307.42342480	24.33
31	08-Isocloso-a118----c4	-307.41732290	28.16
32	08-Isocloso-a116----c4	-307.41732000	28.16
33	01-BicapSqAntipr-a14----c4	-307.41731680	28.16
34	03-BicapCubB-a15----c4	-307.41244520	31.22
35	06-TetrTriPri1-a18----c4	-307.41244420	31.22
36	01-BicapSqAntipr-a113----c4	-307.41061230	32.37
37	06-TetrTriPri1-a14----c4	-307.41060410	32.38
38	07-TetrTriPri2-a122----c4	-307.40895200	33.41

39	08-Isocloso-a124----c4	-307.40894870	33.41
40	07-TetrcTriPri2-a127----c4	-307.40894530	33.42
41	01-BicapSqAntipr-a16----c4	-307.40894120	33.42
42	08-Isocloso-a19----c4	-307.40722980	34.49
43	11-EdgeCoalsced-1vx-a18----c4	-307.40721950	34.50
44	09-DistTetracapOh-a16----c4	-307.40720920	34.51
45	07-TetrcTriPri2-a120----c4	-307.40544580	35.61
46	04-PentagPrism-a13----c4	-307.40489840	35.96
47	07-TetrcTriPri2-a19----c4	-307.40462060	36.13
48	10-BisDisphenoid-Like-a13----c4	-307.40460980	36.14
49	04-PentagPrism-a15----c4	-307.40271140	37.33
50	08-Isocloso-a12----c4	-307.40200600	37.77
51	07-TetrcTriPri2-a114----c4	-307.40199970	37.78
52	01-BicapSqAntipr-a114----c4	-307.40199910	37.78
53	05-PentAntiPr-a12----c4	-307.40093000	38.45
54	06-TetrcTriPri1-a11----c4	-307.39978360	39.17
55	10-BisDisphenoid-Like-a14----c4	-307.39977730	39.17
56	04-PentagPrism-a17----c4	-307.39965450	39.25
57	01-BicapSqAntipr-a111----c4	-307.39965100	39.25
58	04-PentagPrism-a16----c4	-307.39965010	39.25
59	01-BicapSqAntipr-a117----c4	-307.39894640	39.69
60	07-TetrcTriPri2-a111----c4	-307.39893280	39.70
61	03-BicapCubB-a16----c4	-307.39893110	39.70
62	09-DistTetracapOh-a110----c4	-307.39892790	39.70
63	10-BisDisphenoid-Like-a12----c4	-307.39892470	39.71
64	03-BicapCubB-a13----c4	-307.39884220	39.76
65	08-Isocloso-a111----c4	-307.39884140	39.76
66	11-EdgeCoalsced-1vx-a11----c4	-307.39883470	39.76
67	07-TetrcTriPri2-a119----c4	-307.39754850	40.57
68	01-BicapSqAntipr-a118----c4	-307.39711910	40.84
69	01-BicapSqAntipr-a110----c4	-307.39643960	41.26
70	11-EdgeCoalsced-1vx-a15----c4	-307.39611140	41.47
71	08-Isocloso-a16----c4	-307.39591530	41.59
72	07-TetrcTriPri2-a13----c4	-307.39536760	41.94
73	06-TetrcTriPri1-a114----c4	-307.39535560	41.94
74	09-DistTetracapOh-a111----c4	-307.39535360	41.95
75	11-EdgeCoalsced-1vx-a16----c4	-307.39276560	43.57
76	01-BicapSqAntipr-a119----c4	-307.39014600	45.21
77	07-TetrcTriPri2-a126----c4	-307.39014410	45.22
78	08-Isocloso-a14----c4	-307.38901610	45.92
79	10-BisDisphenoid-Like-a17----c4	-307.38886340	46.02
80	09-DistTetracapOh-a11----c4	-307.38886130	46.02

81	02-BicapCubA-a12----c4	-307.38885910	46.02
82	05-PentAntiPr-a14----c4	-307.38885760	46.02
83	03-BicapCubB-a14----c4	-307.38858440	46.19
84	07-TetrTriPri2-a124----c4	-307.38857820	46.20
85	11-EdgeCoalsced-1vx-a13----c4	-307.38857670	46.20
86	07-TetrTriPri2-a117----c4	-307.38803160	46.54
87	10-BisDisphenoid-Like-a113----c4	-307.38802760	46.54
88	06-TetrTriPri1-a110----c4	-307.38580990	47.93
89	09-DistTetracapOh-a17----c4	-307.38579750	47.94
90	08-Isocloso-a17----c4	-307.38578770	47.95
91	09-DistTetracapOh-a12----c4	-307.38496340	48.47
92	05-PentAntiPr-a15----c4	-307.38495980	48.47
93	08-Isocloso-a113----c4	-307.38403800	49.05
94	03-BicapCubB-a115----c4	-307.38390340	49.13
95	05-PentAntiPr-a11----c4	-307.38390330	49.13
96	07-TetrTriPri2-a121----c4	-307.38256130	49.97
97	01-BicapSqAntipr-a19----c4	-307.38255590	49.98
98	07-TetrTriPri2-a113----c4	-307.38254970	49.98
99	11-EdgeCoalsced-1vx-a14----c4	-307.38254390	49.98
100	08-Isocloso-a114----c4	-307.38254310	49.98
101	08-Isocloso-a112----c4	-307.38138780	50.71
102	09-DistTetracapOh-a114----c4	-307.38035600	51.36
103	02-BicapCubA-a11----c4	-307.37970620	51.77
104	07-TetrTriPri2-a17----c4	-307.37936790	51.98
105	07-TetrTriPri2-a115----c4	-307.37420600	55.22
106	03-BicapCubB-a111----c4	-307.37289830	56.04
107	03-BicapCubB-a114----c4	-307.37289830	56.04
108	11-EdgeCoalsced-1vx-a12----c4	-307.37289750	56.04
109	08-Isocloso-a120----c4	-307.37289270	56.04
110	07-TetrTriPri2-a18----c4	-307.37289260	56.04
111	09-DistTetracapOh-a18----c4_r-45	-307.37268120	56.17
112	02-BicapCubA-a18----c4	-307.37249980	56.29
113	09-DistTetracapOh-a14----c4	-307.37233460	56.39
114	07-TetrTriPri2-a118----c4	-307.37136680	57.00
115	01-BicapSqAntipr-a18----c4	-307.37131930	57.03
116	04-PentagPrism-a11----c4	-307.37103730	57.20
117	10-BisDisphenoid-Like-a111----c4	-307.37101570	57.22
118	03-BicapCubB-a17----c4	-307.36732820	59.53
119	08-Isocloso-a117----c4	-307.36649220	60.06
120	01-BicapSqAntipr-a11----c4	-307.36648620	60.06
121	08-Isocloso-a125----c4	-307.36648460	60.06
122	10-BisDisphenoid-Like-a115----c4	-307.36648420	60.06

123	01-BicapSqAntipr-a12----c4	-307.36550960	60.67
124	01-BicapSqAntipr-a13----c4	-307.36534950	60.77
125	06-TetrcTriPri1-a12----c4	-307.36249430	62.57
126	10-BisDisphenoid-Like-a16----c4	-307.36236880	62.64
127	04-PentagPrism-a14----c4	-307.36160070	63.13
128	06-TetrcTriPri1-a15----c4	-307.36080500	63.63
129	10-BisDisphenoid-Like-a19----c4	-307.35990330	64.19
130	02-BicapCubA-a15----c4	-307.35978870	64.26
131	07-TetrcTriPri2-a123----c4	-307.35907560	64.71
132	07-TetrcTriPri2-a16----c4	-307.35772180	65.56
133	03-BicapCubB-a110----c4	-307.35661390	66.26
134	03-BicapCubB-a18----c4	-307.35660990	66.26
135	07-TetrcTriPri2-a110----c4	-307.35641280	66.38
136	06-TetrcTriPri1-a112----c4	-307.35440470	67.64
137	03-BicapCubB-a113----c4	-307.35036520	70.18
138	08-Isocloso-a115----c4	-307.34887810	71.11
139	10-BisDisphenoid-Like-a11----c4	-307.34779940	71.79
140	06-TetrcTriPri1-a111----c4	-307.34463190	73.77
141	03-BicapCubB-a12----c4	-307.34290160	74.86
142	07-TetrcTriPri2-a14----c4	-307.34286710	74.88
143	01-BicapSqAntipr-a17----c4	-307.34276290	74.95
144	08-Isocloso-a13----c4	-307.33985910	76.77
145	03-BicapCubB-a19----c4	-307.33984160	76.78
146	01-BicapSqAntipr-a116----c4	-307.33875410	77.46
147	06-TetrcTriPri1-a115----c4	-307.33793520	77.98
148	09-DistTetracapOh-a18----c4_i-45	-307.33666790	78.77
149	09-DistTetracapOh-a15----c4	-307.33435620	80.22
150	07-TetrcTriPri2-a15----c4	-307.33140990	82.07
151	09-DistTetracapOh-a112----c4	-307.32932360	83.38
152	08-Isocloso-a119----c4	-307.32932130	83.38
153	03-BicapCubB-a11----c4	-307.32931900	83.38
154	04-PentagPrism-a12----c4	-307.32931880	83.38
155	05-PentAntiPr-a13----c4	-307.32931650	83.39
156	01-BicapSqAntipr-a115----c4_r-863	-307.32739750	84.59
157	11-EdgeCoalsced-1vx-a17----c4_r-852	-307.32739630	84.59
158	07-TetrcTriPri2-a11----c4	-307.32739440	84.59
159	01-BicapSqAntipr-a120----c4_r-834	-307.30272120	100.07
160	10-BisDisphenoid-Like-a15----c4	-307.29252650	106.47
161	07-TetrcTriPri2-a12----c4	-307.28640800	110.31
162	06-TetrcTriPri1-a19----c4	-307.20818550	159.40
163	06-TetrcTriPri1-a113----c4	-307.20817050	159.41

Table S6A. Initial $C_4B_7H_{11}$ structures.,a total of 155 structures:

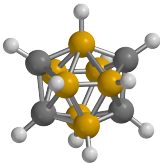
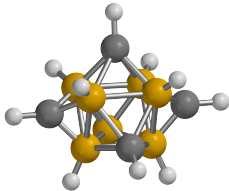
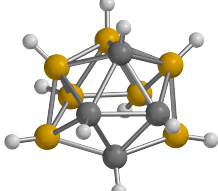
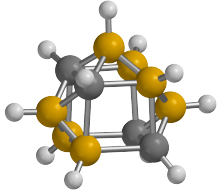
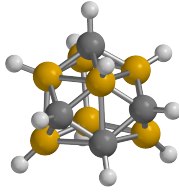
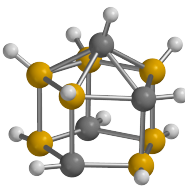
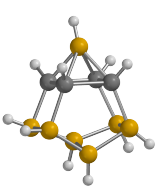
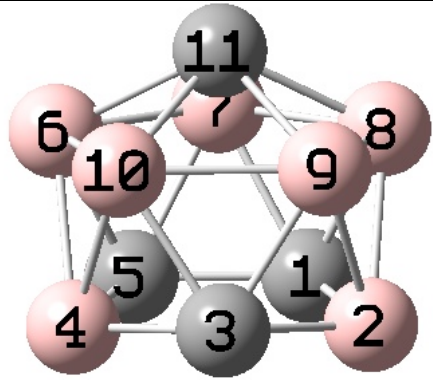
Initial	structures	 Edge-coalesced icos (32)
 Pentacapped trig prism (31)	 Capped pentag antiprism (29)	 Tricapped cube A (28)
 Tricapped cube B (22)	 Capped pentag prism A (5)	 Capped pentag prism B (8)

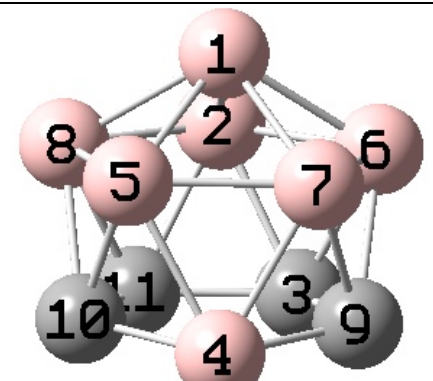
Table S6B. Distance table for the lowest-lying C₄B₇H₁₁ structures. For clarity, only the polyhedral framework is presented.



1. -332.8007615 Cs

	1	2	3	4	5
1 C	0.000000				
2 B	1.605029	0.000000			
3 C	2.591212	1.628262	0.000000		
4 B	2.571368	2.606714	1.629163	0.000000	
5 C	1.549575	2.572539	2.592052	1.604735	0.000000
6 B	2.717088	3.276280	2.721550	1.801357	1.712161
7 B	1.686284	2.807153	3.215708	2.806308	1.685636
8 B	1.711020	1.800907	2.720911	3.275399	2.716237
9 B	2.706350	1.793057	1.674860	2.813652	3.181270
10 B	3.180745	2.813167	1.674879	1.793481	2.706667
11 C	2.599946	2.742782	2.620293	2.742781	2.599990

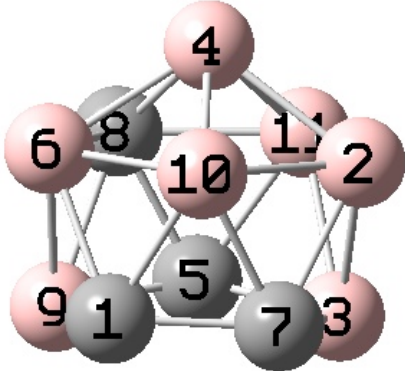
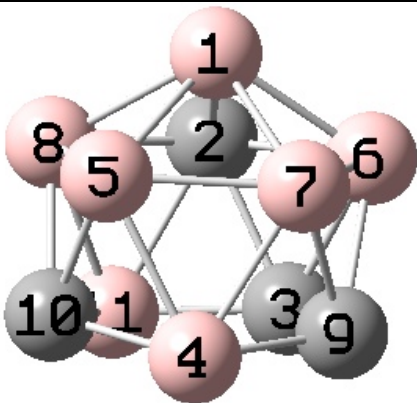
	6	7	8	9	10
6 B	0.000000				
7 B	1.785634	0.000000			
8 B	2.872217	1.785520	0.000000		
9 B	2.862054	2.858433	1.736020	0.000000	
10 B	1.735716	2.858285	2.862055	1.802830	0.000000
11 C	1.697049	1.688179	1.697389	1.725273	1.725398

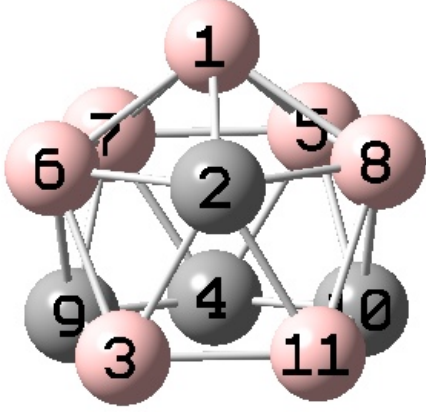
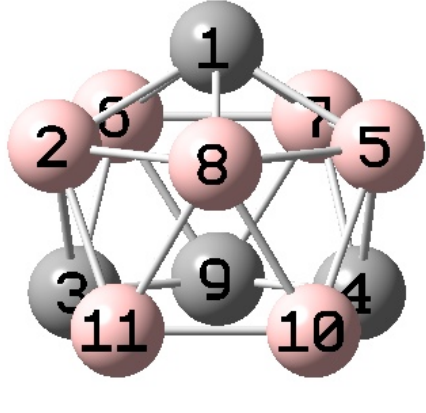


2. -332.7970560 Cs

	1	2	3	4	5
1 B	0.000000				
2 B	1.764878	0.000000			
3 C	2.725557	1.717846	0.000000		
4 B	2.895463	3.303243	2.539186	0.000000	
5 B	1.799512	2.871388	3.138866	1.800694	0.000000
6 B	1.777838	1.780226	1.718952	2.826095	2.859587
7 B	1.800157	2.871006	2.688525	1.800959	1.745293
8 B	1.777835	1.780552	2.695778	2.824052	1.777182
9 C	2.753650	2.717667	1.522348	1.614262	2.712194
10 C	2.754008	2.717852	2.474049	1.612655	1.713243
11 C	2.725765	1.717576	1.499754	2.538873	2.690390

	6	7	8	9	10
6 B	0.000000				
7 B	1.777152	0.000000			
8 B	2.875059	2.859203	0.000000		
9 C	1.701718	1.711222	3.190595	0.000000	
10 C	3.191455	2.712139	1.701053	2.534880	0.000000
11 C	2.695770	3.138296	1.719257	2.473803	1.523052

 3. -332.7863353 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.731164</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.576533</td><td>1.800727</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.742737</td><td>1.778441</td><td>2.873919</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.565238</td><td>2.745017</td><td>1.634379</td><td>2.772400</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.698863</td><td>2.859438</td><td>3.264749</td><td>1.767132</td><td>2.718342</td></tr><tr><td>7 C</td><td>1.548965</td><td>1.720634</td><td>1.598018</td><td>2.735059</td><td>2.568838</td></tr><tr><td>8 C</td><td>2.570636</td><td>2.721778</td><td>2.681395</td><td>1.700965</td><td>1.621746</td></tr><tr><td>9 B</td><td>1.598211</td><td>3.297275</td><td>2.611098</td><td>2.904037</td><td>1.602542</td></tr><tr><td>10 B</td><td>1.706940</td><td>1.792658</td><td>2.814856</td><td>1.775917</td><td>3.228466</td></tr><tr><td>11 B</td><td>3.186702</td><td>1.736392</td><td>1.789229</td><td>1.801446</td><td>1.718224</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 C</td><td>2.691796</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>1.658749</td><td>3.011976</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>1.832111</td><td>2.560812</td><td>1.749127</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>1.770267</td><td>1.696977</td><td>2.722911</td><td>2.835675</td><td>0.000000</td></tr><tr><td>11 B</td><td>2.860403</td><td>2.701568</td><td>1.722255</td><td>2.835575</td><td>2.868150</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	2.731164	0.000000				3 B	2.576533	1.800727	0.000000			4 B	2.742737	1.778441	2.873919	0.000000		5 C	2.565238	2.745017	1.634379	2.772400	0.000000	6 B	1.698863	2.859438	3.264749	1.767132	2.718342	7 C	1.548965	1.720634	1.598018	2.735059	2.568838	8 C	2.570636	2.721778	2.681395	1.700965	1.621746	9 B	1.598211	3.297275	2.611098	2.904037	1.602542	10 B	1.706940	1.792658	2.814856	1.775917	3.228466	11 B	3.186702	1.736392	1.789229	1.801446	1.718224		6	7	8	9	10	6 B	0.000000					7 C	2.691796	0.000000				8 C	1.658749	3.011976	0.000000			9 B	1.832111	2.560812	1.749127	0.000000		10 B	1.770267	1.696977	2.722911	2.835675	0.000000	11 B	2.860403	2.701568	1.722255	2.835575	2.868150
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 4. -332.7843560 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>1.680350</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.765807</td><td>1.651944</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.875717</td><td>3.111243</td><td>2.547916</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.803699</td><td>2.728207</td><td>3.190301</td><td>1.802214</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.762408</td><td>1.709494</td><td>1.763652</td><td>2.802930</td><td>2.859681</td></tr><tr><td>7 B</td><td>1.783635</td><td>2.726849</td><td>2.737672</td><td>1.810751</td><td>1.758675</td></tr><tr><td>8 B</td><td>1.786378</td><td>1.668141</td><td>2.700771</td><td>2.790785</td><td>1.781307</td></tr><tr><td>9 C</td><td>2.736763</td><td>2.568189</td><td>1.543871</td><td>1.612327</td><td>2.723709</td></tr><tr><td>10 C</td><td>2.757638</td><td>2.596552</td><td>2.559822</td><td>1.627226</td><td>1.690613</td></tr><tr><td>11 B</td><td>2.910936</td><td>1.771138</td><td>1.570528</td><td>2.594244</td><td>2.838936</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>1.759622</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.857985</td><td>2.853640</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>1.683746</td><td>1.715372</td><td>3.167033</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>3.228455</td><td>2.741086</td><td>1.668063</td><td>2.596414</td><td>0.000000</td></tr><tr><td>11 B</td><td>2.850948</td><td>3.298796</td><td>1.832669</td><td>2.565377</td><td>1.622452</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 C	1.680350	0.000000				3 C	2.765807	1.651944	0.000000			4 B	2.875717	3.111243	2.547916	0.000000		5 B	1.803699	2.728207	3.190301	1.802214	0.000000	6 B	1.762408	1.709494	1.763652	2.802930	2.859681	7 B	1.783635	2.726849	2.737672	1.810751	1.758675	8 B	1.786378	1.668141	2.700771	2.790785	1.781307	9 C	2.736763	2.568189	1.543871	1.612327	2.723709	10 C	2.757638	2.596552	2.559822	1.627226	1.690613	11 B	2.910936	1.771138	1.570528	2.594244	2.838936		6	7	8	9	10	6 B	0.000000					7 B	1.759622	0.000000				8 B	2.857985	2.853640	0.000000			9 C	1.683746	1.715372	3.167033	0.000000		10 C	3.228455	2.741086	1.668063	2.596414	0.000000	11 B	2.850948	3.298796	1.832669	2.565377	1.622452
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 5. -332.7796661 Cs	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>1.719289</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.928774</td><td>1.741132</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.707427</td><td>2.958224</td><td>2.576951</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.765033</td><td>2.725874</td><td>3.358411</td><td>1.718164</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.785569</td><td>1.664751</td><td>1.803837</td><td>2.660447</td><td>2.862892</td></tr><tr><td>7 B</td><td>1.765810</td><td>2.725813</td><td>2.871162</td><td>1.717552</td><td>1.790369</td></tr><tr><td>8 B</td><td>1.785377</td><td>1.665028</td><td>2.834788</td><td>2.659256</td><td>1.770864</td></tr><tr><td>9 C</td><td>2.737583</td><td>2.564827</td><td>1.636230</td><td>1.514408</td><td>2.720407</td></tr><tr><td>10 C</td><td>2.736925</td><td>2.563925</td><td>2.629249</td><td>1.513588</td><td>1.707812</td></tr><tr><td>11 B</td><td>2.928705</td><td>1.741049</td><td>1.692314</td><td>2.576304</td><td>2.871961</td></tr></table> <table><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>1.771479</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.824965</td><td>2.862412</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>1.691716</td><td>1.706667</td><td>3.151931</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>3.151582</td><td>2.719361</td><td>1.690489</td><td>2.504011</td><td>0.000000</td></tr><tr><td>11 B</td><td>2.834467</td><td>3.357459</td><td>1.804146</td><td>2.629493</td><td>1.635478</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 C	1.719289	0.000000				3 B	2.928774	1.741132	0.000000			4 C	2.707427	2.958224	2.576951	0.000000		5 B	1.765033	2.725874	3.358411	1.718164	0.000000	6 B	1.785569	1.664751	1.803837	2.660447	2.862892	7 B	1.765810	2.725813	2.871162	1.717552	1.790369	8 B	1.785377	1.665028	2.834788	2.659256	1.770864	9 C	2.737583	2.564827	1.636230	1.514408	2.720407	10 C	2.736925	2.563925	2.629249	1.513588	1.707812	11 B	2.928705	1.741049	1.692314	2.576304	2.871961		6	7	8	9	10	6 B	0.000000					7 B	1.771479	0.000000				8 B	2.824965	2.862412	0.000000			9 C	1.691716	1.706667	3.151931	0.000000		10 C	3.151582	2.719361	1.690489	2.504011	0.000000	11 B	2.834467	3.357459	1.804146	2.629493	1.635478
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 6. -332.7682364 Cs	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.718107</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.598791</td><td>1.710429</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.599667</td><td>3.171361</td><td>2.502936</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.717069</td><td>2.846746</td><td>3.169717</td><td>1.711324</td><td>0.000000</td></tr><tr><td>6 B</td><td>1.675779</td><td>1.785092</td><td>1.694835</td><td>2.706319</td><td>2.871231</td></tr><tr><td>7 B</td><td>1.675924</td><td>2.872602</td><td>2.706392</td><td>1.695154</td><td>1.784279</td></tr><tr><td>8 B</td><td>1.746636</td><td>1.751612</td><td>2.707092</td><td>2.708314</td><td>1.751249</td></tr><tr><td>9 C</td><td>2.567648</td><td>2.687170</td><td>1.516274</td><td>1.516159</td><td>2.686592</td></tr><tr><td>10 B</td><td>2.776539</td><td>2.842751</td><td>2.646037</td><td>1.634192</td><td>1.774867</td></tr><tr><td>11 B</td><td>2.775953</td><td>1.774798</td><td>1.633368</td><td>2.645919</td><td>2.841276</td></tr></table> <table><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>1.778453</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.864818</td><td>2.865022</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>1.706570</td><td>1.707020</td><td>3.131824</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>3.340749</td><td>2.842924</td><td>1.794898</td><td>2.591246</td><td>0.000000</td></tr><tr><td>11 B</td><td>2.842544</td><td>3.340329</td><td>1.794152</td><td>2.590721</td><td>1.730753</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.718107	0.000000				3 C	2.598791	1.710429	0.000000			4 C	2.599667	3.171361	2.502936	0.000000		5 B	1.717069	2.846746	3.169717	1.711324	0.000000	6 B	1.675779	1.785092	1.694835	2.706319	2.871231	7 B	1.675924	2.872602	2.706392	1.695154	1.784279	8 B	1.746636	1.751612	2.707092	2.708314	1.751249	9 C	2.567648	2.687170	1.516274	1.516159	2.686592	10 B	2.776539	2.842751	2.646037	1.634192	1.774867	11 B	2.775953	1.774798	1.633368	2.645919	2.841276		6	7	8	9	10	6 B	0.000000					7 B	1.778453	0.000000				8 B	2.864818	2.865022	0.000000			9 C	1.706570	1.707020	3.131824	0.000000		10 B	3.340749	2.842924	1.794898	2.591246	0.000000	11 B	2.842544	3.340329	1.794152	2.590721	1.730753
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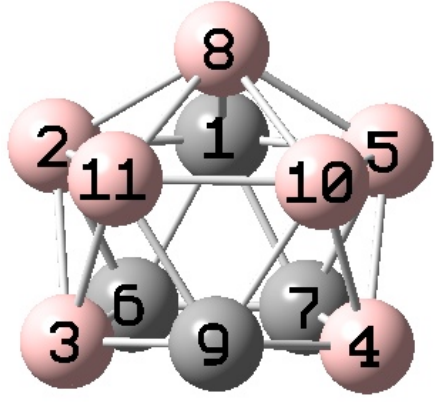
 7. -332.7612186 Cs	1 2 3 4 5				
	1 C	0.000000			
	2 B	1.706920	0.000000		
	3 B	2.682623	1.806493	0.000000	
	4 B	2.682740	3.289027	2.616286	0.000000
	5 B	1.706407	2.887247	3.289038	1.806745
	6 C	1.653417	1.759641	1.600703	2.561120
	7 C	1.653822	2.740032	2.560831	1.600096
	8 B	1.666307	1.777451	2.878097	2.878234
	9 C	3.051573	2.722432	1.624061	1.624211
	10 B	2.717774	2.870675	2.823049	1.801636
	11 B	2.717795	1.740034	1.801469	2.823025
		6 7 8 9 10			
	6 C	0.000000			
	7 C	1.527860	0.000000		
	8 B	2.767430	2.767460	0.000000	
	9 C	2.569947	2.569456	2.748518	0.000000
	10 B	3.196999	2.731324	1.800030	1.685351
	11 B	2.731698	3.196699	1.800088	1.685116

Table S6C. Energy ranking for all of the C₄B₇H₁₁ structures.

		E w zpc	delta E w zpc
1	03-CapPentAnPr-a39----c4	-332.9208882	0.00
2	07-CapPentPrB-a34----c4	-332.9208875	0.00
3	07-CapPentPrB-a33----c4	-332.9208826	0.00
4	05-TricapCubeB-a16----c4	-332.9208487	0.02
5	06-CapPentPrA-a35----c4	-332.9208436	0.03
6	01-EdgeCoalscedlh-a121----c4	-332.9208433	0.03
7	06-CapPentPrA-a22----c4	-332.9193533	0.96
8	03-CapPentAnPr-a22----c4	-332.9193164	0.99
9	02-PentaCapTriPri-a35----c4	-332.9074543	8.43
10	06-CapPentPrA-a27----c4	-332.9074542	8.43
11	07-CapPentPrB-a26----c4	-332.9074354	8.44
12	01-EdgeCoalscedlh-a125----c4	-332.9074305	8.44
13	03-CapPentAnPr-a38----c4	-332.9055506	9.62
14	01-EdgeCoalscedlh-a122----c4	-332.9055403	9.63
15	07-CapPentPrB-a25----c4	-332.9055265	9.64
16	07-CapPentPrB-a21----c4	-332.9055229	9.64
17	05-TricapCubeB-a18----c4	-332.9055205	9.64
18	06-CapPentPrA-a17----c4	-332.9055039	9.65
19	01-EdgeCoalscedlh-a124----c4	-332.9055030	9.65
20	03-CapPentAnPr-a36----c4	-332.9003510	12.89
21	01-EdgeCoalscedlh-a115----c4	-332.9003376	12.90
22	07-CapPentPrB-a31----c4	-332.9003353	12.90
23	01-EdgeCoalscedlh-a112----c4	-332.8954068	15.99
24	05-TricapCubeB-a15----c4	-332.8953995	15.99
25	03-CapPentAnPr-a21----c4	-332.8876210	20.88
26	03-CapPentAnPr-a13----c4	-332.8832534	23.62
27	01-EdgeCoalscedlh-a116----c4	-332.8832417	23.62
28	02-PentaCapTriPri-a27----c4	-332.8832112	23.64
29	01-EdgeCoalscedlh-a114----c4	-332.8809240	25.08
30	01-EdgeCoalscedlh-a129----c4	-332.8781978	26.79
31	05-TricapCubeB-a17----c4	-332.8781925	26.79
32	03-CapPentAnPr-a37----c4	-332.8781730	26.80
33	03-CapPentAnPr-a11----c4	-332.8781642	26.81
34	01-EdgeCoalscedlh-a131----c4	-332.8735146	29.73
35	06-CapPentPrA-a34----c4	-332.8728796	30.13
36	02-PentaCapTriPri-a39----c4	-332.8728500	30.14
37	04-TricapCubeA-a12----c4	-332.8683916	32.94
38	05-TricapCubeB-a13----c4	-332.8679960	33.19
39	05-TricapCubeB-a20----c4	-332.8679960	33.19

40	06-CapPentPrA-a15----c4	-332.8679910	33.19
41	07-CapPentPrB-a30----c4	-332.8679643	33.21
42	04-TricapCubeA-a31----c4	-332.8672478	33.66
43	02-PentaCapTriPri-a20----c4	-332.8664919	34.13
44	05-TricapCubeB-a28----c4	-332.8650272	35.05
45	02-PentaCapTriPri-a29----c4	-332.8649928	35.08
46	01-EdgeCoalscedlh-a126----c4	-332.8649847	35.08
47	01-EdgeCoalscedlh-a18----c4	-332.8634231	36.06
48	01-EdgeCoalscedlh-a19----c4	-332.8608814	37.66
49	04-TricapCubeA-a20----c4	-332.8604156	37.95
50	03-CapPentAnPr-a33----c4	-332.8599632	38.23
51	06-CapPentPrA-a33----c4	-332.8598645	38.29
52	04-TricapCubeA-a30----c4	-332.8596582	38.42
53	03-CapPentAnPr-a35----c4	-332.8587332	39.00
54	05-TricapCubeB-a29----c4	-332.8581459	39.37
55	02-PentaCapTriPri-a16----c4	-332.8570315	40.07
56	06-CapPentPrA-a28----c4	-332.8561669	40.61
57	01-EdgeCoalscedlh-a119----c4	-332.8560998	40.66
58	06-CapPentPrA-a21----c4	-332.8560954	40.66
59	03-CapPentAnPr-a23----c4	-332.8559578	40.75
60	02-PentaCapTriPri-a40----c4	-332.8557819	40.86
61	03-CapPentAnPr-a12----c4	-332.8545291	41.64
62	05-TricapCubeB-a23----c4	-332.8545058	41.66
63	06-CapPentPrA-a24----c4	-332.8545012	41.66
64	03-CapPentAnPr-a14----c4	-332.8544947	41.66
65	07-CapPentPrB-a20----c4	-332.8544903	41.67
66	04-TricapCubeA-a15----c4	-332.8544854	41.67
67	07-CapPentPrB-a19----c4	-332.8544849	41.67
68	04-TricapCubeA-a24----c4	-332.8544790	41.67
69	03-CapPentAnPr-a30----c4	-332.8544782	41.67
70	01-EdgeCoalscedlh-a132----c4	-332.8544756	41.68
71	05-TricapCubeB-a11----c4	-332.8544632	41.68
72	05-TricapCubeB-a30----c4	-332.8537320	42.14
73	01-EdgeCoalscedlh-a14----c4	-332.8537061	42.16
74	02-PentaCapTriPri-a38----c4	-332.8533525	42.38
75	03-CapPentAnPr-a20----c4	-332.8530733	42.56
76	04-TricapCubeA-a17----c4	-332.8530523	42.57
77	02-PentaCapTriPri-a33----c4	-332.8515899	43.49
78	05-TricapCubeB-a32----c4	-332.8515673	43.50
79	02-PentaCapTriPri-a31----c4	-332.8503677	44.25
80	04-TricapCubeA-a23----c4	-332.8490883	45.06
81	05-TricapCubeB-a21----c4	-332.8475897	46.00

82	04-TricapCubeA-a16----c4	-332.8475760	46.00
83	01-EdgeCoalscedlh-a123----c4	-332.8475732	46.01
84	01-EdgeCoalscedlh-a113----c4	-332.8475678	46.01
85	07-CapPentPrB-a28----c4	-332.8472161	46.23
86	05-TricapCubeB-a12----c4	-332.8457962	47.12
87	07-CapPentPrB-a22----c4	-332.8450864	47.57
88	05-TricapCubeB-a24----c4	-332.8433176	48.68
89	06-CapPentPrA-a25----c4	-332.8424885	49.20
90	07-CapPentPrB-a36----c4	-332.8410580	50.10
91	04-TricapCubeA-a29----c4	-332.8410567	50.10
92	01-EdgeCoalscedlh-a110----c4	-332.8410554	50.10
93	03-CapPentAnPr-a31----c4	-332.8410520	50.10
94	01-EdgeCoalscedlh-a120----c4	-332.8380831	51.96
95	02-PentaCapTriPri-a28----c4	-332.8380749	51.97
96	07-CapPentPrB-a11----c4	-332.8378728	52.09
97	02-PentaCapTriPri-a11----c4	-332.8378408	52.11
98	07-CapPentPrB-a32----c4	-332.8377647	52.16
99	03-CapPentAnPr-a32----c4	-332.8342922	54.34
100	04-TricapCubeA-a25----c4	-332.8339933	54.53
101	03-CapPentAnPr-a15----c4	-332.8339758	54.54
102	02-PentaCapTriPri-a32----c4	-332.8328448	55.25
103	01-EdgeCoalscedlh-a118----c4	-332.8312281	56.26
104	06-CapPentPrA-a29----c4	-332.8306661	56.62
105	04-TricapCubeA-a11----c4	-332.8306600	56.62
106	03-CapPentAnPr-a34----c4	-332.8301649	56.93
107	01-EdgeCoalscedlh-a130----c4	-332.8283706	58.06
108	06-CapPentPrA-a23----c4	-332.8283369	58.08
109	05-TricapCubeB-a14----c4	-332.8281458	58.20
110	01-EdgeCoalscedlh-a16----c4	-332.8245517	60.45
111	04-TricapCubeA-a22----c4	-332.8237840	60.93
112	07-CapPentPrB-a37----c4	-332.8230758	61.38
113	01-EdgeCoalscedlh-a12----c4	-332.8213334	62.47
114	02-PentaCapTriPri-a30----c4	-332.8198789	63.39
115	05-TricapCubeB-a19----c4	-332.8197999	63.43
116	06-CapPentPrA-a18----c4	-332.8197886	63.44
117	03-CapPentAnPr-a19----c4	-332.8197686	63.45
118	04-TricapCubeA-a37----c4	-332.8182652	64.40
119	06-CapPentPrA-a13----c4	-332.8182648	64.40
120	01-EdgeCoalscedlh-a11----c4	-332.8182628	64.40
121	04-TricapCubeA-a21----c4	-332.8182353	64.42
122	01-EdgeCoalscedlh-a15----c4	-332.8178867	64.64
123	06-CapPentPrA-a32----c4	-332.8174905	64.88

124	06-CapPentPrA-a20----c4	-332.8173567	64.97
125	04-TricapCubeA-a34----c4	-332.8124161	68.07
126	07-CapPentPrB-a38----c4	-332.8120209	68.32
127	06-CapPentPrA-a31----c4	-332.8120028	68.33
128	01-EdgeCoalscedlh-a127----c4	-332.8119882	68.34
129	04-TricapCubeA-a32----c4	-332.8108848	69.03
130	02-PentaCapTriPri-a41----c4	-332.8108809	69.03
131	04-TricapCubeA-a36----c4	-332.8107346	69.12
132	03-CapPentAnPr-a29----c4	-332.8104517	69.30
133	07-CapPentPrB-a29----c4	-332.8099823	69.60
134	03-CapPentAnPr-a26----c4	-332.8089336	70.25
135	04-TricapCubeA-a19----c4	-332.8089294	70.26
136	01-EdgeCoalscedlh-a13----c4	-332.8088075	70.33
137	03-CapPentAnPr-a28----c4	-332.8081653	70.74
138	07-CapPentPrB-a13----c4	-332.8066921	71.66
139	07-CapPentPrB-a14----c4	-332.8066921	71.66
140	07-CapPentPrB-a35----c4	-332.8066752	71.67
141	04-TricapCubeA-a38----c4	-332.8066568	71.68
142	04-TricapCubeA-a13----c4	-332.8062166	71.96
143	06-CapPentPrA-a11----c4	-332.8062163	71.96
144	04-TricapCubeA-a14----c4	-332.8061015	72.03
145	06-CapPentPrA-a14----c4	-332.8060863	72.04
146	02-PentaCapTriPri-a34----c4	-332.8057756	72.24
147	01-EdgeCoalscedlh-a17----c4	-332.8048330	72.83
148	04-TricapCubeA-a27----c4	-332.8047888	72.85
149	07-CapPentPrB-a27----c4	-332.8046753	72.93
150	04-TricapCubeA-a26----c4	-332.8046427	72.95
151	03-CapPentAnPr-a18----c4	-332.8007609	75.38
152	05-TricapCubeB-a27----c4	-332.7999148	75.91
153	05-TricapCubeB-a26----c4	-332.7978241	77.23
154	04-TricapCubeA-a28----c4	-332.7978132	77.23
155	04-TricapCubeA-a18----c4	-332.7975333	77.41
156	07-CapPentPrB-a15----c4	-332.7965964	78.00
157	07-CapPentPrB-a24----c4	-332.7956123	78.61
158	03-CapPentAnPr-a27----c4	-332.7951082	78.93
159	01-EdgeCoalscedlh-a117----c4	-332.7948361	79.10
160	06-CapPentPrA-a16----c4	-332.7929532	80.28
161	01-EdgeCoalscedlh-a128----c4	-332.7901307	82.05
162	02-PentaCapTriPri-a14----c4	-332.7893807	82.52
163	02-PentaCapTriPri-a22----c4	-332.7891947	82.64
164	06-CapPentPrA-a19----c4	-332.7890210	82.75
165	06-CapPentPrA-a12----c4	-332.7883198	83.19

166	01-EdgeCoalscedlh-a111----c4	-332.7865216	84.32
167	03-CapPentAnPr-a25----c4	-332.7862175	84.51
168	07-CapPentPrB-a16----c4	-332.7855332	84.94
169	03-CapPentAnPr-a17----c4	-332.7823730	86.92
170	05-TricapCubeB-a31----c4	-332.7823430	86.94
171	02-PentaCapTriPri-a25----c4	-332.7811732	87.67
172	06-CapPentPrA-a26----c4	-332.7800068	88.41
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174	02-PentaCapTriPri-a13----c4	-332.7752500	91.39
175	02-PentaCapTriPri-a36----c4	-332.7751997	91.42
176	03-CapPentAnPr-a16----c4	-332.7747763	91.69
177	02-PentaCapTriPri-a15----c4	-332.7742793	92.00
178	02-PentaCapTriPri-a19----c4	-332.7712796	93.88
179	04-TricapCubeA-a35----c4	-332.7666863	96.76
180	03-CapPentAnPr-a24----c4	-332.7624571	99.42
181	04-TricapCubeA-a33----c4	-332.7599482	100.99
182	05-TricapCubeB-a22----c4	-332.7596601	101.17
183	05-TricapCubeB-a25----c4	-332.7593316	101.38
184	06-CapPentPrA-a30----c4	-332.7547080	104.28
185	02-PentaCapTriPri-a37----c4	-332.7503511	107.02
186	02-PentaCapTriPri-a18----c4	-332.7488637	107.95
187	02-PentaCapTriPri-a12----c4	-332.7485433	108.15
188	02-PentaCapTriPri-a23----c4	-332.7455311	110.04
189	02-PentaCapTriPri-a24----c4	-332.7410952	112.82
190	02-PentaCapTriPri-a26----c4	-332.7300624	119.75
191	07-CapPentPrB-a12----c4	-332.7283012	120.85
192	02-PentaCapTriPri-a17----c4	-332.7273480	121.45
193	07-CapPentPrB-a23----c4_r-14	-332.7261204	122.22
194	07-CapPentPrB-a23----c4_i-14	-332.7259211	122.35
195	07-CapPentPrB-a18----c4_i-29	-332.7251986	122.80
196	07-CapPentPrB-a18----c4_r-29	-332.7249146	122.98
197	07-CapPentPrB-a17----c4_i-28	-332.6752878	154.12
198	07-CapPentPrB-a17----c4_r-28	-332.6749638	154.32

Table S7A. Initial $C_4B_8H_{12}$ structures a total of 191 structures:

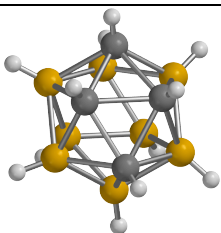
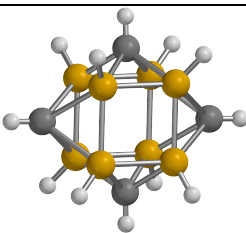
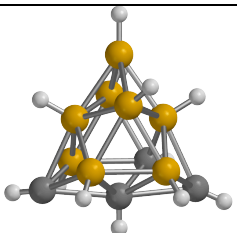
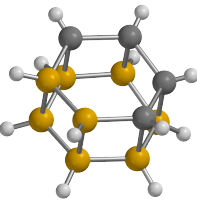
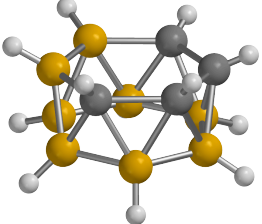
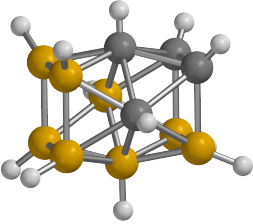
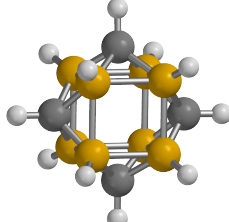
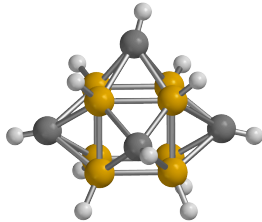
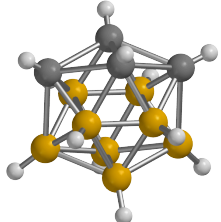
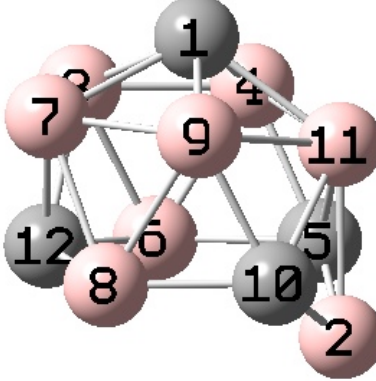
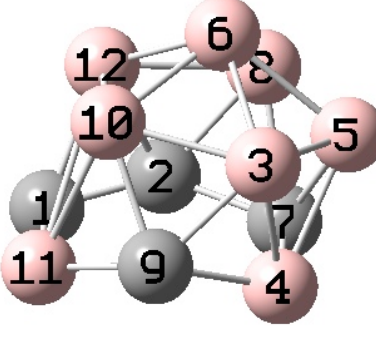
 Icosahedron (6)	 Cube octahedron (26)	 Anticube octahedron (28)
 Hexagonal prism (16)	 Hexagonal antiprism (15)	 Double square antiprism (18)
 Tetracapped cube A (26)	 Tetracapped cube B (40)	 2v6 structure (16)

Table S7B. Distance table for the lowest-lying C₄B₈H₁₂ structures. For clarity, only the polyhedral framework is presented.



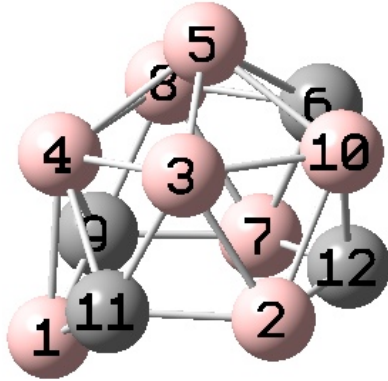
1. -358.2237943 C_s

	1	2	3	4	5
1 C	0.000000				
2 B	3.261740	0.000000			
3 B	1.727106	3.665007	0.000000		
4 B	1.685065	2.904447	1.716712	0.000000	
5 C	2.725307	1.526760	2.794292	1.655176	0.000000
6 B	2.720978	2.599842	1.776683	1.792479	1.652033
7 B	1.727102	3.665012	1.777403	2.875027	3.508597
8 B	2.720976	2.599839	2.848871	3.400385	3.130021
9 B	1.685062	2.904458	2.875028	2.992392	3.212382
10 C	2.725284	1.526768	3.508590	3.212358	2.533000
11 B	1.747839	1.910738	2.898116	1.900021	1.781392
12 C	2.577412	3.026998	1.694138	2.701425	2.782914
	6	7	8	9	10
6 B	0.000000				
7 B	2.848881	0.000000			
8 B	2.790296	1.776689	0.000000		
9 B	3.400396	1.716709	1.792487	0.000000	
10 C	3.130033	2.794292	1.652054	1.655165	0.000000
11 B	2.780643	2.898078	2.780578	1.899930	1.781272
12 C	1.628920	1.694151	1.628925	2.701436	2.782935
	11	12			
12 C	3.098600	0.000000			



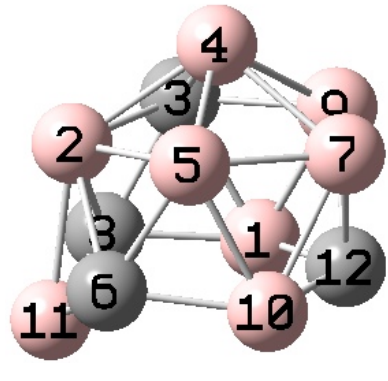
2. -358.2116750 C₁

	1	2	3	4	5
1 C	0.000000				
2 C	1.458327	0.000000			
3 B	3.556228	3.422414	0.000000		
4 B	3.035017	2.684204	1.813373	0.000000	
5 B	3.595965	2.759326	1.734120	1.833466	0.000000
6 B	3.143082	2.791463	1.816462	2.846832	1.811297
7 C	2.604542	1.535360	2.738388	1.607193	1.706132
8 B	2.828716	1.713857	2.894828	2.823925	1.734183
9 C	2.644174	3.066666	1.656113	1.639500	2.778483
10 B	2.548029	3.019739	1.792834	2.748473	2.847749
11 B	1.499145	2.597753	2.982845	2.653126	3.690568
12 B	1.738632	1.755127	3.001481	3.256915	2.897937
	6	7	8	9	10
7 C	2.716144	0.000000			
8 B	1.768648	1.706755	0.000000		
9 C	2.739176	2.759498	3.419656	0.000000	
10 B	1.725371	3.206401	2.964085	1.660885	0.000000
11 B	3.265736	3.070442	3.590893	1.578377	1.989024
12 B	1.781850	2.678607	1.842416	2.927147	1.935299
	11	12			
12 B	2.494706	0.000000			



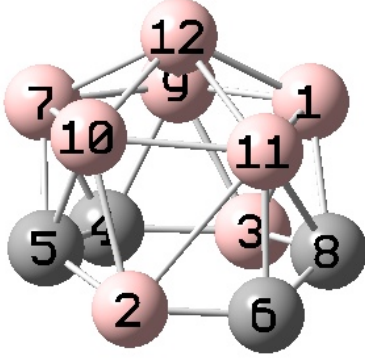
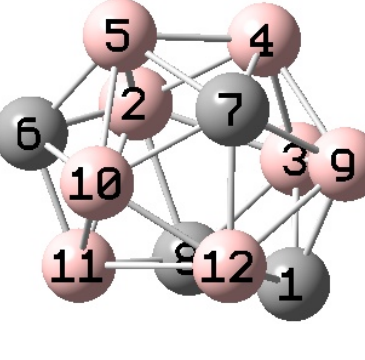
3. -358.2090681 C₁

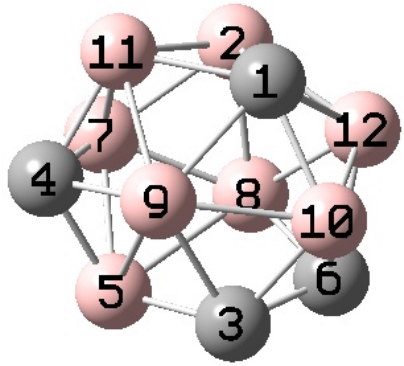
	1	2	3	4	5
1 B	0.000000				
2 B	2.636447	0.000000			
3 B	2.916127	1.787009	0.000000		
4 B	1.896750	2.787645	1.914550	0.000000	
5 B	3.385602	2.849899	1.765745	1.820388	0.000000
6 C	3.525773	2.716260	2.740885	2.744454	1.699191
7 B	2.622903	2.793810	3.434014	2.814248	2.888951
8 B	2.874498	3.388575	2.997417	1.880579	1.752942
9 C	1.530177	3.134499	3.259084	1.842847	2.877768
10 B	3.686986	1.780674	1.713038	2.895392	1.797524
11 C	1.524732	1.638157	1.672992	1.803964	2.853455
12 C	3.035014	1.633165	2.724729	3.102198	2.736244
	6	7	8	9	10
6 C	0.000000				
7 B	1.740790	0.000000			
8 B	1.640561	1.826170	0.000000		
9 C	2.671310	1.628239	1.656728	0.000000	
10 B	1.695493	2.875128	2.872005	3.522046	0.000000
11 C	3.340068	3.123564	3.194755	2.549839	2.794755
12 C	1.637884	1.600372	2.695393	2.740268	1.744608
	11	12			
11 C	0.000000				
12 C	2.758039	0.000000			



4. -358.2054453 C₁

	1	2	3	4	5
1 B	0.000000				
2 B	2.886998	0.000000			
3 C	1.746673	1.842158	0.000000		
4 B	2.890746	1.797421	1.665209	0.000000	
5 B	3.455910	1.844886	2.862248	1.772153	0.000000
6 C	3.152775	1.732158	3.029229	2.831730	1.660150
7 B	2.873868	2.876339	2.738943	1.807378	1.736701
8 C	1.602482	1.975901	1.616718	2.905916	3.291790
9 B	1.810005	2.911987	1.657966	1.790478	2.874162
10 B	2.773847	2.747732	3.202056	2.848976	1.808939
11 B	2.638691	1.918934	2.747287	3.370897	2.914605
12 C	1.624967	3.127364	2.561103	2.722197	2.730836
	6	7	8	9	10
6 C	0.000000				
7 B	2.812275	0.000000			
8 C	2.558855	3.528619	0.000000		
9 B	3.491175	1.747399	2.793111	0.000000	
10 B	1.660340	1.797527	3.093398	2.817873	0.000000
11 B	1.523229	3.689071	1.525978	3.665859	2.609476
12 C	2.802485	1.707908	2.741118	1.685047	1.621243
	11	12			
12 C	3.067729	0.000000			

 5. -358.2031294 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.472736</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.790843</td><td>3.149424</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.697360</td><td>2.697292</td><td>1.593928</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>3.325892</td><td>1.609776</td><td>2.735487</td><td>1.541463</td><td>0.000000</td></tr><tr><td>6 C</td><td>2.822082</td><td>1.487869</td><td>2.654327</td><td>3.023295</td><td>2.643889</td></tr><tr><td>7 B</td><td>2.891622</td><td>2.976927</td><td>2.837030</td><td>1.716424</td><td>1.672802</td></tr><tr><td>8 C</td><td>1.700923</td><td>2.588520</td><td>1.657202</td><td>2.711347</td><td>3.054410</td></tr><tr><td>9 B</td><td>1.710300</td><td>3.675745</td><td>1.774177</td><td>1.738411</td><td>2.749688</td></tr><tr><td>10 B</td><td>2.969285</td><td>1.913551</td><td>3.339686</td><td>2.648139</td><td>1.671615</td></tr><tr><td>11 B</td><td>1.891064</td><td>2.240075</td><td>2.811985</td><td>3.126168</td><td>2.804235</td></tr><tr><td>12 B</td><td>1.783931</td><td>3.150824</td><td>2.846984</td><td>2.705530</td><td>2.704465</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>3.644289</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>1.438851</td><td>3.505130</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>3.634078</td><td>1.768340</td><td>2.805620</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>2.713778</td><td>1.759989</td><td>3.118553</td><td>2.855957</td><td>0.000000</td></tr><tr><td>11 B</td><td>1.773031</td><td>2.971236</td><td>1.791086</td><td>2.910388</td><td>1.905483</td></tr><tr><td>12 B</td><td>3.236477</td><td>1.799621</td><td>2.847514</td><td>1.809553</td><td>1.713549</td></tr></table> <table><tr><th></th><th>11</th><th>12</th></tr><tr><td>11 B</td><td>0.000000</td><td></td></tr><tr><td>12 B</td><td>1.805661</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	3.472736	0.000000				3 B	1.790843	3.149424	0.000000			4 C	2.697360	2.697292	1.593928	0.000000		5 C	3.325892	1.609776	2.735487	1.541463	0.000000	6 C	2.822082	1.487869	2.654327	3.023295	2.643889	7 B	2.891622	2.976927	2.837030	1.716424	1.672802	8 C	1.700923	2.588520	1.657202	2.711347	3.054410	9 B	1.710300	3.675745	1.774177	1.738411	2.749688	10 B	2.969285	1.913551	3.339686	2.648139	1.671615	11 B	1.891064	2.240075	2.811985	3.126168	2.804235	12 B	1.783931	3.150824	2.846984	2.705530	2.704465		6	7	8	9	10	6 C	0.000000					7 B	3.644289	0.000000				8 C	1.438851	3.505130	0.000000			9 B	3.634078	1.768340	2.805620	0.000000		10 B	2.713778	1.759989	3.118553	2.855957	0.000000	11 B	1.773031	2.971236	1.791086	2.910388	1.905483	12 B	3.236477	1.799621	2.847514	1.809553	1.713549		11	12	11 B	0.000000		12 B	1.805661	0.000000
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 6. -358.1976892 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.807392</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.675343</td><td>1.909072</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.751087</td><td>1.890987</td><td>1.761008</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>3.495523</td><td>1.880985</td><td>3.007758</td><td>1.756752</td><td>0.000000</td></tr><tr><td>6 C</td><td>3.393719</td><td>1.665934</td><td>3.227587</td><td>2.809230</td><td>1.587629</td></tr><tr><td>7 C</td><td>2.642847</td><td>2.721950</td><td>2.733209</td><td>1.713330</td><td>1.700146</td></tr><tr><td>8 C</td><td>1.532757</td><td>1.835780</td><td>1.639326</td><td>2.813922</td><td>3.183915</td></tr><tr><td>9 B</td><td>1.645884</td><td>2.922410</td><td>1.777963</td><td>1.766634</td><td>2.902762</td></tr><tr><td>10 B</td><td>2.965503</td><td>2.681796</td><td>3.419059</td><td>2.866793</td><td>1.840927</td></tr><tr><td>11 B</td><td>2.406169</td><td>2.118833</td><td>2.885224</td><td>3.261374</td><td>2.733410</td></tr><tr><td>12 B</td><td>1.647700</td><td>3.125057</td><td>2.783335</td><td>2.868562</td><td>2.916079</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.647781</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.577262</td><td>3.131895</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>3.561880</td><td>1.654752</td><td>2.667332</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>1.644271</td><td>1.720043</td><td>2.926177</td><td>2.914117</td><td>0.000000</td></tr><tr><td>11 B</td><td>1.586984</td><td>2.921515</td><td>1.597737</td><td>3.261599</td><td>1.853238</td></tr><tr><td>12 B</td><td>2.919977</td><td>1.756360</td><td>2.472617</td><td>1.856961</td><td>1.755088</td></tr></table> <table><tr><th></th><th>11</th><th>12</th></tr><tr><td>12 B</td><td>2.202136</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	2.807392	0.000000				3 B	1.675343	1.909072	0.000000			4 B	2.751087	1.890987	1.761008	0.000000		5 B	3.495523	1.880985	3.007758	1.756752	0.000000	6 C	3.393719	1.665934	3.227587	2.809230	1.587629	7 C	2.642847	2.721950	2.733209	1.713330	1.700146	8 C	1.532757	1.835780	1.639326	2.813922	3.183915	9 B	1.645884	2.922410	1.777963	1.766634	2.902762	10 B	2.965503	2.681796	3.419059	2.866793	1.840927	11 B	2.406169	2.118833	2.885224	3.261374	2.733410	12 B	1.647700	3.125057	2.783335	2.868562	2.916079		6	7	8	9	10	6 C	0.000000					7 C	2.647781	0.000000				8 C	2.577262	3.131895	0.000000			9 B	3.561880	1.654752	2.667332	0.000000		10 B	1.644271	1.720043	2.926177	2.914117	0.000000	11 B	1.586984	2.921515	1.597737	3.261599	1.853238	12 B	2.919977	1.756360	2.472617	1.856961	1.755088		11	12	12 B	2.202136	0.000000			
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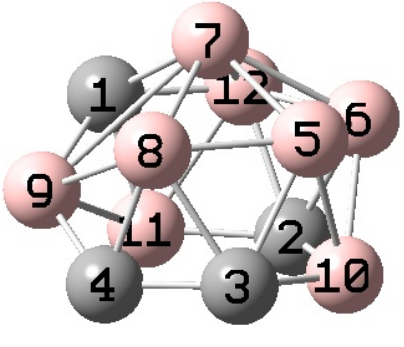


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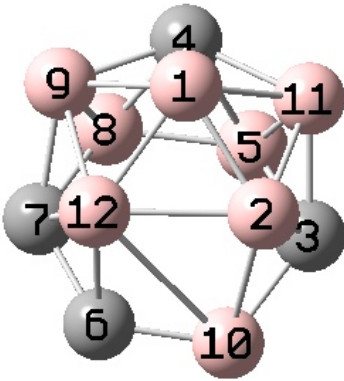
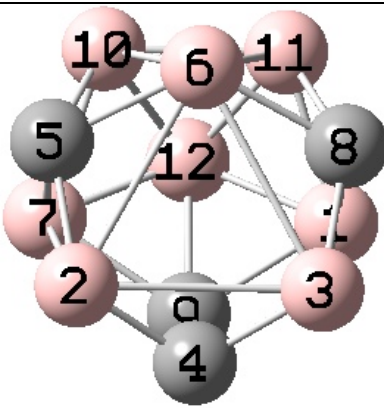


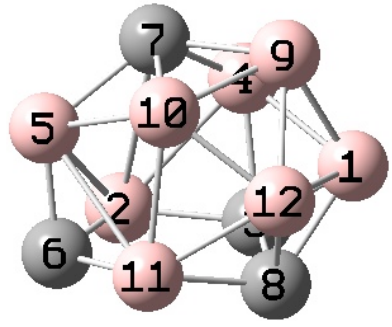
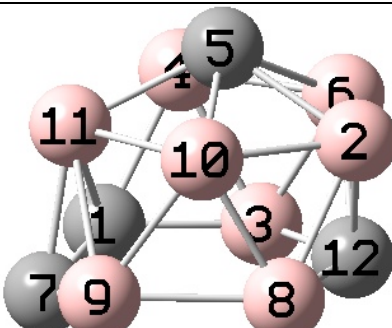
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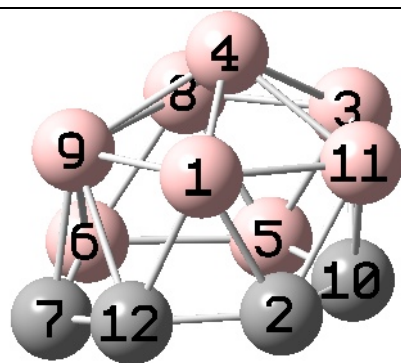
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6 B	2.785668	1.703814	2.793388	3.533792	1.723705
7 B	1.688329	2.709958	2.869125	2.943524	1.816239
8 B	2.692087	3.419738	1.741842	1.639650	1.730087
9 B	1.610297	3.062011	2.637216	1.498470	3.113675
10 B	3.379665	1.628526	1.606500	2.685088	1.823160
11 B	1.598251	1.579004	3.064886	2.615303	3.380182
12 B	1.595402	1.700023	3.578996	3.624045	2.923332

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12 B	1.832056	0.000000

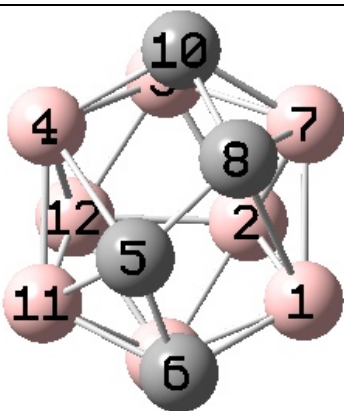
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3 B	2.878922	2.742473	0.000000		
4 B	1.730855	2.700327	1.792783	0.000000	
5 B	3.412737	2.721061	1.763889	2.826008	0.000000
6 B	3.370747	3.194016	3.019687	3.021208	1.837071
7 C	2.787626	2.590330	3.656068	3.239264	2.703452
8 B	3.005088	3.263046	1.725049	1.786714	1.730986
9 B	1.879847	2.721734	2.963344	1.816882	2.888183
10 C	2.698246	1.532835	1.745444	2.702861	1.590408
11 B	1.754673	1.700319	1.747913	1.792909	2.825716
12 C	1.751129	1.496365	3.477502	2.889723	3.058957
	6	7	8	9	10
6 B	0.000000				
7 C	1.478374	0.000000			
8 B	1.786473	2.788392	0.000000		
9 B	1.974722	1.768140	1.971235	0.000000	
10 C	2.901325	3.022232	2.659164	3.131754	0.000000
11 B	3.714485	3.642898	2.875092	2.942406	1.725087
12 C	2.587488	1.439439	3.213521	1.929290	2.593703
	11	12			
12 C	2.788720	0.000000			



14. -358.1759190 C₂

	1	2	3	4	5
1 B	0.000000				
2 B	1.801558	0.000000			
3 B	2.942677	1.783118	0.000000		
4 B	3.257756	2.872087	1.833565	0.000000	
5 C	2.328973	3.193672	3.158956	2.088894	0.000000
6 C	1.660174	2.789833	3.549356	2.968967	1.492947
7 B	1.849903	1.775525	1.794128	2.736813	2.783937
8 C	2.087741	2.875281	2.638967	2.330480	1.500676
9 B	1.834211	1.746777	2.918644	2.943233	2.638851
10 C	2.967797	2.808231	1.659445	1.660770	2.396282
11 B	2.736299	2.846926	2.951212	1.850587	1.672374
12 B	2.872538	1.821919	1.747176	1.800158	2.874307
	6	7	8	9	10
6 C	0.000000				
7 B	3.039116	0.000000			
8 C	2.396732	1.673379	0.000000		
9 B	1.659334	2.950942	3.159549	0.000000	
10 C	3.373276	1.680088	1.492814	3.549570	0.000000
11 B	1.679710	3.343606	2.783843	1.794831	3.038987
12 B	2.807921	2.846948	3.193939	1.783588	2.789836
	11	12			
11 B	0.000000				
12 B	1.775438	0.000000			

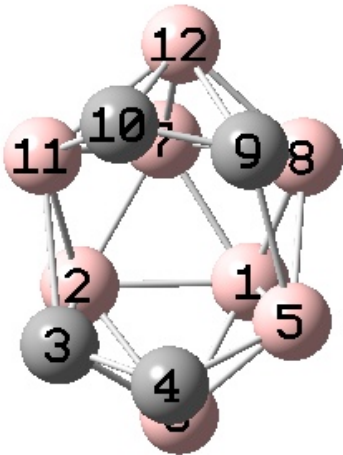
 15. -358.1737850 C₂	1 2 3 4 5					
	1 B	0.000000				
	2 B	1.807267	0.000000			
	3 C	2.687621	1.622412	0.000000		
	4 C	2.707054	2.578555	1.408035	0.000000	
	5 B	1.876627	2.779555	2.467030	1.556079	0.000000
	6 B	1.748000	1.808394	1.736512	1.642633	1.873457
	7 B	1.759896	1.773346	2.912546	3.457716	2.925147
	8 B	1.774085	2.862247	3.309193	3.074255	1.887338
	9 C	2.912907	3.309406	3.011713	2.630827	2.020737
	10 C	3.457789	3.074302	2.630864	2.830736	2.916380
	11 B	2.925705	1.887901	2.021173	2.916701	3.180305
	12 B	2.988454	3.042472	3.430012	3.708214	3.170737
	6 7 8 9 10					
	6 B	0.000000				
	7 B	2.988415	0.000000			
	8 B	3.042507	1.808287	0.000000		
	9 C	3.429901	2.687529	1.621534	0.000000	
	10 C	3.708135	2.705913	2.578135	1.408824	0.000000
	11 B	3.171037	1.876277	2.780675	2.468424	1.556224
	12 B	3.983597	1.747573	1.808652	1.736975	1.642184
	11 12					
	11 B	0.000000				
	12 B	1.874181	0.000000			

Table S7C. Energy ranking for all of the C₄B₈H₁₂ structures.

		E w zpc	delta E w zpc
1	02-CubeOh-6----c4	-358.3584189	0.00
2	07-TetraCappedCube-D4h-6----c4	-358.3584189	0.00
3	09-2v6-Dh-12----c4	-358.3584132	0.00
4	08-TetraCappedCube-C2v-7----c4	-358.3584109	0.01
5	08-TetraCappedCube-C2v-37----c4	-358.3584093	0.01
6	09-2v6-Dh-16----c4	-358.3569688	0.91
7	02-CubeOh-19----c4	-358.3569572	0.92
8	07-TetraCappedCube-D4h-19----c4	-358.3569572	0.92
9	08-TetraCappedCube-C2v-3----c4	-358.3569559	0.92
10	06-DsqAnPr-13----c4	-358.3569531	0.92
11	03-AnticubeOh-3_r-35----c4	-358.3487712	6.05
12	09-2v6-Dh-8----c4	-358.3487690	6.06
13	02-CubeOh-14----c4	-358.3487688	6.06
14	07-TetraCappedCube-D4h-14----c4	-358.3487688	6.06
15	08-TetraCappedCube-C2v-17_r-64----c4	-358.3487688	6.06
16	06-DsqAnPr-14----c4	-358.3487662	6.06
17	02-CubeOh-12----c4	-358.3475009	6.85
18	07-TetraCappedCube-D4h-12----c4	-358.3475009	6.85
19	02-CubeOh-11----c4	-358.3474613	6.88
20	07-TetraCappedCube-D4h-11----c4	-358.3474613	6.88
21	08-TetraCappedCube-C2v-6----c4	-358.3467677	7.31
22	08-TetraCappedCube-C2v-18----c4	-358.3467668	7.31
23	08-TetraCappedCube-C2v-5----c4	-358.3467610	7.32
24	08-TetraCappedCube-C2v-25----c4	-358.3467542	7.32
25	03-AnticubeOh-8----c4	-358.3455961	8.05
26	08-TetraCappedCube-C2v-16----c4	-358.3455910	8.05
27	03-AnticubeOh-3_i-35----c4	-358.3442786	8.87
28	08-TetraCappedCube-C2v-17_i-64----c4	-358.3442615	8.88
29	03-AnticubeOh-18----c4	-358.3441881	8.93
30	08-TetraCappedCube-C2v-38----c4	-358.3410699	10.89
31	08-TetraCappedCube-C2v-39----c4	-358.3370999	13.38
32	01-Icos-4----c4	-358.3351526	14.60
33	03-AnticubeOh-9----c4	-358.3346115	14.94
34	02-CubeOh-16----c4	-358.3346094	14.94
35	07-TetraCappedCube-D4h-16----c4	-358.3346094	14.94
36	03-AnticubeOh-13----c4	-358.3346076	14.94
37	02-CubeOh-26----c4	-358.3346026	14.95
38	07-TetraCappedCube-D4h-26----c4	-358.3346026	14.95
39	09-2v6-Dh-14----c4	-358.3346022	14.95

40	02-CubeOh-3----c4	-358.3346005	14.95
41	07-TetraCappedCube-D4h-3----c4	-358.3346005	14.95
42	03-AnticubeOh-17----c4	-358.3332750	15.78
43	08-TetraCappedCube-C2v-9----c4	-358.3332722	15.78
44	08-TetraCappedCube-C2v-15----c4	-358.3332636	15.79
45	08-TetraCappedCube-C2v-26----c4	-358.3331859	15.83
46	09-2v6-Dh-6----c4	-358.3316944	16.77
47	08-TetraCappedCube-C2v-23----c4	-358.3283159	18.89
48	02-CubeOh-4----c4	-358.3283158	18.89
49	07-TetraCappedCube-D4h-4----c4	-358.3283158	18.89
50	09-2v6-Dh-3----c4	-358.3281642	18.99
51	02-CubeOh-10----c4	-358.3279912	19.09
52	07-TetraCappedCube-D4h-10----c4	-358.3279912	19.09
53	08-TetraCappedCube-C2v-36_r-159----c4	-358.3279901	19.09
54	04-HexPr-11----c4	-358.3279850	19.10
55	06-DsqAnPr-5----c4	-358.3240116	21.59
56	08-TetraCappedCube-C2v-20----c4	-358.3240072	21.59
57	09-2v6-Dh-1----c4	-358.3240061	21.59
58	08-TetraCappedCube-C2v-12----c4	-358.3240058	21.59
59	02-CubeOh-21----c4	-358.3240024	21.60
60	07-TetraCappedCube-D4h-21----c4	-358.3240024	21.60
61	02-CubeOh-18----c4	-358.3240016	21.60
62	07-TetraCappedCube-D4h-18----c4	-358.3240016	21.60
63	03-AnticubeOh-7----c4	-358.3240010	21.60
64	03-AnticubeOh-19----c4	-358.3228837	22.30
65	09-2v6-Dh-15----c4	-358.3228750	22.30
66	08-TetraCappedCube-C2v-1----c4	-358.3216756	23.06
67	03-AnticubeOh-20----c4	-358.3216667	23.06
68	04-HexPr-3----c4	-358.3209551	23.51
69	09-2v6-Dh-10----c4	-358.3208803	23.56
70	08-TetraCappedCube-C2v-36_i-159----c4	-358.3208424	23.58
71	09-2v6-Dh-4----c4	-358.3204459	23.83
72	04-HexPr-12----c4	-358.3192152	24.60
73	08-TetraCappedCube-C2v-30----c4	-358.3192106	24.60
74	09-2v6-Dh-7----c4	-358.3190518	24.70
75	06-DsqAnPr-12----c4	-358.3190450	24.71
76	08-TetraCappedCube-C2v-8----c4	-358.3190429	24.71
77	08-TetraCappedCube-C2v-34----c4	-358.3190420	24.71
78	08-TetraCappedCube-C2v-31----c4	-358.3172660	25.82
79	02-CubeOh-20----c4	-358.3171124	25.92
80	07-TetraCappedCube-D4h-20----c4	-358.3171124	25.92
81	02-CubeOh-17----c4	-358.3171107	25.92

82	07-TetraCappedCube-D4h-17----c4	-358.3171107	25.92
83	01-Icos-5----c4	-358.3171027	25.93
84	09-2v6-Dh-9----c4	-358.3165772	26.26
85	02-CubeOh-1----c4	-358.3165759	26.26
86	07-TetraCappedCube-D4h-1----c4	-358.3165759	26.26
87	08-TetraCappedCube-C2v-27----c4	-358.3165643	26.26
88	04-HexPr-1----c4	-358.3165633	26.27
89	03-AnticubeOh-10----c4	-358.3158009	26.74
90	08-TetraCappedCube-C2v-19----c4	-358.3147600	27.40
91	08-TetraCappedCube-C2v-11----c4	-358.3147565	27.40
92	03-AnticubeOh-23----c4	-358.3131824	28.39
93	08-TetraCappedCube-C2v-13----c4	-358.3130456	28.47
94	02-CubeOh-9----c4	-358.3130432	28.47
95	07-TetraCappedCube-D4h-9----c4	-358.3130432	28.47
96	08-TetraCappedCube-C2v-21----c4	-358.3130417	28.48
97	06-DsqAnPr-8----c4	-358.3121893	29.01
98	02-CubeOh-23----c4	-358.3115180	29.43
99	07-TetraCappedCube-D4h-23----c4	-358.3115180	29.43
100	06-DsqAnPr-6----c4	-358.3109644	29.78
101	08-TetraCappedCube-C2v-35----c4	-358.3109585	29.78
102	08-TetraCappedCube-C2v-40----c4	-358.3109492	29.79
103	06-DsqAnPr-11----c4	-358.3108976	29.82
104	02-CubeOh-22----c4	-358.3108970	29.82
105	07-TetraCappedCube-D4h-22----c4	-358.3108970	29.82
106	09-2v6-Dh-11----c4	-358.3108944	29.82
107	02-CubeOh-15----c4	-358.3108925	29.82
108	07-TetraCappedCube-D4h-15----c4	-358.3108925	29.82
109	01-Icos-3----c4	-358.3105302	30.05
110	03-AnticubeOh-2----c4	-358.3105238	30.06
111	09-2v6-Dh-2----c4	-358.3098764	30.46
112	01-Icos-1----c4	-358.3087092	31.19
113	02-CubeOh-24----c4	-358.3085460	31.30
114	07-TetraCappedCube-D4h-24----c4	-358.3085460	31.30
115	06-DsqAnPr-3----c4	-358.3079968	31.64
116	08-TetraCappedCube-C2v-29----c4	-358.3077692	31.78
117	03-AnticubeOh-24----c4	-358.3064655	32.60
118	03-AnticubeOh-14----c4	-358.3063692	32.66
119	08-TetraCappedCube-C2v-33----c4	-358.3060438	32.87
120	01-Icos-6----c4	-358.3037824	34.29
121	02-CubeOh-2----c4	-358.3037785	34.29
122	07-TetraCappedCube-D4h-2----c4	-358.3037785	34.29
123	02-CubeOh-25----c4	-358.3024666	35.11

124	07-TetraCappedCube-D4h-25----c4	-358.3024666	35.11
125	04-HexPr-8----c4	-358.3009946	36.03
126	09-2v6-Dh-5----c4	-358.3009860	36.04
127	03-AnticubeOh-4----c4	-358.3005030	36.34
128	06-DsqAnPr-1----c4	-358.2981146	37.84
129	08-TetraCappedCube-C2v-32----c4	-358.2952987	39.61
130	03-AnticubeOh-15----c4	-358.2952937	39.61
131	02-CubeOh-5----c4	-358.2949208	39.85
132	07-TetraCappedCube-D4h-5----c4	-358.2949208	39.85
133	03-AnticubeOh-16----c4	-358.2929980	41.05
134	01-Icos-2----c4	-358.2902943	42.75
135	06-DsqAnPr-9----c4	-358.2897538	43.09
136	03-AnticubeOh-6----c4	-358.2887181	43.74
137	08-TetraCappedCube-C2v-14----c4	-358.2869738	44.83
138	08-TetraCappedCube-C2v-24----c4	-358.2869676	44.84
139	03-AnticubeOh-25----c4	-358.2865173	45.12
140	04-HexPr-2----c4	-358.2850491	46.04
141	06-DsqAnPr-4----c4	-358.2841895	46.58
142	03-AnticubeOh-1----c4	-358.2841067	46.63
143	04-HexPr-4----c4	-358.2828263	47.44
144	04-HexPr-13----c4	-358.2807080	48.77
145	08-TetraCappedCube-C2v-2----c4	-358.2803273	49.00
146	02-CubeOh-7----c4	-358.2803225	49.01
147	07-TetraCappedCube-D4h-7----c4	-358.2803225	49.01
148	08-TetraCappedCube-C2v-4----c4	-358.2736355	53.20
149	06-DsqAnPr-10----c4	-358.2734575	53.31
150	04-HexPr-9----c4	-358.2715756	54.50
151	05-HexAnPr-3----c4	-358.2711211	54.78
152	05-HexAnPr-11----c4	-358.2698197	55.60
153	08-TetraCappedCube-C2v-28----c4	-358.2676223	56.98
154	02-CubeOh-13----c4	-358.2676164	56.98
155	07-TetraCappedCube-D4h-13----c4	-358.2676164	56.98
156	02-CubeOh-8----c4	-358.2670264	57.35
157	07-TetraCappedCube-D4h-8----c4	-358.2670264	57.35
158	03-AnticubeOh-5----c4	-358.2666998	57.56
159	05-HexAnPr-2----c4	-358.2652496	58.47
160	06-DsqAnPr-2----c4	-358.2645498	58.90
161	05-HexAnPr-10----c4	-358.2644670	58.96
162	04-HexPr-10----c4	-358.2640633	59.21
163	04-HexPr-5----c4	-358.2596841	61.96
164	06-DsqAnPr-16----c4	-358.2596824	61.96
165	05-HexAnPr-8----c4	-358.2593971	62.14

166	09-2v6-Dh-13_r-168----c4	-358.2576949	63.21
167	05-HexAnPr-6----c4	-358.2568799	63.72
168	05-HexAnPr-12----c4	-358.2551795	64.78
169	03-AnticubeOh-22----c4	-358.2506925	67.60
170	05-HexAnPr-15----c4	-358.2506321	67.64
171	04-HexPr-6----c4	-358.2476055	69.54
172	06-DsqAnPr-15----c4	-358.2466883	70.11
173	06-DsqAnPr-17----c4	-358.2418682	73.14
174	05-HexAnPr-9----c4	-358.2405660	73.96
175	03-AnticubeOh-11----c4	-358.2397477	74.47
176	03-AnticubeOh-12----c4	-358.2397468	74.47
177	04-HexPr-15----c4	-358.2388639	75.02
178	04-HexPr-14----c4	-358.2384040	75.31
179	05-HexAnPr-14----c4	-358.2368336	76.30
180	09-2v6-Dh-13_i-168----c4	-358.2336455	78.30
181	08-TetraCappedCube-C2v-10----c4	-358.2317006	79.52
182	08-TetraCappedCube-C2v-22----c4	-358.2316996	79.52
183	04-HexPr-16----c4	-358.2316977	79.52
184	06-DsqAnPr-7----c4	-358.2315697	79.60
185	06-DsqAnPr-18----c4	-358.2315685	79.60
186	05-HexAnPr-1----c4	-358.2307886	80.09
187	05-HexAnPr-7----c4	-358.2284479	81.56
188	03-AnticubeOh-21----c4	-358.2226492	85.20
189	04-HexPr-7----c4	-358.2224652	85.31
190	05-HexAnPr-5----c4	-358.2187569	87.64
191	03-AnticubeOh-26_i-30----c4	-358.2138766	90.70
192	03-AnticubeOh-26_r-30----c4	-358.2137947	90.75
193	05-HexAnPr-4----c4	-358.2122977	91.69
194	05-HexAnPr-13----c4	-358.1714746	117.31

Table S8A. Initial $C_4B_9H_{13}$ structures, a total of 240 structures.

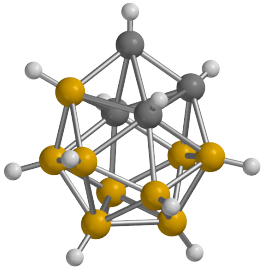
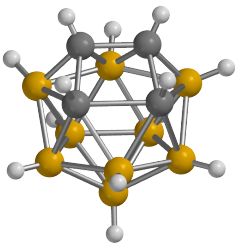
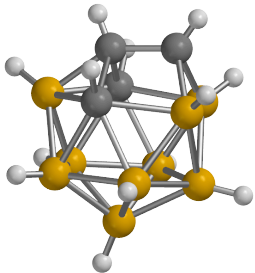
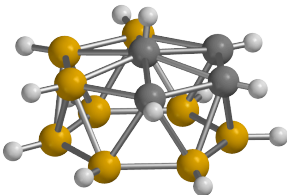
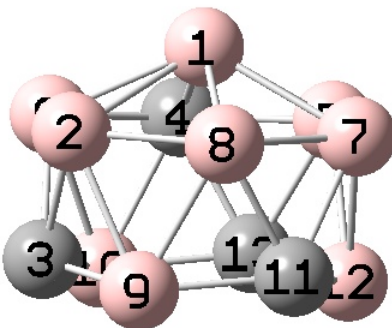
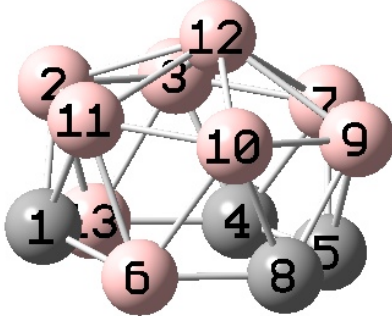
 Docosahedron (64)	 Henicosahedron (64)
 Ditrapezoidal icos (66)	 Capped hexag antiprism (46)

Table S8B. Distance table for the lowest-lying C₄B₉H₁₃ structures. For clarity, only the polyhedral framework is presented.



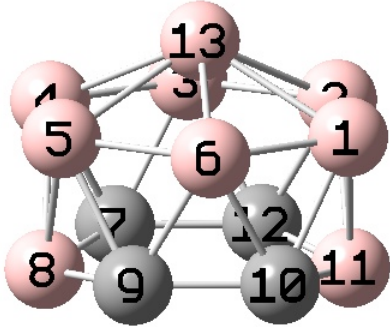
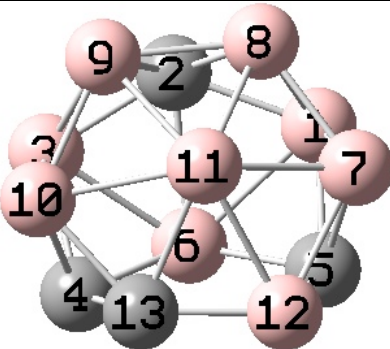
1. -383.6561241 C₁

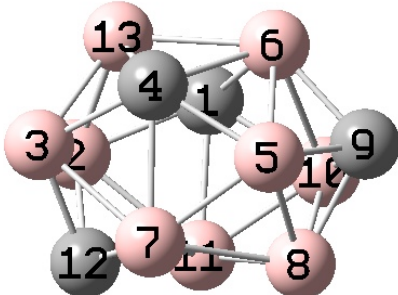
	1	2	3	4	5
1 B	0.000000				
2 B	1.907778	0.000000			
3 C	2.768339	1.682551	0.000000		
4 C	1.810265	2.860539	2.621443	0.000000	
5 B	1.925027	3.457607	3.529552	1.658218	0.000000
6 B	1.896371	1.739793	1.667319	1.631359	2.971233
7 B	1.913142	2.996060	3.542145	2.849107	1.713189
8 B	1.922719	1.716233	2.766941	3.306530	3.007028
9 B	2.888326	1.809251	1.617950	3.405280	3.576392
10 B	2.935056	2.862680	1.596969	1.776734	2.870912
11 C	2.762746	2.757446	2.813576	3.358533	2.752309
12 B	2.897456	3.574425	3.212766	2.711342	1.816985
13 C	2.791258	3.525518	2.769063	1.604405	1.705486
	6	7	8	9	10
6 B	0.000000				
7 B	3.436571	0.000000			
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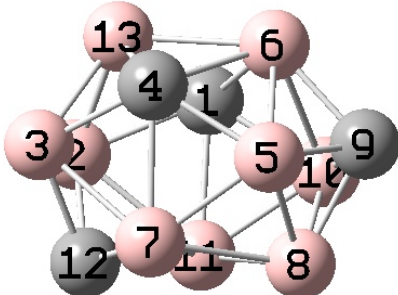


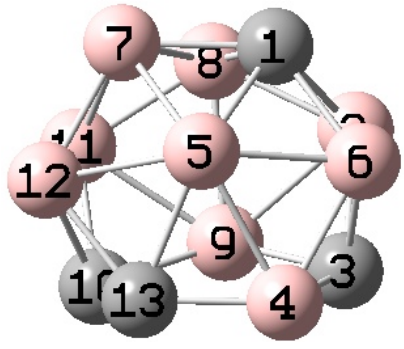
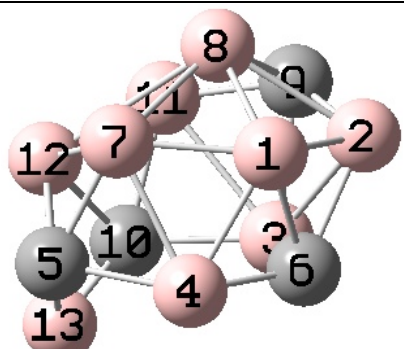
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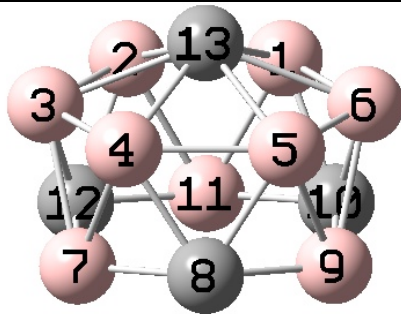
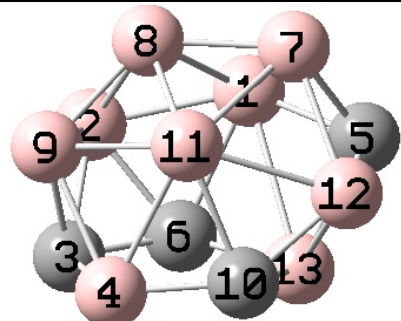
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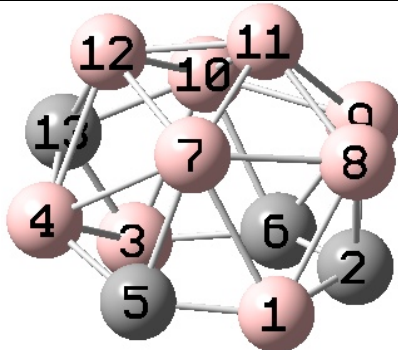
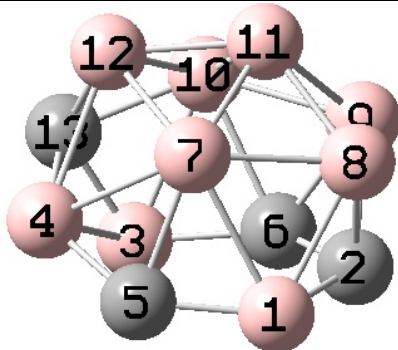
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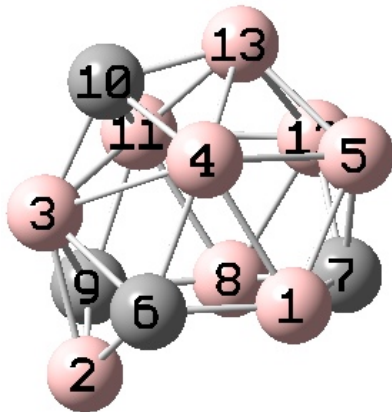
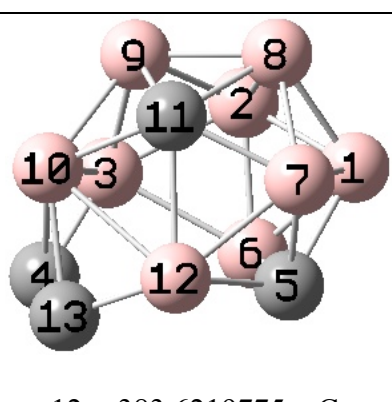
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 7. -383.6323770 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.747385</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.841968</td><td>1.971905</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.780577</td><td>2.892938</td><td>2.804373</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.803486</td><td>3.809484</td><td>3.208409</td><td>1.662654</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.710953</td><td>1.672907</td><td>1.691651</td><td>1.592460</td><td>2.820353</td></tr><tr><td>7 B</td><td>1.723316</td><td>3.009593</td><td>3.268749</td><td>1.861319</td><td>1.627340</td></tr><tr><td>8 B</td><td>1.815316</td><td>1.914084</td><td>2.680150</td><td>2.975632</td><td>3.101460</td></tr><tr><td>9 C</td><td>2.735805</td><td>1.546019</td><td>1.766103</td><td>3.611687</td><td>3.889568</td></tr><tr><td>10 C</td><td>3.553155</td><td>3.308480</td><td>1.699717</td><td>3.040130</td><td>2.491582</td></tr><tr><td>11 B</td><td>3.270693</td><td>2.763691</td><td>2.032322</td><td>3.602719</td><td>3.201173</td></tr><tr><td>12 B</td><td>3.121295</td><td>3.578005</td><td>2.843462</td><td>2.800083</td><td>1.664566</td></tr><tr><td>13 B</td><td>3.652105</td><td>4.032413</td><td>2.669926</td><td>2.449327</td><td>1.532592</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>2.679253</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.686111</td><td>1.882938</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>2.613459</td><td>3.217776</td><td>1.673060</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>2.797798</td><td>3.072232</td><td>3.007769</td><td>2.624878</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.747385	0.000000				3 B	2.841968	1.971905	0.000000			4 B	1.780577	2.892938	2.804373	0.000000		5 C	2.803486	3.809484	3.208409	1.662654	0.000000	6 C	1.710953	1.672907	1.691651	1.592460	2.820353	7 B	1.723316	3.009593	3.268749	1.861319	1.627340	8 B	1.815316	1.914084	2.680150	2.975632	3.101460	9 C	2.735805	1.546019	1.766103	3.611687	3.889568	10 C	3.553155	3.308480	1.699717	3.040130	2.491582	11 B	3.270693	2.763691	2.032322	3.602719	3.201173	12 B	3.121295	3.578005	2.843462	2.800083	1.664566	13 B	3.652105	4.032413	2.669926	2.449327	1.532592		6	7	8	9	10	6 C	0.000000					7 B	2.679253	0.000000				8 B	2.686111	1.882938	0.000000			9 C	2.613459	3.217776	1.673060	0.000000		10 C	2.797798	3.072232	3.007769	2.624878	0.000000																																		
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6 C	1.710953	1.672907	1.691651	1.592460	2.820353																																																																																																																																																						
7 B	1.723316	3.009593	3.268749	1.861319	1.627340																																																																																																																																																						
8 B	1.815316	1.914084	2.680150	2.975632	3.101460																																																																																																																																																						
9 C	2.735805	1.546019	1.766103	3.611687	3.889568																																																																																																																																																						
10 C	3.553155	3.308480	1.699717	3.040130	2.491582																																																																																																																																																						
11 B	3.270693	2.763691	2.032322	3.602719	3.201173																																																																																																																																																						
12 B	3.121295	3.578005	2.843462	2.800083	1.664566																																																																																																																																																						
13 B	3.652105	4.032413	2.669926	2.449327	1.532592																																																																																																																																																						
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6 C	0.000000																																																																																																																																																										
7 B	2.679253	0.000000																																																																																																																																																									
8 B	2.686111	1.882938	0.000000																																																																																																																																																								
9 C	2.613459	3.217776	1.673060	0.000000																																																																																																																																																							
10 C	2.797798	3.072232	3.007769	2.624878	0.000000																																																																																																																																																						

	<table><tr><td>11</td><td>B</td><td>3.136799</td><td>2.911511</td><td>1.950951</td><td>1.527361</td><td>1.655969</td></tr><tr><td>12</td><td>B</td><td>3.233678</td><td>1.887697</td><td>2.386265</td><td>3.005732</td><td>1.739011</td></tr><tr><td>13</td><td>B</td><td>2.953284</td><td>2.857080</td><td>3.671910</td><td>3.811428</td><td>1.530504</td></tr><tr><td></td><td></td><td>11</td><td>12</td><td>13</td><td></td><td></td></tr><tr><td>11</td><td>B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>12</td><td>B</td><td>1.857427</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>13</td><td>B</td><td>2.931030</td><td>1.868547</td><td>0.000000</td><td></td><td></td></tr></table>	11	B	3.136799	2.911511	1.950951	1.527361	1.655969	12	B	3.233678	1.887697	2.386265	3.005732	1.739011	13	B	2.953284	2.857080	3.671910	3.811428	1.530504			11	12	13			11	B	0.000000					12	B	1.857427	0.000000				13	B	2.931030	1.868547	0.000000																																																																																																																																														
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	13 B	2.217993	2.961377	2.636198	2.637904	1.683959
		6	7	8	9	10
	6 C	0.000000				
	7 B	3.143238	0.000000			
	8 B	2.783439	1.694044	0.000000		
	9 B	2.639276	3.054245	1.710568	0.000000	
	10 C	2.664437	2.851818	3.131853	2.809039	0.000000
	11 B	3.096576	1.975868	1.846872	1.905743	1.753140
	12 B	3.089822	1.866380	2.984561	3.511943	1.576421
	13 B	1.617515	2.759631	3.237196	3.380608	1.821031
		11	12	13		
	11 B	0.000000				
	12 B	1.983570	0.000000			
13 B	2.840308	1.880238	0.000000			
		1	2	3	4	5
	1 B	0.000000				
	2 C	1.640559	0.000000			
	3 B	3.186270	2.769168	0.000000		
	4 B	2.795577	3.447773	2.199415	0.000000	
	5 C	1.503645	2.710308	2.746756	1.512198	0.000000
	6 C	2.675562	1.522710	1.568710	3.108268	3.031879
	7 B	1.997352	2.777625	3.341113	2.112831	1.758854
	8 B	1.861955	1.671485	3.643439	3.495590	2.812033
	9 B	2.895564	1.656275	2.941351	3.758331	3.585794
	10 B	3.572661	2.831861	1.982187	2.855506	3.463544
	11 B	3.004705	2.715499	3.305694	3.068331	3.182980
	12 B	3.455084	3.570529	2.775642	1.942144	2.827098
	13 C	3.656561	3.555962	1.535224	1.651965	2.857500
		6	7	8	9	10
	6 C	0.000000				
	7 B	3.238201	0.000000			
	8 B	2.691396	1.863657	0.000000		
	9 B	1.689333	2.920871	1.745276	0.000000	
	10 B	1.874056	2.947816	2.948937	1.863458	0.000000
	11 B	2.808977	1.806348	1.717710	1.784768	1.889175
	12 B	3.167400	1.922876	3.027518	3.003464	1.873629
	13 C	2.602095	2.893858	3.752735	3.256084	1.685239
		11	12	13		
	11 B	0.000000				
	12 B	1.710585	0.000000			
	13 C	2.795505	1.587766	0.000000		

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>2.524919</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.915530</td><td>1.811540</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.899979</td><td>2.977907</td><td>2.105987</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.816761</td><td>3.771687</td><td>3.411320</td><td>1.899963</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.599206</td><td>1.541510</td><td>1.783519</td><td>1.752106</td><td>2.915235</td></tr><tr><td>7 C</td><td>1.627858</td><td>3.046749</td><td>3.414196</td><td>2.779505</td><td>1.642672</td></tr><tr><td>8 B</td><td>2.680458</td><td>2.524337</td><td>2.916547</td><td>3.334863</td><td>2.822536</td></tr><tr><td>9 C</td><td>3.054445</td><td>1.541719</td><td>1.783832</td><td>3.184644</td><td>3.590467</td></tr><tr><td>10 C</td><td>3.198714</td><td>3.168324</td><td>1.561012</td><td>1.734473</td><td>2.809602</td></tr><tr><td>11 B</td><td>3.333406</td><td>2.977068</td><td>2.105629</td><td>2.799408</td><td>2.911592</td></tr><tr><td>12 B</td><td>2.822721</td><td>3.771954</td><td>3.411775</td><td>2.912810</td><td>1.740198</td></tr><tr><td>13 B</td><td>3.016335</td><td>3.924171</td><td>2.803956</td><td>1.925605</td><td>1.783864</td></tr></table> <table><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.812962</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.054099</td><td>1.626936</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 C</td><td>2.525854</td><td>2.812796</td><td>1.599628</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>2.679030</td><td>3.420127</td><td>3.200700</td><td>2.679436</td><td>0.000000</td></tr><tr><td>11 B</td><td>3.183788</td><td>2.778689</td><td>1.901472</td><td>1.751228</td><td>1.735112</td></tr><tr><td>12 B</td><td>3.591081</td><td>1.642860</td><td>1.817909</td><td>2.915090</td><td>2.810350</td></tr><tr><td>13 B</td><td>3.292714</td><td>2.779114</td><td>3.016843</td><td>3.291642</td><td>1.538681</td></tr></table> <table><tr><th></th><th>11</th><th>12</th><th>13</th></tr><tr><td>11 B</td><td>0.000000</td><td></td><td></td></tr><tr><td>12 B</td><td>1.899716</td><td>0.000000</td><td></td></tr><tr><td>13 B</td><td>1.923752</td><td>1.783199</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	2.524919	0.000000				3 B	2.915530	1.811540	0.000000			4 B	1.899979	2.977907	2.105987	0.000000		5 B	1.816761	3.771687	3.411320	1.899963	0.000000	6 C	1.599206	1.541510	1.783519	1.752106	2.915235	7 C	1.627858	3.046749	3.414196	2.779505	1.642672	8 B	2.680458	2.524337	2.916547	3.334863	2.822536	9 C	3.054445	1.541719	1.783832	3.184644	3.590467	10 C	3.198714	3.168324	1.561012	1.734473	2.809602	11 B	3.333406	2.977068	2.105629	2.799408	2.911592	12 B	2.822721	3.771954	3.411775	2.912810	1.740198	13 B	3.016335	3.924171	2.803956	1.925605	1.783864		6	7	8	9	10	6 C	0.000000					7 C	2.812962	0.000000				8 B	3.054099	1.626936	0.000000			9 C	2.525854	2.812796	1.599628	0.000000		10 C	2.679030	3.420127	3.200700	2.679436	0.000000	11 B	3.183788	2.778689	1.901472	1.751228	1.735112	12 B	3.591081	1.642860	1.817909	2.915090	2.810350	13 B	3.292714	2.779114	3.016843	3.291642	1.538681		11	12	13	11 B	0.000000			12 B	1.899716	0.000000		13 B	1.923752	1.783199	0.000000
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	11 C	3.134729	1.679820	1.710640	1.660721	1.741552
	12 B	2.734100	1.858480	3.043855	3.042455	2.131224
	13 C	2.956439	3.272181	3.966048	3.255745	1.746834
		11	12	13		
	11 C	0.000000				
	12 B	1.898643	0.000000			
	13 C	2.749496	1.568217	0.000000		

Table S8C. Energy ranking for all of the C₄B₉H₁₃ structures.

		E w zpc	delta E w zpc
1	04-CapHexAnPr----C4---31	-383.8106809	0.00
2	04-CapHexAnPr----C4---45	-383.8106076	0.05
3	01-Doc----C4---20	-383.8091695	0.95
4	04-CapHexAnPr----C4---38	-383.8091694	0.95
5	04-CapHexAnPr----C4---3	-383.8091664	0.95
6	04-CapHexAnPr----C4---46	-383.8082973	1.50
7	02-Hen----C4---45	-383.7976292	8.19
8	02-Hen----C4---48	-383.7883183	14.03
9	04-CapHexAnPr----C4---16	-383.7883125	14.04
10	04-CapHexAnPr----C4---24	-383.7883001	14.04
11	01-Doc----C4---26	-383.7882964	14.05
12	03-Ditrapicos----C4---9	-383.7881761	14.12
13	03-Ditrapicos----C4---3	-383.7865722	15.13
14	01-Doc----C4---33	-383.7855920	15.74
15	02-Hen----C4---33	-383.7855920	15.74
16	02-Hen----C4---31	-383.7855788	15.75
17	01-Doc----C4---55	-383.7854467	15.83
18	04-CapHexAnPr----C4---37	-383.7854275	15.85
19	01-Doc----C4---51	-383.7853072	15.92
20	02-Hen----C4---51	-383.7853072	15.92
21	01-Doc----C4---35	-383.7852808	15.94
22	02-Hen----C4---54	-383.7849997	16.12
23	01-Doc----C4---8	-383.7849690	16.13
24	01-Doc----C4---52	-383.7844592	16.45
25	04-CapHexAnPr----C4---41	-383.7844549	16.46
26	01-Doc----C4---5	-383.7841971	16.62
27	03-Ditrapicos----C4---5	-383.7841971	16.62
28	04-CapHexAnPr----C4---22	-383.7834744	17.07
29	01-Doc----C4---59	-383.7820859	17.94
30	01-Doc----C4---53	-383.7820840	17.95
31	01-Doc----C4---37	-383.7820240	17.98
32	02-Hen----C4---37	-383.7820240	17.98
33	03-Ditrapicos----C4---43	-383.7819641	18.02
34	03-Ditrapicos----C4---59	-383.7811985	18.50
35	01-Doc----C4---7	-383.7811602	18.52
36	04-CapHexAnPr----C4---39	-383.7809936	18.63
37	01-Doc----C4---9	-383.7786206	20.12
38	04-CapHexAnPr----C4---14	-383.7786103	20.12
39	01-Doc----C4---28	-383.7786037	20.13

40	01-Doc---C4---18	-383.7786003	20.13
41	02-Hen---C4---18	-383.7786003	20.13
42	04-CapHexAnPr---C4---17	-383.7784667	20.22
43	03-Ditrapicos---C4---31	-383.7783273	20.30
44	01-Doc---C4---43	-383.7782578	20.35
45	03-Ditrapicos---C4---16	-383.7782517	20.35
46	01-Doc---C4---40	-383.7766159	21.38
47	02-Hen---C4---40	-383.7766159	21.38
48	03-Ditrapicos---C4---36	-383.7766132	21.38
49	02-Hen---C4---27	-383.7765942	21.39
50	04-CapHexAnPr---C4---44	-383.7751303	22.31
51	03-Ditrapicos---C4---30	-383.7748920	22.46
52	01-Doc---C4---60	-383.7748908	22.46
53	03-Ditrapicos---C4---60	-383.7748908	22.46
54	04-CapHexAnPr---C4---25	-383.7748646	22.48
55	01-Doc---C4---32	-383.7748510	22.48
56	01-Doc---C4---63	-383.7748326	22.50
57	02-Hen---C4---63	-383.7748326	22.50
58	04-CapHexAnPr---C4---5	-383.7739366	23.06
59	04-CapHexAnPr---C4---20	-383.7739247	23.07
60	03-Ditrapicos---C4---44	-383.7735328	23.31
61	04-CapHexAnPr---C4---6	-383.7735238	23.32
62	03-Ditrapicos---C4---54	-383.7735097	23.33
63	02-Hen---C4---16	-383.7734991	23.33
64	04-CapHexAnPr---C4---18	-383.7734580	23.36
65	02-Hen---C4---44	-383.7733607	23.42
66	04-CapHexAnPr---C4---28	-383.7733478	23.43
67	01-Doc---C4---50	-383.7733438	23.43
68	03-Ditrapicos---C4---33	-383.7732892	23.46
69	04-CapHexAnPr---C4---10	-383.7732543	23.49
70	01-Doc---C4---27	-383.7726789	23.85
71	02-Hen---C4---22	-383.7726714	23.85
72	02-Hen---C4---25	-383.7726494	23.87
73	03-Ditrapicos---C4---34	-383.7726467	23.87
74	03-Ditrapicos---C4---37	-383.7726464	23.87
75	03-Ditrapicos---C4---1	-383.7726312	23.88
76	01-Doc---C4---24	-383.7718869	24.34
77	02-Hen---C4---24	-383.7718869	24.34
78	03-Ditrapicos---C4---24	-383.7718869	24.34
79	03-Ditrapicos---C4---40	-383.7718751	24.35
80	03-Ditrapicos---C4---42	-383.7718747	24.35
81	02-Hen---C4---14	-383.7718708	24.35

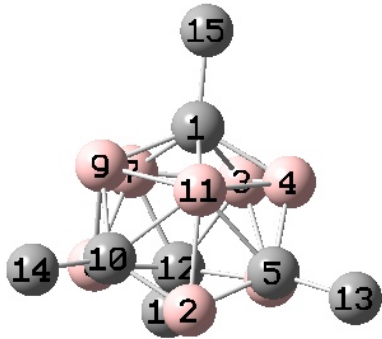
82	04-CapHexAnPr---C4---15	-383.7718502	24.37
83	02-Hen---C4---17	-383.7718448	24.37
84	03-Ditrapicos---C4---17	-383.7718058	24.39
85	01-Doc---C4---31	-383.7717549	24.43
86	01-Doc---C4---58	-383.7698407	25.63
87	03-Ditrapicos---C4---58	-383.7698407	25.63
88	04-CapHexAnPr---C4---36	-383.7698312	25.63
89	01-Doc---C4---45	-383.7694138	25.90
90	03-Ditrapicos---C4---7	-383.7694068	25.90
91	01-Doc---C4---39	-383.7694031	25.90
92	01-Doc---C4---56	-383.7693880	25.91
93	02-Hen---C4---56	-383.7693880	25.91
94	03-Ditrapicos---C4---56	-383.7693880	25.91
95	02-Hen---C4---57	-383.7693855	25.91
96	03-Ditrapicos---C4---45	-383.7693791	25.92
97	01-Doc---C4---46	-383.7693688	25.92
98	03-Ditrapicos---C4---46	-383.7693688	25.92
99	04-CapHexAnPr---C4---42	-383.7686099	26.40
100	03-Ditrapicos---C4---4	-383.7685903	26.41
101	01-Doc---C4---17	-383.7681373	26.70
102	02-Hen---C4---5	-383.7681047	26.72
103	04-CapHexAnPr---C4---27	-383.7680630	26.74
104	02-Hen---C4---36	-383.7680270	26.77
105	01-Doc---C4---16	-383.7669835	27.42
106	03-Ditrapicos---C4---20	-383.7667051	27.60
107	01-Doc---C4---11	-383.7656948	28.23
108	01-Doc---C4---2	-383.7656948	28.23
109	04-CapHexAnPr---C4---11	-383.7645060	28.98
110	02-Hen---C4---49	-383.7637489	29.45
111	04-CapHexAnPr---C4---4	-383.7637416	29.46
112	01-Doc---C4---1	-383.7637116	29.47
113	01-Doc---C4---6	-383.7634747	29.62
114	02-Hen---C4---6	-383.7634747	29.62
115	03-Ditrapicos---C4---6	-383.7634747	29.62
116	04-CapHexAnPr---C4---34	-383.7634594	29.63
117	01-Doc---C4---4	-383.7634397	29.64
118	01-Doc---C4---10	-383.7634360	29.65
119	03-Ditrapicos---C4---55	-383.7634211	29.66
120	02-Hen---C4---38	-383.7621754	30.44
121	03-Ditrapicos---C4---8	-383.7621723	30.44
122	04-CapHexAnPr---C4---19	-383.7621514	30.45
123	01-Doc---C4---13	-383.7618830	30.62

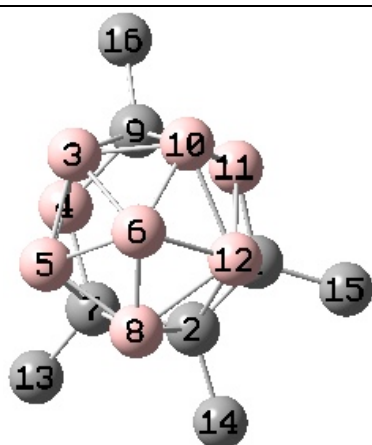
124	03-Ditrapicos----C4---13	-383.7618830	30.62
125	03-Ditrapicos----C4---11	-383.7618792	30.62
126	03-Ditrapicos----C4---2	-383.7618792	30.62
127	03-Ditrapicos----C4---12	-383.7618693	30.63
128	02-Hen----C4---12	-383.7615532	30.83
129	03-Ditrapicos----C4---62	-383.7598152	31.92
130	02-Hen----C4---13	-383.7597748	31.94
131	01-Doc----C4---49	-383.7597739	31.95
132	01-Doc----C4---14	-383.7597638	31.95
133	03-Ditrapicos----C4---53	-383.7588862	32.50
134	03-Ditrapicos----C4---51	-383.7588465	32.53
135	02-Hen----C4---46	-383.7588009	32.56
136	03-Ditrapicos----C4---27	-383.7583118	32.86
137	01-Doc----C4---25	-383.7583031	32.87
138	01-Doc----C4---23	-383.7582611	32.89
139	03-Ditrapicos----C4---23	-383.7582611	32.89
140	04-CapHexAnPr----C4---43	-383.7580064	33.05
141	02-Hen----C4---26	-383.7577795	33.20
142	03-Ditrapicos----C4---26	-383.7572184	33.55
143	02-Hen----C4---11	-383.7559605	34.34
144	02-Hen----C4---2	-383.7559605	34.34
145	01-Doc----C4---12	-383.7559071	34.37
146	03-Ditrapicos----C4---61	-383.7559058	34.37
147	01-Doc----C4---54	-383.7547479	35.10
148	02-Hen----C4---59	-383.7545506	35.22
149	01-Doc----C4---48	-383.7543099	35.37
150	02-Hen----C4---20	-383.7538002	35.69
151	02-Hen----C4---30	-383.7527139	36.38
152	02-Hen----C4---32	-383.7515885	37.08
153	03-Ditrapicos----C4---18	-383.7509653	37.47
154	02-Hen----C4---9	-383.7506489	37.67
155	04-CapHexAnPr----C4---40	-383.7506246	37.69
156	02-Hen----C4---39	-383.7501349	37.99
157	03-Ditrapicos----C4---35	-383.7497637	38.23
158	02-Hen----C4---60	-383.7490708	38.66
159	02-Hen----C4---3	-383.7490607	38.67
160	03-Ditrapicos----C4---49	-383.7490547	38.67
161	01-Doc----C4---30	-383.7489533	38.74
162	01-Doc----C4---21	-383.7489513	38.74
163	01-Doc----C4---3	-383.7489009	38.77
164	02-Hen----C4---21	-383.7473116	39.77
165	01-Doc----C4---62	-383.7472880	39.78

166	02-Hen---C4---62	-383.7472880	39.78
167	02-Hen---C4---23	-383.7463567	40.36
168	02-Hen---C4---19	-383.7463457	40.37
169	02-Hen---C4---29	-383.7463380	40.38
170	03-Ditrapicos---C4---14	-383.7463328	40.38
171	01-Doc---C4---22	-383.7456212	40.83
172	03-Ditrapicos---C4---22	-383.7456212	40.83
173	01-Doc---C4---61	-383.7455977	40.84
174	02-Hen---C4---53	-383.7452281	41.07
175	04-CapHexAnPr---C4---35	-383.7451993	41.09
176	02-Hen---C4---7	-383.7451760	41.11
177	03-Ditrapicos---C4---39	-383.7446441	41.44
178	01-Doc---C4---19	-383.7443405	41.63
179	04-CapHexAnPr---C4---1	-383.7440820	41.79
180	03-Ditrapicos---C4---10	-383.7434390	42.20
181	04-CapHexAnPr---C4---2	-383.7433520	42.25
182	01-Doc---C4---34	-383.7419804	43.11
183	04-CapHexAnPr---C4---30	-383.7419193	43.15
184	01-Doc---C4---44	-383.7411061	43.66
185	03-Ditrapicos---C4---19	-383.7410596	43.69
186	03-Ditrapicos---C4---38	-383.7410596	43.69
187	02-Hen---C4---61	-383.7408216	43.84
188	02-Hen---C4---1	-383.7400733	44.31
189	03-Ditrapicos---C4---28	-383.7394215	44.72
190	02-Hen---C4---34	-383.7392835	44.80
191	03-Ditrapicos---C4---64	-383.7392535	44.82
192	03-Ditrapicos---C4---32	-383.7384841	45.30
193	02-Hen---C4---10	-383.7380065	45.60
194	01-Doc---C4---15	-383.7379827	45.62
195	01-Doc---C4---47	-383.7377653	45.76
196	02-Hen---C4---47	-383.7377653	45.76
197	03-Ditrapicos---C4---47	-383.7377653	45.76
198	01-Doc---C4---38	-383.7369214	46.29
199	04-CapHexAnPr---C4---9	-383.7353406	47.28
200	03-Ditrapicos---C4---63	-383.7310007	50.00
201	03-Ditrapicos---C4---15	-383.7308068	50.12
202	02-Hen---C4---15	-383.7295136	50.93
203	04-CapHexAnPr---C4---7	-383.7281129	51.81
204	03-Ditrapicos---C4---52	-383.7273845	52.27
205	04-CapHexAnPr---C4---21	-383.7273842	52.27
206	01-Doc---C4---36	-383.7263497	52.92
207	02-Hen---C4---55	-383.7261032	53.07

208	02-Hen----C4---41	-383.7242008	54.27
209	02-Hen----C4---58	-383.7222815	55.47
210	04-CapHexAnPr----C4---33	-383.7222132	55.52
211	02-Hen----C4---8	-383.7218992	55.71
212	04-CapHexAnPr----C4---8	-383.7199726	56.92
213	02-Hen----C4---35	-383.7192417	57.38
214	02-Hen----C4---4	-383.7178529	58.25
215	04-CapHexAnPr----C4---23	-383.7132699	61.13
216	01-Doc----C4---42	-383.7129791	61.31
217	02-Hen----C4---42	-383.7129791	61.31
218	01-Doc----C4---29	-383.7114488	62.27
219	03-Ditrapicos----C4---29	-383.7114488	62.27
220	01-Doc----C4---64	-383.7083516	64.21
221	02-Hen----C4---64	-383.7083516	64.21
222	01-Doc----C4---41	-383.7075879	64.69
223	03-Ditrapicos----C4---41	-383.7075879	64.69
224	02-Hen----C4---28	-383.7035490	67.23
225	03-Ditrapicos----C4---25	-383.7034286	67.30
226	03-Ditrapicos----C4---21	-383.7009476	68.86
227	04-CapHexAnPr----C4---29	-383.6989211	70.13
228	04-CapHexAnPr----C4---32	-383.6975844	70.97
229	02-Hen----C4---52	-383.6974540	71.05
230	04-CapHexAnPr----C4---12	-383.6969754	71.35
231	04-CapHexAnPr----C4---13	-383.6956390	72.19
232	03-Ditrapicos----C4---48	-383.6942975	73.03
233	03-Ditrapicos----C4---50	-383.6942428	73.07
234	01-Doc----C4---57	-383.6849900	78.87
235	03-Ditrapicos----C4---57	-383.6849900	78.87
236	04-CapHexAnPr----C4---26	-383.6812111	81.24
237	02-Hen----C4---50	-383.6766745	84.09
238	02-Hen----C4---43	-383.6608835	94.00

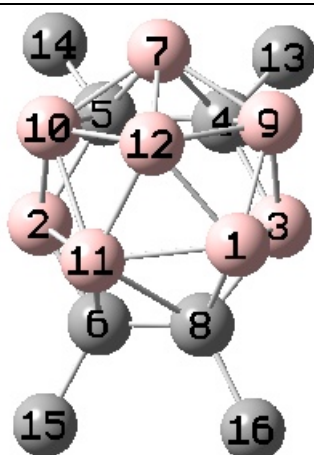
Table S9. Distance table for the lowest-lying $C_4Me_4B_8H_8$ structures. For clarity, only the polyhedral framework is presented.

 Me₄C₄B₈H₈_1 -515.4680544 C_s		1	2	3	4	5	
	1 C	0.000000					
	2 B	3.258653	0.000000				
	3 B	1.721376	3.617570	0.000000			
	4 B	1.676256	2.862156	1.712341	0.000000		
	5 C	2.756840	1.523573	2.797942	1.646413	0.000000	
	6 B	2.716831	2.558399	1.758006	1.773409	1.652513	
	7 B	1.721363	3.617568	1.749347	2.841860	3.510038	
	8 B	2.716839	2.558388	2.816301	3.358943	3.136331	
	9 B	1.676276	2.862141	2.841879	2.940589	3.203337	
	10 C	2.756842	1.523589	3.510059	3.203351	2.567780	
	11 B	1.766913	1.886429	2.879536	1.871639	1.779369	
	12 C	2.605623	3.009929	1.684802	2.704757	2.821157	
	13 C	4.027624	2.595275	3.989944	2.586148	1.522743	
	14 C	4.027658	2.595256	4.977210	4.644276	3.913188	
	15 C	1.519524	4.621901	2.797686	2.697680	4.035632	
	16 C	3.987527	4.298213	2.729045	4.043616	4.144380	
		6	7	8	9	10	
	6 B	0.000000					
	7 B	2.816316	0.000000				
	8 B	2.767312	1.758018	0.000000			
	9 B	3.358953	1.712341	1.773421	0.000000		
	10 C	3.136374	2.797951	1.652548	1.646384	0.000000	
	11 B	2.748925	2.879500	2.748886	1.871569	1.779298	
	12 C	1.634104	1.684820	1.634089	2.704764	2.821192	
	13 C	2.730263	4.977179	4.632330	4.644259	3.913206	
	14 C	4.632355	3.989984	2.730315	2.586171	1.522736	
	15 C	4.085967	2.797651	4.085959	2.697669	4.035605	
	16 C	2.692497	2.729069	2.692485	4.043626	4.144420	
		11	12	13	14	15	
	11 B	0.000000					
	12 C	3.107068	0.000000				
	13 C	2.965855	4.195880	0.000000			
	14 C	2.965792	4.195913	5.060548	0.000000		
	15 C	2.856601	4.003447	5.063467	5.063475	0.000000	
	16 C	4.628600	1.523376	5.355392	5.355430	5.238626	



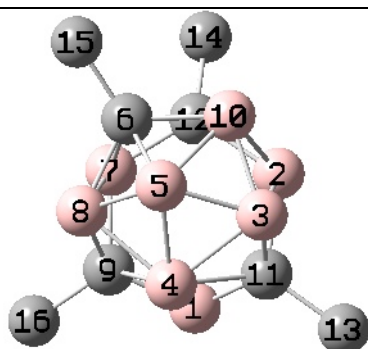
Me₄C₄B₈H₈⁻²
-515.4633024 C₁

	1	2	3	4	5
1 C	0.000000				
2 C	1.439173	0.000000			
3 B	3.659778	3.522393	0.000000		
4 B	3.028665	2.705112	1.800761	0.000000	
5 B	3.608795	2.795566	1.735595	1.808563	0.000000
6 B	3.235836	2.895737	1.794394	2.797500	1.793966
7 C	2.607810	1.559832	2.772892	1.625934	1.684562
8 B	2.784124	1.737245	2.862910	2.774245	1.719750
9 C	2.741024	3.149277	1.654065	1.615152	2.759023
10 B	2.797806	3.226433	1.739177	2.720595	2.839817
11 B	1.494962	2.562119	2.912808	2.670553	3.571651
12 B	1.767671	1.889735	2.932317	3.155097	2.881582
13 C	3.808782	2.601701	4.050685	2.693840	2.687837
14 C	2.511993	1.519263	4.971054	4.060033	3.953728
15 C	1.507741	2.534023	5.125074	4.498242	5.059670
16 C	3.947798	4.566689	2.690680	2.717433	4.070687
	6	7	8	9	10
6 B	0.000000				
7 C	2.727776	0.000000			
8 B	1.732206	1.700163	0.000000		
9 C	2.708245	2.802557	3.361474	0.000000	
10 B	1.725060	3.297603	2.962228	1.640950	0.000000
11 B	3.035151	3.077525	3.347977	1.630076	1.856703
12 B	1.783503	2.711441	1.859100	2.797292	1.913969
13 C	4.084202	1.521373	2.784969	4.145520	4.806564
14 C	4.129744	2.626088	2.621259	4.654739	4.670283
15 C	4.529868	3.948136	3.980299	4.105106	4.027800
16 C	4.071539	4.164646	4.876498	1.523227	2.746063
	11	12	13	14	15
11 B	0.000000				
12 B	2.087512	0.000000			
13 C	4.466873	4.120975	0.000000		
14 C	3.914368	3.040112	2.925027	0.000000	
15 C	2.596006	2.816467	4.914578	2.835034	0.000000
16 C	2.609936	4.208746	5.334078	6.031761	5.103300



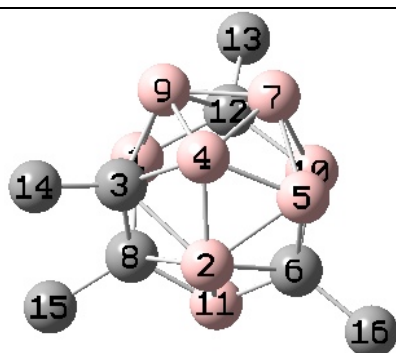
Me4C4B8H8_3
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	1	2	3	4	5
1 B	0.000000				
2 B	3.267983	0.000000			
3 B	1.769444	3.096315	0.000000		
4 C	2.696281	2.705918	1.608269	0.000000	
5 C	3.285851	1.639337	2.736165	1.545599	0.000000
6 C	2.754353	1.505190	2.633163	3.068987	2.718534
7 B	2.852446	2.899776	2.819798	1.720460	1.672077
8 C	1.731646	2.558075	1.651532	2.770904	3.127914
9 B	1.714100	3.558199	1.747826	1.731910	2.730988
10 B	2.942378	1.801714	3.347224	2.660651	1.668287
11 B	1.884849	1.978341	2.820649	3.120871	2.745756
12 B	1.742065	2.985903	2.817080	2.711394	2.704362
13 C	4.042870	3.956698	2.650687	1.517749	2.600957
14 C	4.795076	2.624538	4.049676	2.634590	1.518421
15 C	3.990852	2.590590	3.972559	4.531848	4.068031
16 C	2.622137	3.923781	2.704501	4.131643	4.632080
	6	7	8	9	10
6 C	0.000000				
7 B	3.689621	0.000000			
8 C	1.419710	3.578522	0.000000		
9 B	3.629315	1.747588	2.850848	0.000000	
10 B	2.827535	1.729476	3.257171	2.841725	0.000000
11 B	1.798526	2.909388	1.946288	2.899570	1.863907
12 B	3.271033	1.780775	2.943291	1.787270	1.729089
13 C	4.366981	2.748523	4.054718	2.785283	3.986381
14 C	3.904002	2.694666	4.522547	4.029215	2.774946
15 C	1.503678	5.151836	2.518308	5.090847	4.063739
16 C	2.514576	5.015325	1.515667	3.993542	4.694874
	11	12	13	14	15
11 B	0.000000				
12 B	1.790593	0.000000			
13 C	4.635594	4.090666	0.000000		
14 C	4.151863	4.072067	2.943012	0.000000	
15 C	2.885578	4.592882	5.732129	5.029317	0.000000
16 C	3.107435	4.161600	5.244369	5.985719	2.855689



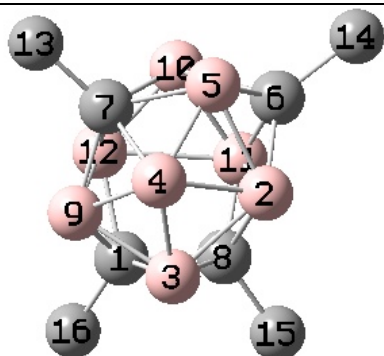
Me₄C₄B₈H₈_4
-515.4598372 °C₁

	1	2	3	4	5
1 B	0.000000				
2 B	2.600649	0.000000			
3 B	2.867362	1.769390	0.000000		
4 B	1.879796	2.758838	1.876984	0.000000	
5 B	3.351719	2.814928	1.745628	1.811171	0.000000
6 C	3.527060	2.723385	2.755217	2.765508	1.705494
7 B	2.581625	2.761928	3.384108	2.777849	2.845944
8 B	2.843072	3.349922	2.954158	1.864153	1.732914
9 C	1.527721	3.139271	3.242253	1.842131	2.873855
10 B	3.635066	1.755307	1.709283	2.864437	1.770637
11 C	1.520114	1.642534	1.663237	1.814610	2.864240
12 C	3.032695	1.641033	2.732101	3.115166	2.730395
13 C	2.579085	2.725137	2.594232	2.992138	4.113973
14 C	4.372119	2.719902	4.050961	4.632630	4.050078
15 C	4.989562	4.043187	4.080469	4.168188	2.810258
16 C	2.591746	4.639175	4.679596	3.014688	4.116678
	6	7	8	9	10
6 C	0.000000				
7 B	1.734820	0.000000			
8 B	1.645853	1.796154	0.000000		
9 C	2.705736	1.626284	1.650401	0.000000	
10 B	1.692263	2.830078	2.832428	3.512320	0.000000
11 C	3.397690	3.126623	3.203350	2.586831	2.796553
12 C	1.650615	1.602344	2.694400	2.782579	1.728287
13 C	4.867617	4.620775	4.644265	3.933353	3.991551
14 C	2.691319	2.660811	4.005185	4.113950	2.721655
15 C	1.510266	2.810157	2.720278	3.984804	2.720261
16 C	3.920394	2.714844	2.589109	1.523460	4.978088
	11	12	13	14	15
11 C	0.000000				
12 C	2.806953	0.000000			
13 C	1.523394	4.186475	0.000000		
14 C	4.153753	1.517812	5.378243	0.000000	
15 C	4.895427	2.753780	6.343492	3.103455	0.000000
16 C	3.933245	4.159573	5.083501	5.326551	4.930891



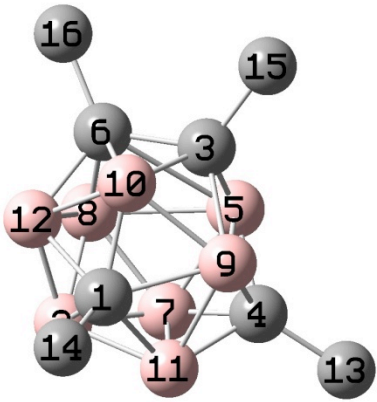
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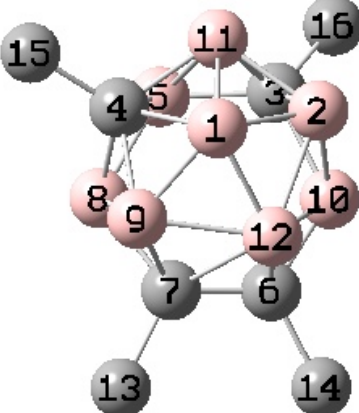
	1	2	3	4	5
1 B	0.000000				
2 B	2.838486	0.000000			
3 C	1.729328	1.875860	0.000000		
4 B	2.835069	1.791407	1.671640	0.000000	
5 B	3.407905	1.830021	2.885914	1.751091	0.000000
6 C	3.172215	1.749144	3.118419	2.838025	1.648117
7 B	2.835121	2.860432	2.754122	1.786838	1.728123
8 C	1.611579	1.930859	1.618114	2.865873	3.264978
9 B	1.777454	2.897999	1.657677	1.775030	2.853764
10 B	2.755428	2.723829	3.234737	2.810568	1.784794
11 B	2.588733	1.872913	2.759603	3.307017	2.847671
12 C	1.625922	3.131259	2.603464	2.713068	2.732201
13 C	2.675705	4.653544	3.956789	4.084939	4.064380
14 C	2.895990	2.965979	1.514225	2.666757	4.180483
15 C	2.696456	3.102835	2.624897	4.115961	4.697368
16 C	4.659633	2.934068	4.573364	4.109138	2.600663
	6	7	8	9	10
7 B	2.816172	0.000000			
8 C	2.607863	3.516593	0.000000		
9 B	3.513479	1.732118	2.784255	0.000000	
10 B	1.664312	1.772200	3.109662	2.794097	0.000000
11 B	1.512702	3.616312	1.530227	3.606416	2.552808
12 C	2.846805	1.701034	2.781272	1.678184	1.628087
13 C	4.171222	2.741460	4.092015	2.728119	2.691559
14 C	4.496268	4.047582	2.638019	2.713040	4.742866
15 C	3.934468	4.982491	1.517060	3.988410	4.597751
16 C	1.522099	4.022085	3.954491	4.985846	2.753075
	11	12	13	14	15
12 C	3.029694	0.000000			
13 C	4.333555	1.523780	0.000000		
14 C	3.972394	3.994914	5.189178	0.000000	
15 C	2.586294	4.156958	5.299131	2.864002	0.000000
16 C	2.578131	4.219276	5.377781	5.862081	5.081445

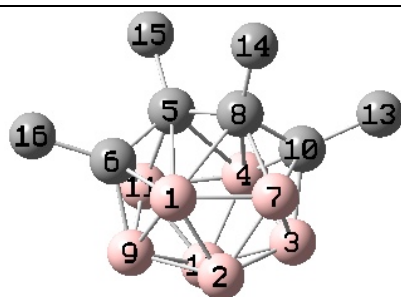


Me4C4B8H8_6
-515.4537160 C₁

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3 B	1.673487	1.870634	0.000000		
4 B	2.756650	1.863825	1.749790	0.000000	
5 B	3.496898	1.849234	2.970154	1.737437	0.000000
6 C	3.419440	1.676038	3.214893	2.811823	1.586713
7 C	2.681983	2.719659	2.740929	1.714785	1.704039
8 C	1.541730	1.840976	1.637302	2.822724	3.176827
9 B	1.635560	2.873721	1.752067	1.749597	2.879453
10 B	2.987457	2.650252	3.387018	2.831868	1.807506
11 B	2.381675	2.117488	2.843059	3.220907	2.695435
12 B	1.652589	3.077221	2.744037	2.825542	2.878580

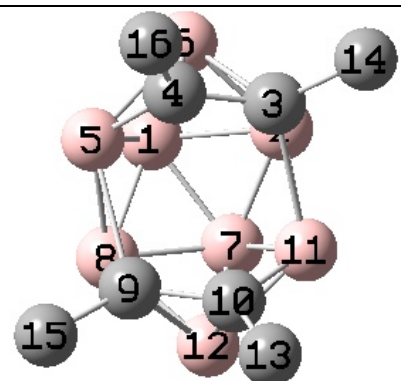
	13 C 3.975227 4.136520 4.086340 2.812497 2.728013					
	14 C 4.881506 2.889750 4.635319 4.140117 2.654878					
	15 C 2.650204 2.917803 2.669828 4.141613 4.544833					
	16 C 1.507217 4.197744 2.791512 4.108860 4.998825					
	6 7 8 9 10					
	7 C 2.673996 0.000000					
	8 C 2.590104 3.168973 0.000000					
	9 B 3.553908 1.667718 2.652679 0.000000					
	10 B 1.634480 1.713019 2.931641 2.894817 0.000000					
	11 B 1.592966 2.894079 1.592698 3.192473 1.818296					
	12 B 2.908219 1.745756 2.461242 1.825482 1.753563					
	13 C 3.927764 1.518502 4.671046 2.687167 2.770699					
	14 C 1.510678 3.996647 3.891042 5.048351 2.757118					
	15 C 3.724672 4.675742 1.509478 3.981098 4.321439					
	16 C 4.853889 4.023582 2.645205 2.720575 4.347514					
	11 12 13 14 15					
	12 B 2.135128 0.000000					
	13 C 4.301758 2.855324 0.000000					
	14 C 2.749286 4.285343 5.015725 0.000000					
	15 C 2.669915 3.829283 6.173983 4.728874 0.000000					
	16 C 3.600329 2.775629 5.112520 6.264342 3.075532					
 Me₄C₄B₈H₈_7 -515.4526389 C₁	1 2 3 4 5					
	1 C 0.000000					
	2 B 1.731015 0.000000					
	3 C 2.710301 3.299433 0.000000					
	4 C 2.713953 2.772462 2.582491 0.000000					
	5 B 3.089762 2.973345 1.604630 1.617236 0.000000					
	6 C 2.648109 2.788621 1.539949 3.416949 2.352494					
	7 B 2.733377 1.773684 2.959716 1.639864 1.808579					
	8 B 2.713293 1.806790 2.479726 2.923123 2.096165					
	9 B 1.834624 2.851965 1.792751 1.624083 2.082344					
	10 B 1.664223 2.832011 1.627092 3.183566 2.822459					
	11 B 1.694821 1.748698 3.185336 1.595225 2.698056					
	12 B 1.706742 1.715811 2.667509 3.555160 3.158253					
	13 C 4.059761 4.081798 3.873955 1.510718 2.782554					
	14 C 1.521108 2.830160 4.049219 3.960857 4.575503					
	15 C 4.041100 4.805382 1.508918 3.712806 2.699563					
	16 C 4.006973 4.110366 2.642346 4.854457 3.579130					
	6 7 8 9 10					
	7 B 3.022904 0.000000					
	8 B 1.668824 1.788388 0.000000					
	9 B 2.776188 2.630284 3.063587 0.000000					
	10 B 1.659699 3.382409 2.732479 1.868059 0.000000					
	11 B 3.497740 1.781184 2.872295 1.886909 2.954699					
	12 B 1.638804 2.900972 1.797075 2.906738 1.770885					
	13 C 4.877532 2.764486 4.308372 2.831455 4.596719					
	14 C 3.955198 4.096111 4.128943 2.972622 2.689238					

	15 C	2.650568	4.349678	3.851488	2.864420	2.669255
	16 C	1.505709	4.392213	2.796233	4.165921	2.776543
		11	12	13	14	15
	12 B	2.878634	0.000000			
	13 C	2.666134	5.051094	0.000000		
	14 C	2.685406	2.765528	5.084793	0.000000	
	15 C	4.552677	3.999227	4.699337	5.192113	0.000000
	16 C	4.997186	2.713008	6.264435	5.123535	3.076053
 Me₄C₄B₈H₈_8 -515.4485922 C₁		1	2	3	4	5
	1 B	0.000000				
	2 B	1.727495	0.000000			
	3 C	2.700034	1.655024	0.000000		
	4 C	1.729257	2.745008	2.637963	0.000000	
	5 B	2.827934	2.765377	1.617470	1.739862	0.000000
	6 C	3.225496	2.834508	2.753928	3.477048	3.118172
	7 C	2.946699	3.302222	3.167726	2.725762	2.803162
	8 B	2.846851	3.439127	2.866978	1.677411	1.711865
	9 B	1.725583	2.947963	3.305283	1.650641	2.792760
	10 B	2.956605	1.808357	1.652391	3.411182	2.753132
	11 B	1.779549	1.725874	1.652058	1.674083	1.791450
	12 B	1.770129	1.885321	2.769838	2.790091	3.232977
	13 C	4.167068	4.736445	4.676683	3.910392	4.165467
	14 C	4.527697	4.056828	4.105650	4.937896	4.581272
	15 C	2.820916	4.065892	3.965889	1.517963	2.851391
	16 C	4.062512	2.735515	1.523114	3.977780	2.696087
		6	7	8	9	10
	7 C	1.430133	0.000000			
	8 B	2.687972	1.637296	0.000000		
	9 B	2.714709	1.732790	1.767677	0.000000	
	10 B	1.505250	2.569640	3.175202	3.242490	0.000000
	11 B	3.660444	3.557421	2.856473	2.830275	2.880919
	12 B	1.776584	2.000707	2.884228	1.875719	1.972110
	13 C	2.516619	1.518315	2.669693	2.635581	3.929657
	14 C	1.505793	2.527611	4.020105	3.936310	2.593071
	15 C	4.946074	4.006113	2.728152	2.714781	4.918352
	16 C	3.955267	4.575879	4.212335	4.822956	2.642371
		11	12	13	14	15
	12 B	2.902225	0.000000			
	13 C	5.000628	3.145344	0.000000		
	14 C	5.121151	2.834777	2.849696	0.000000	
	15 C	2.690491	4.175345	4.910926	6.374127	0.000000
	16 C	2.697582	4.162901	6.047935	5.089109	5.104199



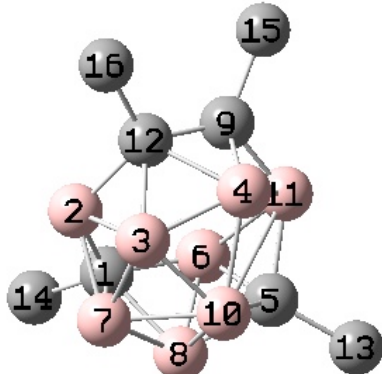
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-515.4482372 C₂

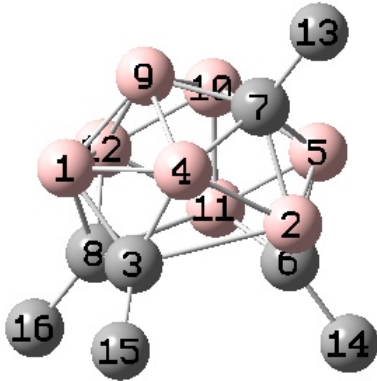
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1 B	0.000000				
2 B	1.786721	0.000000			
3 B	2.902279	1.770351	0.000000		
4 B	3.210043	2.840048	1.807859	0.000000	
5 C	2.333017	3.206328	3.148553	2.078250	0.000000
6 C	1.667037	2.803030	3.541140	2.950805	1.500437
7 B	1.818750	1.758853	1.768617	2.705490	2.782020
8 C	2.078120	2.886324	2.634640	2.333928	1.508102
9 B	1.807385	1.740397	2.897729	2.902735	2.634639
10 C	2.950574	2.814424	1.657156	1.667572	2.398995
11 B	2.704638	2.819602	2.915533	1.819181	1.677808
12 B	2.839826	1.800367	1.740816	1.786573	2.885933
13 C	4.319414	4.134110	2.731714	2.842635	3.671160
14 C	3.040069	4.180200	3.988441	3.726831	2.569250
15 C	3.724313	4.710504	4.458293	3.042623	1.506964
16 C	2.841086	4.141992	5.040246	4.320460	2.635788
	6	7	8	9	10
7 B	3.029957	0.000000			
8 C	2.399501	1.678255	0.000000		
9 B	1.656992	2.915036	3.149015	0.000000	
10 C	3.380240	1.681445	1.500346	3.541357	0.000000
11 B	1.680650	3.303903	2.782274	1.768901	3.030128
12 B	2.814106	2.819661	3.206758	1.770558	2.803282
13 C	4.817307	2.786317	2.634685	5.040426	1.506953
14 C	3.407368	2.702332	1.507107	4.457385	2.627202
15 C	2.626014	4.131717	2.567843	3.988599	3.407574
16 C	1.506978	4.436517	3.671568	2.731163	4.817531
	11	12	13	14	15
12 B	1.759142	0.000000			
13 C	4.437341	4.142946	0.000000		
14 C	4.132491	4.710835	3.103433	0.000000	
15 C	2.703626	4.181595	4.305176	2.977310	0.000000
16 C	2.786586	4.134114	6.194654	4.304629	3.103115

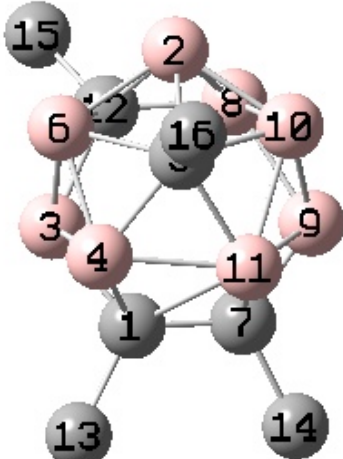
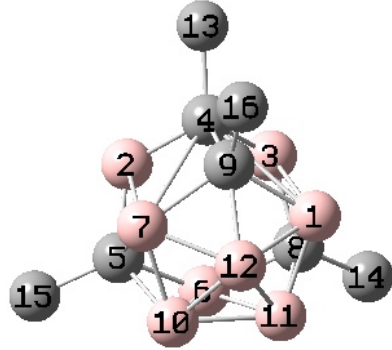


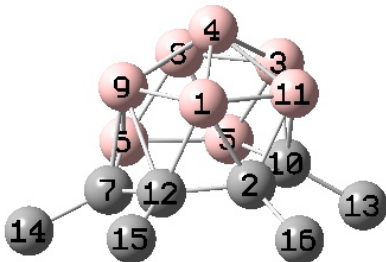
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2 B	1.788781	0.000000			
3 C	2.696990	1.630700	0.000000		
4 C	2.704190	2.568462	1.408378	0.000000	
5 B	1.824519	2.723283	2.462983	1.562714	0.000000
6 B	1.738543	1.784221	1.722974	1.644775	1.838329
7 B	1.755715	1.766628	2.934994	3.454394	2.883827
8 B	1.767581	2.833253	3.320094	3.066048	1.867061
9 C	2.936838	3.321804	3.064199	2.658856	2.065699
10 C	3.455814	3.067739	2.658970	2.830765	2.923955
11 B	2.884588	1.867731	2.064837	2.923510	3.143975
12 B	2.975421	3.029151	3.455170	3.699978	3.147969

	13 C 4.937149 4.374990 3.661119 3.812051 4.193336					
	14 C 4.111100 2.706955 1.502631 2.544629 3.895791					
	15 C 4.179263 4.789149 4.343083 3.608364 2.948708					
	16 C 4.127513 3.980448 2.559691 1.497397 2.709929					
	6 7 8 9 10					
	7 B 2.974808 0.000000					
	8 B 3.028674 1.789165 0.000000					
	9 C 3.456183 2.697062 1.629971 0.000000					
	10 C 3.700941 2.703490 2.567683 1.408717 0.000000					
	11 B 3.148103 1.823708 2.723429 2.464401 1.563725					
	12 B 3.964626 1.738292 1.784017 1.722951 1.644212					
	13 C 4.970363 4.125877 3.980097 2.561082 1.497380					
	14 C 2.912723 4.177413 4.787055 4.341574 3.606382					
	15 C 4.636000 4.110675 2.705736 1.502684 2.545529					
	16 C 2.857303 4.935414 4.373616 3.660084 3.810040					
	11 12 13 14 15					
	12 B 1.838970 0.000000					
	13 C 2.709439 2.855878 0.000000					
	14 C 2.946387 4.633870 4.156203 0.000000					
	15 C 3.897464 2.911860 3.032506 5.521455 0.000000					
	16 C 4.191175 4.968389 4.355590 3.029100 4.158191					
 Me₄C₄B₈H₈⁻ 11 -515.4471807 C₁	1 2 3 4 5					
	1 C 0.000000					
	2 B 1.627015 0.000000					
	3 B 2.731977 1.788732 0.000000					
	4 B 3.378322 2.807176 1.733716 0.000000					
	5 C 2.563114 3.357622 3.065591 2.559265 0.000000					
	6 B 1.590710 2.740836 3.346520 3.154941 1.596693					
	7 B 1.705405 1.741017 1.719525 2.994381 2.781047					
	8 B 1.692785 2.821901 2.890867 3.303121 1.596127					
	9 C 3.115735 2.666405 2.689070 1.654971 2.840238					
	10 B 2.705773 2.827266 1.784452 1.925376 1.687040					
	11 B 3.011230 3.275420 3.105620 1.935105 1.629311					
	12 C 2.785943 1.622414 1.720285 1.758792 3.380376					
	13 C 3.951034 4.868321 4.407067 3.675331 1.514296					
	14 C 1.524522 2.659378 4.071182 4.887465 3.864976					
	15 C 4.515587 3.954461 3.992030 2.767993 4.148396					
	16 C 4.113601 2.658069 2.715320 2.844414 4.876021					
	6 7 8 9 10					
	7 B 2.778129 0.000000					
	8 B 1.786144 1.728688 0.000000					
	9 C 2.643325 3.554949 3.636617 0.000000					
	10 B 2.694817 1.857667 1.814247 3.019015 0.000000					
	11 B 1.917138 3.505460 2.901910 1.498205 2.496485					
	12 C 3.108328 2.810357 3.585412 1.472031 2.883871					
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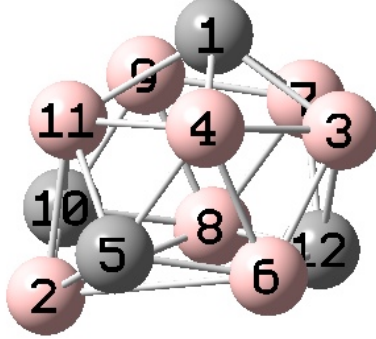
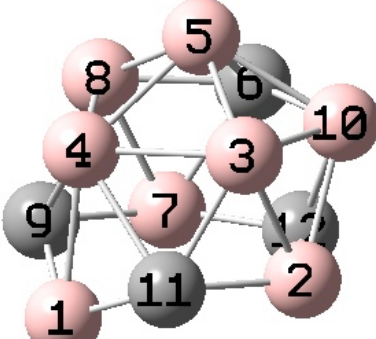
	15 C	3.920351	5.036501	5.111998	1.510393	4.428766
	16 C	4.574413	4.012460	5.050796	2.564618	4.220206
		11	12	13	14	15
	12 C	2.621770	0.000000			
	13 C	2.600230	4.798358	0.000000		
	14 C	4.387752	4.060659	5.064815	0.000000	
	15 C	2.569400	2.555381	5.112734	5.723393	0.000000
	16 C	3.961011	1.519304	6.251098	5.175302	2.895293
 Me₄C₄B₈H₈·12 -515.4467815 C₁		1	2	3	4	5
	1 B	0.000000				
	2 B	3.294950	0.000000			
	3 C	1.657547	2.339413	0.000000		
	4 B	1.802480	1.941735	1.586979	0.000000	
	5 B	3.919119	1.824631	3.541644	3.054624	0.000000
	6 C	3.768636	1.520590	2.822797	3.050626	1.595123
	7 C	2.883196	1.719022	2.879109	1.729250	1.726039
	8 C	1.684252	2.974555	1.406575	2.509315	3.492828
	9 B	1.747371	2.954544	2.704605	1.805767	2.956851
	10 B	2.969265	2.769345	3.366619	2.827462	1.751479
	11 B	3.262582	2.524435	2.956863	3.238158	1.825899
	12 B	1.811716	3.280722	2.532684	2.719114	3.045603
	13 C	4.073198	2.802552	4.192008	2.747794	2.706558
	14 C	5.135695	2.677315	3.953989	4.402722	2.764842
	15 C	2.870267	3.236875	1.497213	2.700054	4.758301
	16 C	2.888733	4.235779	2.548505	3.934853	4.705463
		6	7	8	9	10
	7 C	2.590801	0.000000			
	8 C	2.790400	3.228397	0.000000		
	9 B	3.538379	1.684769	2.700355	0.000000	
	10 B	2.692183	1.707759	2.944416	1.739459	0.000000
	11 B	1.543799	2.671726	2.241906	2.951741	1.804315
	12 B	3.091402	2.727273	1.596392	1.801429	1.779370
	13 C	3.858058	1.523503	4.709193	2.661416	2.837733
	14 C	1.507474	4.004800	3.925410	5.045230	4.093442
	15 C	3.748860	4.164130	2.561101	4.123107	4.837250
	16 C	3.722936	4.700648	1.500108	4.119502	4.215731
		11	12	13	14	15
	12 B	1.937883	0.000000			
	13 C	4.083804	4.100166	0.000000		
	14 C	2.703295	4.448467	5.097299	0.000000	
	15 C	4.209899	3.957268	5.316305	4.478552	0.000000
	16 C	3.135431	2.702581	6.197770	4.454561	3.043905

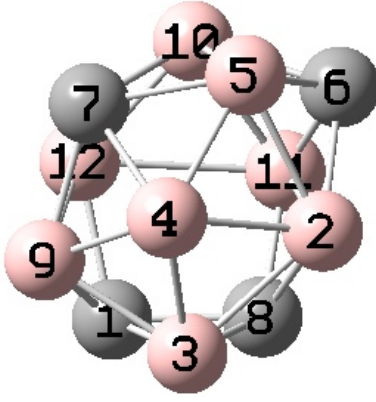
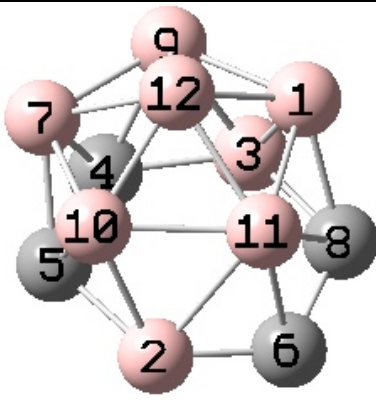
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	1 C	0.000000				
	2 B	3.559905	0.000000			
	3 B	1.596456	2.833154	0.000000		
	4 B	1.747876	2.831258	1.778308	0.000000	
	5 C	2.861667	1.715681	2.714457	1.651720	0.000000
	6 B	2.824274	1.747867	1.738772	1.721183	1.728472
	7 C	1.443845	3.681931	2.661878	2.724013	3.150194
	8 B	3.138350	1.742517	2.786733	3.336488	2.693317
	9 B	2.600614	2.965342	3.230633	3.241175	2.857765
	10 B	3.286613	1.716179	3.372434	2.933378	1.700834
	11 B	2.038122	2.896114	2.863237	1.881131	1.723506
	12 C	2.776166	1.697573	1.647961	2.704718	2.600312
	13 C	1.517573	4.993002	2.634596	2.632846	4.092553
	14 C	2.517337	5.161038	3.967939	3.942440	4.497596
	15 C	4.052732	2.750871	2.682289	4.043931	3.988924
16 C	4.163652	2.783122	4.076152	2.673424	1.521411	
 Me4C4B8H8_14 -515.4382818 C_s	6	7	8	9	10	
	7 C	3.624770	0.000000			
	8 B	2.788151	2.748412	0.000000		
	9 B	3.627174	1.496812	1.816986	0.000000	
	10 B	2.853250	2.820771	1.731101	1.752455	0.000000
	11 B	2.917449	1.788801	2.814689	1.858798	1.863604
	12 C	1.681048	3.156944	1.606709	2.934945	2.683433
	13 C	3.956093	2.536185	4.641382	3.947138	4.727299
	14 C	5.076201	1.506515	4.112449	2.576036	4.096036
	15 C	2.722730	4.489816	2.672810	4.255837	4.028212
	16 C	2.802878	4.462591	4.062424	4.128645	2.734184
	11	12	13	14	15	
	12 C	3.179102	0.000000			
	13 C	3.190426	4.128036	0.000000		
	14 C	2.891549	4.619522	2.838760	0.000000	
	15 C	4.701954	1.523690	5.221829	5.862315	0.000000
16 C	2.763179	3.999379	5.158852	5.645190	5.243793	

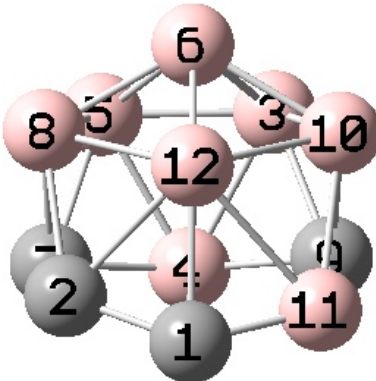
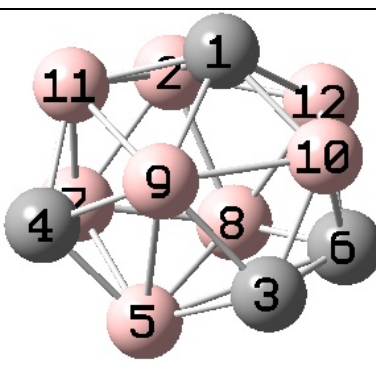
		13 C	3.643301	2.602206	2.602225	1.522095	3.983732
		14 C	2.833117	4.451366	2.593872	4.003725	4.318020
		15 C	4.869948	2.593877	4.451273	4.003734	1.526120
		16 C	2.754349	3.690919	3.691000	2.638561	4.153633
			6	7	8	9	10
		7 B	2.765577	0.000000			
		8 C	1.673984	3.369520	0.000000		
		9 C	3.108965	1.712616	2.785498	0.000000	
		10 B	1.828924	1.755899	2.818242	2.766625	0.000000
		11 B	1.828933	2.856979	1.631133	2.766621	1.780696
		12 B	2.794454	1.736210	2.749110	1.682681	1.746042
		13 C	4.395332	3.643313	3.983719	2.640214	4.855214
		14 C	2.757888	4.869948	1.526121	4.224917	4.061634
		15 C	2.757907	2.833113	4.318030	4.224925	2.588786
		16 C	4.629655	2.754338	4.153632	1.522149	4.072425
			11	12	13	14	15
		12 B	1.746037	0.000000			
		13 C	4.855215	4.276604	0.000000		
		14 C	2.588796	4.049549	5.161232	0.000000	
		15 C	4.061646	4.049546	5.161249	5.500704	0.000000
		16 C	4.072426	2.682480	2.898245	5.470860	5.470847
 Me4C4B8H8_15 -515.4368847 C₁			1	2	3	4	5
		1 B	0.000000				
		2 C	1.721775	0.000000			
		3 B	2.845185	2.751630	0.000000		
		4 B	1.719001	2.727906	1.774532	0.000000	
		5 B	3.355324	2.735860	1.751448	2.800018	0.000000
		6 B	3.267846	3.182310	2.966649	2.964842	1.796922
		7 C	2.740405	2.605740	3.657637	3.256864	2.699438
		8 B	2.959056	3.298967	1.724230	1.769392	1.728065
		9 B	1.861187	2.768781	2.913271	1.796166	2.827079
		10 C	2.692645	1.559384	1.735629	2.709445	1.596767
		11 B	1.738208	1.696633	1.730619	1.769544	2.800276
		12 C	1.750132	1.520898	3.511208	2.947360	3.083400
		13 C	4.026098	2.616757	2.781967	4.087568	2.643442
		14 C	3.946113	3.914197	5.145337	4.598059	4.069551
		15 C	2.658710	2.579449	4.958910	4.197840	4.574116
		16 C	2.816953	1.520781	4.009011	4.066378	4.054780
			6	7	8	9	10
		7 C	1.489967	0.000000			
		8 B	1.755291	2.817375	0.000000		
		9 B	1.895478	1.802107	1.906119	0.000000	
		10 C	2.881342	3.043890	2.680426	3.136551	0.000000
		11 B	3.637779	3.620100	2.852986	2.908734	1.721580
		12 C	2.595572	1.447846	3.272106	2.021419	2.640814
		13 C	4.182609	4.348752	4.020911	4.655017	1.520741
		14 C	2.576176	1.509429	4.105991	2.903561	4.500336

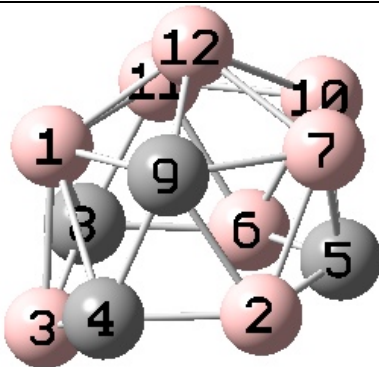
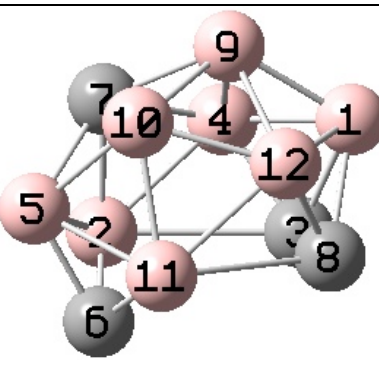
	15 C	3.931477	2.520376	4.732394	3.192820	3.979912
	16 C	4.608956	3.826430	4.800876	4.191170	2.632245
		11	12	13	14	15
	11 B	0.000000				
	12 C	2.798579	0.000000			
	13 C	2.756054	3.894222	0.000000		
	14 C	5.069565	2.522428	5.698036	0.000000	
	15 C	3.949393	1.518771	5.017338	2.807823	0.000000
	16 C	2.667925	2.569190	2.936491	4.881459	2.860840

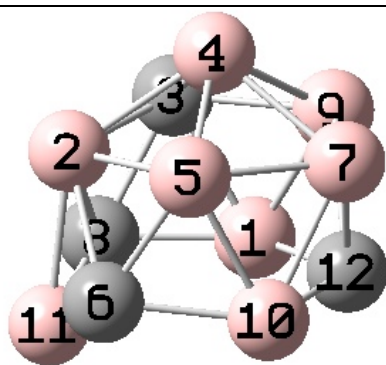
Table S10. Distance table for the lowest-lying C₄Et₄B₈H₈ structures. For clarity, only the polyhedral framework is presented.

 1. -672.57887200 Cs	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.252885</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>1.721872</td><td>3.596064</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.678791</td><td>2.857584</td><td>1.710419</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.761146</td><td>1.527515</td><td>2.798498</td><td>1.645346</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.720159</td><td>2.539531</td><td>1.755651</td><td>1.772380</td><td>1.657565</td></tr><tr><td>7 B</td><td>1.722396</td><td>3.595252</td><td>1.748409</td><td>2.841756</td><td>3.514115</td></tr><tr><td>8 B</td><td>2.720341</td><td>2.538341</td><td>2.818055</td><td>3.364602</td><td>3.150301</td></tr><tr><td>9 B</td><td>1.678165</td><td>2.856970</td><td>2.841737</td><td>2.944838</td><td>3.212372</td></tr><tr><td>10 C</td><td>2.761342</td><td>1.526842</td><td>3.514732</td><td>3.213004</td><td>2.585492</td></tr><tr><td>11 B</td><td>1.774473</td><td>1.880118</td><td>2.877616</td><td>1.875177</td><td>1.773102</td></tr><tr><td>12 C</td><td>2.605688</td><td>2.973450</td><td>1.685181</td><td>2.701943</td><td>2.821835</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>2.816617</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.776946</td><td>1.755557</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>3.364393</td><td>1.711127</td><td>1.772864</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>3.150651</td><td>2.798171</td><td>1.656483</td><td>1.645557</td><td>0.000000</td></tr><tr><td>11 B</td><td>2.744335</td><td>2.878026</td><td>2.744550</td><td>1.875446</td><td>1.774336</td></tr><tr><td>12 C</td><td>1.633232</td><td>1.683852</td><td>1.633725</td><td>2.702130</td><td>2.821665</td></tr><tr><th></th><th>11</th><th>12</th></tr><tr><td>12 C</td><td>3.094879</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	3.252885	0.000000				3 B	1.721872	3.596064	0.000000			4 B	1.678791	2.857584	1.710419	0.000000		5 C	2.761146	1.527515	2.798498	1.645346	0.000000	6 B	2.720159	2.539531	1.755651	1.772380	1.657565	7 B	1.722396	3.595252	1.748409	2.841756	3.514115	8 B	2.720341	2.538341	2.818055	3.364602	3.150301	9 B	1.678165	2.856970	2.841737	2.944838	3.212372	10 C	2.761342	1.526842	3.514732	3.213004	2.585492	11 B	1.774473	1.880118	2.877616	1.875177	1.773102	12 C	2.605688	2.973450	1.685181	2.701943	2.821835		6	7	8	9	10	6 B	0.000000					7 B	2.816617	0.000000				8 B	2.776946	1.755557	0.000000			9 B	3.364393	1.711127	1.772864	0.000000		10 C	3.150651	2.798171	1.656483	1.645557	0.000000	11 B	2.744335	2.878026	2.744550	1.875446	1.774336	12 C	1.633232	1.683852	1.633725	2.702130	2.821665		11	12	12 C	3.094879	0.000000
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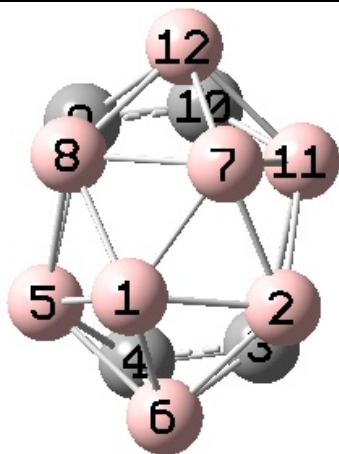
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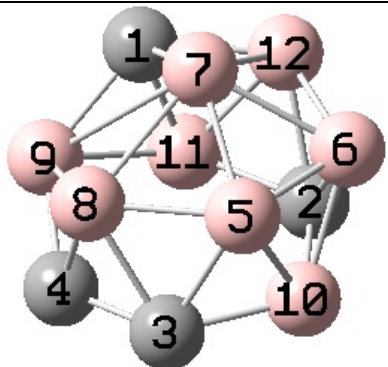
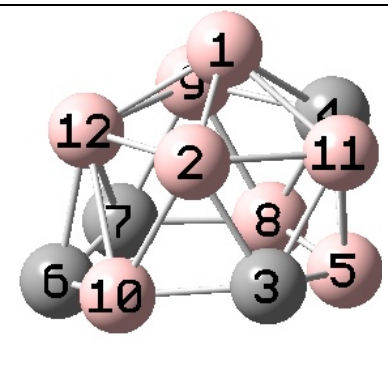
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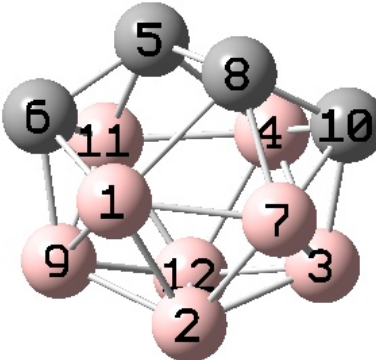
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6 C	3.188998	1.744519	3.104375	2.829512	1.643278	
7 B	2.835084	2.853876	2.757630	1.781189	1.726331	
8 C	1.588309	1.992142	1.652950	2.909885	3.297119	
9 B	1.772932	2.891154	1.670759	1.774297	2.857718	
10 B	2.751557	2.722974	3.226876	2.803573	1.780524	
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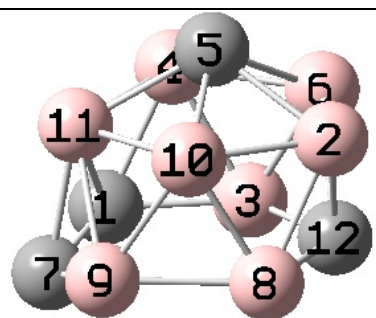
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12 B	3.977326	1.739259	1.783424	1.721131	1.650614	
	11	12				
12 B	1.835495	0.000000				

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 12. -672.55444100 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.722416</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.698383</td><td>1.657082</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>1.734519</td><td>2.747818</td><td>2.640031</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>2.821148</td><td>2.760489</td><td>1.614848</td><td>1.734999</td><td>0.000000</td></tr><tr><td>6 C</td><td>3.224287</td><td>2.837545</td><td>2.771230</td><td>3.484627</td><td>3.124690</td></tr><tr><td>7 C</td><td>2.957768</td><td>3.316809</td><td>3.188727</td><td>2.735414</td><td>2.809574</td></tr><tr><td>8 B</td><td>2.848733</td><td>3.436358</td><td>2.866935</td><td>1.681747</td><td>1.708442</td></tr><tr><td>9 B</td><td>1.726277</td><td>2.949124</td><td>3.310299</td><td>1.646854</td><td>2.785867</td></tr><tr><td>10 B</td><td>2.949673</td><td>1.808545</td><td>1.654585</td><td>3.406684</td><td>2.741359</td></tr><tr><td>11 B</td><td>1.779268</td><td>1.727818</td><td>1.651638</td><td>1.677778</td><td>1.790690</td></tr><tr><td>12 B</td><td>1.765046</td><td>1.884582</td><td>2.772201</td><td>2.787064</td><td>3.221100</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>1.440479</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>2.687202</td><td>1.634080</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>2.721601</td><td>1.743446</td><td>1.768418</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>1.508040</td><td>2.577268</td><td>3.160244</td><td>3.241495</td><td>0.000000</td></tr><tr><td>11 B</td><td>3.671343</td><td>3.574690</td><td>2.861060</td><td>2.830528</td><td>2.879834</td></tr><tr><td>12 B</td><td>1.770152</td><td>2.006582</td><td>2.873424</td><td>1.875711</td><td>1.969760</td></tr><tr><th></th><th>11</th><th>12</th><th></th><th></th><th></th></tr><tr><td>12 B</td><td>2.901499</td><td>0.000000</td><td></td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.722416	0.000000				3 C	2.698383	1.657082	0.000000			4 C	1.734519	2.747818	2.640031	0.000000		5 B	2.821148	2.760489	1.614848	1.734999	0.000000	6 C	3.224287	2.837545	2.771230	3.484627	3.124690	7 C	2.957768	3.316809	3.188727	2.735414	2.809574	8 B	2.848733	3.436358	2.866935	1.681747	1.708442	9 B	1.726277	2.949124	3.310299	1.646854	2.785867	10 B	2.949673	1.808545	1.654585	3.406684	2.741359	11 B	1.779268	1.727818	1.651638	1.677778	1.790690	12 B	1.765046	1.884582	2.772201	2.787064	3.221100		6	7	8	9	10	6 C	0.000000					7 C	1.440479	0.000000				8 B	2.687202	1.634080	0.000000			9 B	2.721601	1.743446	1.768418	0.000000		10 B	1.508040	2.577268	3.160244	3.241495	0.000000	11 B	3.671343	3.574690	2.861060	2.830528	2.879834	12 B	1.770152	2.006582	2.873424	1.875711	1.969760		11	12				12 B	2.901499	0.000000									
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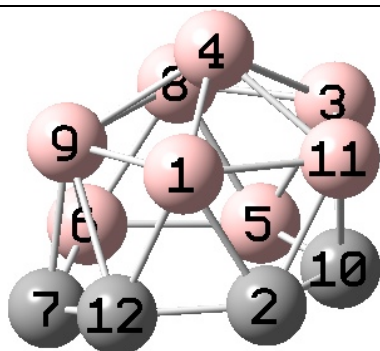
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9 B	1.809884	1.742163	2.896695	2.891843	2.632343
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9 B	1.656351	2.921622	3.112198	0.000000	
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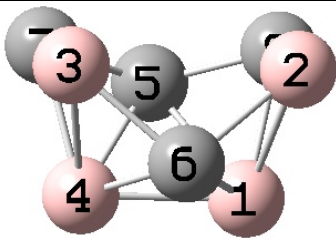
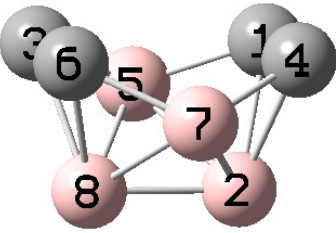
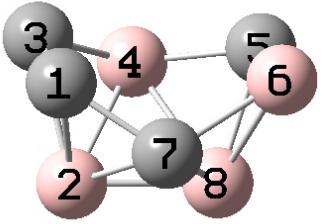
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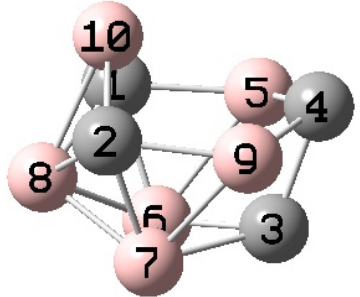
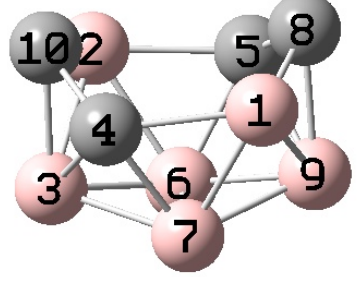
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3 B	2.842850	2.765377	0.000000		
4 B	1.719475	2.730523	1.772513	0.000000	
5 B	3.350392	2.751077	1.749218	2.797444	0.000000
6 B	3.272072	3.199168	2.958746	2.962717	1.790278
7 C	2.755024	2.616120	3.651214	3.262744	2.682450
8 B	2.954069	3.306871	1.720051	1.764677	1.728181
9 B	1.862600	2.766556	2.921205	1.809271	2.828233
10 C	2.697032	1.580120	1.745498	2.719351	1.596805
11 B	1.735580	1.692549	1.729043	1.771587	2.790350
12 C	1.734561	1.543746	3.513815	2.931417	3.090108
	6	7	8	9	10
6 B	0.000000				
7 C	1.485438	0.000000			
8 B	1.747064	2.808734	0.000000		
9 B	1.896990	1.799690	1.913435	0.000000	
10 C	2.884730	3.040141	2.686640	3.145839	0.000000
11 B	3.631842	3.618405	2.846384	2.912166	1.720673
12 C	2.595797	1.451478	3.256256	1.978105	2.666486
	11	12			
11 B	0.000000				
12 C	2.800828	0.000000			

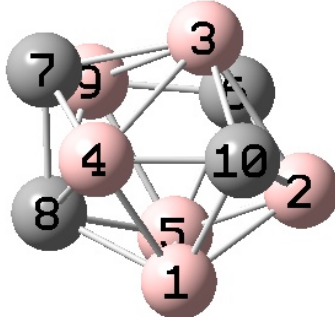
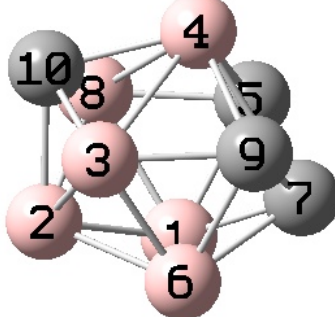
Table S11. Distance table for the lowest-lying B₄Et₄C₄H₄ structures. For clarity, only the polyhedral framework is presented.

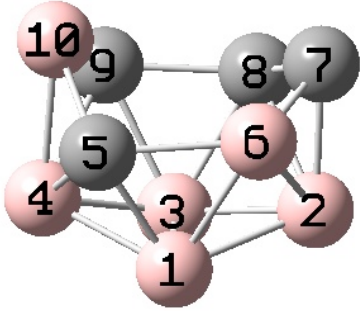
 1. -570.607768 0.0 C_s	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.848348</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.808567</td><td>2.477725</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.804877</td><td>2.807825</td><td>1.847043</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>1.804705</td><td>2.492062</td><td>2.492145</td><td>1.803820</td><td>0.000000</td></tr><tr><td>6 C</td><td>1.690267</td><td>1.622336</td><td>1.622533</td><td>1.690046</td><td>2.514579</td></tr><tr><td>7 C</td><td>2.723562</td><td>2.935698</td><td>1.501216</td><td>1.666327</td><td>1.496597</td></tr><tr><td>8 C</td><td>1.666017</td><td>1.501475</td><td>2.936722</td><td>2.722291</td><td>1.496533</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.458247</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.457881</td><td>2.569815</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.848348	0.000000				3 B	2.808567	2.477725	0.000000			4 B	1.804877	2.807825	1.847043	0.000000		5 C	1.804705	2.492062	2.492145	1.803820	0.000000	6 C	1.690267	1.622336	1.622533	1.690046	2.514579	7 C	2.723562	2.935698	1.501216	1.666327	1.496597	8 C	1.666017	1.501475	2.936722	2.722291	1.496533		6	7	8			6 C	0.000000					7 C	2.458247	0.000000				8 C	2.457881	2.569815	0.000000		
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 2. -570.600942 +4.3 C_{2v}	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.745576</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.605553</td><td>2.739496</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>1.385483</td><td>1.746355</td><td>2.948836</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.586850</td><td>1.898283</td><td>1.587457</td><td>2.525099</td><td>0.000000</td></tr><tr><td>6 C</td><td>2.952545</td><td>2.737356</td><td>1.385319</td><td>2.604926</td><td>2.525755</td></tr><tr><td>7 B</td><td>2.525559</td><td>1.894159</td><td>2.525275</td><td>1.586795</td><td>2.785529</td></tr><tr><td>8 B</td><td>2.736660</td><td>1.708189</td><td>1.745172</td><td>2.738873</td><td>1.893511</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 B</td><td>1.587065</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.745123</td><td>1.898242</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.745576	0.000000				3 C	2.605553	2.739496	0.000000			4 C	1.385483	1.746355	2.948836	0.000000		5 B	1.586850	1.898283	1.587457	2.525099	0.000000	6 C	2.952545	2.737356	1.385319	2.604926	2.525755	7 B	2.525559	1.894159	2.525275	1.586795	2.785529	8 B	2.736660	1.708189	1.745172	2.738873	1.893511		6	7	8			6 C	0.000000					7 B	1.587065	0.000000				8 B	1.745123	1.898242	0.000000		
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 3. -570.593247 +9.1 C₁	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.736620</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>1.392773</td><td>1.757424</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>2.504089</td><td>1.923660</td><td>1.575366</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.966954</td><td>2.766112</td><td>2.658165</td><td>1.610932</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.606517</td><td>2.880497</td><td>3.021319</td><td>2.642927</td><td>1.477647</td></tr><tr><td>7 C</td><td>1.486045</td><td>1.757366</td><td>2.407388</td><td>2.650449</td><td>2.458970</td></tr><tr><td>8 B</td><td>2.689830</td><td>1.735716</td><td>2.721667</td><td>1.891430</td><td>1.660824</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th></th><th></th></tr><tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>1.645943</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>1.864296</td><td>1.769055</td><td>0.000000</td><td></td><td></td></tr></table>		1	2	3	4	5	1 C	0.000000					2 B	1.736620	0.000000				3 C	1.392773	1.757424	0.000000			4 B	2.504089	1.923660	1.575366	0.000000		5 C	2.966954	2.766112	2.658165	1.610932	0.000000	6 B	2.606517	2.880497	3.021319	2.642927	1.477647	7 C	1.486045	1.757366	2.407388	2.650449	2.458970	8 B	2.689830	1.735716	2.721667	1.891430	1.660824		6	7	8			6 B	0.000000					7 C	1.645943	0.000000				8 B	1.864296	1.769055	0.000000		
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	3 C	1.764331	1.735469	0.000000		
	4 B	1.860130	2.847877	1.606985	0.000000	
	5 B	2.848023	1.859727	2.552718	3.062610	0.000000
	6 C	1.735592	1.764195	2.507724	2.552655	1.606961
	7 C	2.725898	1.656084	1.543676	2.613862	1.486784
	8 C	1.655904	2.725622	2.420625	1.486709	2.614232
		6	7	8		
	6 C	0.000000				
	7 C	2.420709	0.000000			
	8 C	1.543665	2.932707	0.000000		

Table S12. Distance table for the lowest-lying B₆C₄Et₁₀ structures (and relation to B₆C₄H₁₀). For clarity, only the polyhedral framework is presented.

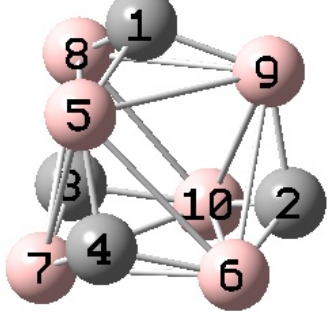
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 2. -1092.720431 +0.7 C₂ (from B6C4-5)	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>3.130096</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.984481</td><td>1.844142</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>1.781784</td><td>2.501677</td><td>1.758283</td><td>0.000000</td><td></td></tr><tr><td>5 C</td><td>2.503449</td><td>1.784141</td><td>2.868407</td><td>3.002714</td><td>0.000000</td></tr><tr><td>6 B</td><td>2.844021</td><td>1.834525</td><td>1.786295</td><td>2.721235</td><td>1.693624</td></tr><tr><td>7 B</td><td>1.843291</td><td>2.844839</td><td>1.798673</td><td>1.701797</td><td>2.723216</td></tr><tr><td>8 C</td><td>1.517807</td><td>2.715775</td><td>3.414207</td><td>2.730540</td><td>1.454879</td></tr><tr><td>9 B</td><td>1.851565</td><td>2.987631</td><td>2.988911</td><td>2.868700</td><td>1.765089</td></tr><tr><td>10 C</td><td>2.721956</td><td>1.516596</td><td>1.701563</td><td>1.461018</td><td>2.735719</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>1.848450</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.660692</td><td>2.701544</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>1.795151</td><td>1.780332</td><td>1.710313</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>2.700285</td><td>2.672851</td><td>2.939806</td><td>3.423646</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	3.130096	0.000000				3 B	2.984481	1.844142	0.000000			4 C	1.781784	2.501677	1.758283	0.000000		5 C	2.503449	1.784141	2.868407	3.002714	0.000000	6 B	2.844021	1.834525	1.786295	2.721235	1.693624	7 B	1.843291	2.844839	1.798673	1.701797	2.723216	8 C	1.517807	2.715775	3.414207	2.730540	1.454879	9 B	1.851565	2.987631	2.988911	2.868700	1.765089	10 C	2.721956	1.516596	1.701563	1.461018	2.735719		6	7	8	9	10	6 B	0.000000					7 B	1.848450	0.000000				8 C	2.660692	2.701544	0.000000			9 B	1.795151	1.780332	1.710313	0.000000		10 C	2.700285	2.672851	2.939806	3.423646	0.000000
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1 B	0.000000																																																																																																						
2 B	3.130096	0.000000																																																																																																					
3 B	2.984481	1.844142	0.000000																																																																																																				
4 C	1.781784	2.501677	1.758283	0.000000																																																																																																			
5 C	2.503449	1.784141	2.868407	3.002714	0.000000																																																																																																		
6 B	2.844021	1.834525	1.786295	2.721235	1.693624																																																																																																		
7 B	1.843291	2.844839	1.798673	1.701797	2.723216																																																																																																		
8 C	1.517807	2.715775	3.414207	2.730540	1.454879																																																																																																		
9 B	1.851565	2.987631	2.988911	2.868700	1.765089																																																																																																		
10 C	2.721956	1.516596	1.701563	1.461018	2.735719																																																																																																		
	6	7	8	9	10																																																																																																		
6 B	0.000000																																																																																																						
7 B	1.848450	0.000000																																																																																																					
8 C	2.660692	2.701544	0.000000																																																																																																				
9 B	1.795151	1.780332	1.710313	0.000000																																																																																																			
10 C	2.700285	2.672851	2.939806	3.423646	0.000000																																																																																																		

	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 B</td><td>1.792680</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 B</td><td>2.679427</td><td>2.038896</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 B</td><td>1.863552</td><td>2.771247</td><td>2.078354</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.787963</td><td>1.798911</td><td>2.678918</td><td>2.901287</td><td>0.000000</td></tr><tr><td>6 C</td><td>2.739824</td><td>1.643707</td><td>1.706233</td><td>3.130560</td><td>1.680940</td></tr><tr><td>7 C</td><td>2.745351</td><td>3.132971</td><td>1.789631</td><td>1.604278</td><td>2.742585</td></tr><tr><td>8 C</td><td>1.738008</td><td>2.761832</td><td>2.618159</td><td>1.800714</td><td>1.726541</td></tr><tr><td>9 B</td><td>2.936791</td><td>2.795969</td><td>2.065373</td><td>2.781191</td><td>1.904042</td></tr><tr><td>10 C</td><td>1.695660</td><td>1.633175</td><td>1.683490</td><td>1.597825</td><td>2.739893</td></tr><tr><th></th><th>6</th><th>7</th><th>8</th><th>9</th><th>10</th></tr><tr><td>6 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7 C</td><td>2.588195</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 C</td><td>2.630738</td><td>1.639383</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>1.600485</td><td>1.594696</td><td>1.822687</td><td>0.000000</td><td></td></tr><tr><td>10 C</td><td>2.604400</td><td>2.578313</td><td>2.641191</td><td>3.129935</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 B	0.000000					2 B	1.792680	0.000000				3 B	2.679427	2.038896	0.000000			4 B	1.863552	2.771247	2.078354	0.000000		5 B	1.787963	1.798911	2.678918	2.901287	0.000000	6 C	2.739824	1.643707	1.706233	3.130560	1.680940	7 C	2.745351	3.132971	1.789631	1.604278	2.742585	8 C	1.738008	2.761832	2.618159	1.800714	1.726541	9 B	2.936791	2.795969	2.065373	2.781191	1.904042	10 C	1.695660	1.633175	1.683490	1.597825	2.739893		6	7	8	9	10	6 C	0.000000					7 C	2.588195	0.000000				8 C	2.630738	1.639383	0.000000			9 B	1.600485	1.594696	1.822687	0.000000		10 C	2.604400	2.578313	2.641191	3.129935	0.000000
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	1	2	3	4	5																																																																																																		
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5. -1092.697652 +14.9 C₁
(from B6C4-3)

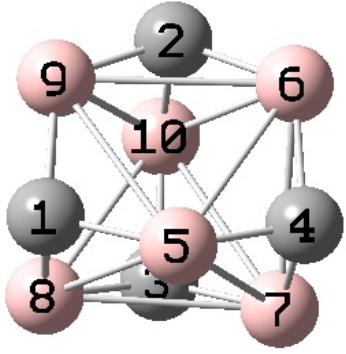
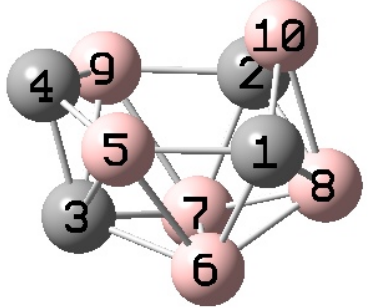
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4 B	1.759808	2.940907	1.749945	0.000000	
5 C	1.707613	2.875392	2.737052	1.702559	0.000000
6 B	1.870867	1.881240	2.860155	2.885779	1.739947
7 C	2.723956	1.652364	2.700585	3.367288	2.783610
8 C	2.753630	1.789158	1.759799	2.795787	3.010993
9 C	2.751931	2.848001	1.754552	1.758804	2.482587
10 B	2.781740	3.416564	2.807324	1.835210	1.549883
	6	7	8	9	10
6 B	0.000000				
7 C	1.532410	0.000000			
8 C	2.508027	1.473213	0.000000		
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10 B	2.617939	2.882553	2.641846	1.567920	0.000000

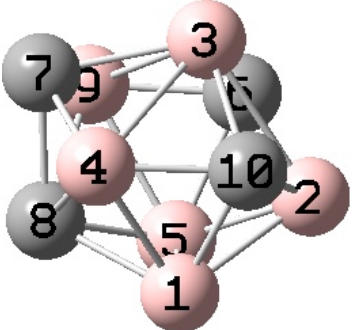
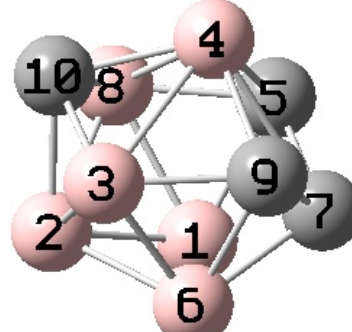
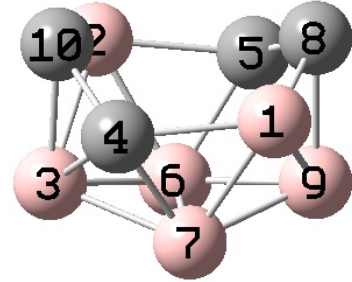


6. -1092.692946 +17.9 C_s
(from B6C4-4)

	1	2	3	4	5
1 C	0.000000				
2 C	2.776717	0.000000			
3 C	2.744801	2.764029	0.000000		
4 C	2.742135	2.718620	2.772549	0.000000	
5 B	1.592404	3.141342	2.957079	1.576977	0.000000
6 B	3.103671	1.590314	3.142496	1.594041	2.610768
7 B	3.097524	2.962577	1.588892	1.599690	2.437532
8 B	1.594926	3.050742	1.597529	3.146291	2.471332
9 B	1.584159	1.608707	3.071527	3.004573	2.552605
10 B	3.002765	1.589289	1.614028	3.131357	3.515993
	6	7	8	9	10
6 B	0.000000				
7 B	2.463960	0.000000			
8 B	3.612803	2.624105	0.000000		
9 B	2.481661	3.481064	2.464711	0.000000	
10 B	2.624527	2.496052	2.386947	2.435134	0.000000

Table S13. Distance table for the lowest-lying B₆Et₆C₄Me₄ structures (and relation to B₆C₄H₁₀). For clarity, only the polyhedral framework is presented.

 1. -935.677692 0.0 C_{3v} (from B6C4-4)	<table><tr><th></th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th></tr><tr><td>1 C</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2 C</td><td>2.745315</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3 C</td><td>2.743510</td><td>2.739537</td><td>0.000000</td><td></td><td></td></tr><tr><td>4 C</td><td>2.739519</td><td>2.732976</td><td>2.741230</td><td>0.000000</td><td></td></tr><tr><td>5 B</td><td>1.581052</td><td>3.061926</td><td>3.062470</td><td>1.591348</td><td>0.000000</td></tr><tr><td>6 B</td><td>3.059415</td><td>1.584083</td><td>3.074506</td><td>1.585412</td><td>2.500048</td></tr><tr><td>7 B</td><td>3.035920</td><td>3.080529</td><td>1.588967</td><td>1.585872</td><td>2.473698</td></tr><tr><td>8 B</td><td>1.587319</td><td>3.053408</td><td>1.590321</td><td>3.073900</td><td>2.511056</td></tr><tr><td>9 B</td><td>1.587528</td><td>1.586035</td><td>3.026084</td><td>3.078998</td><td>2.526723</td></tr><tr><td>10 B</td><td>3.062921</td><td>1.588937</td><td>1.586718</td><td>3.067018</td><td>3.541714</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>2.538631</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8 B</td><td>3.544402</td><td>2.488934</td><td>0.000000</td><td></td><td></td></tr><tr><td>9 B</td><td>2.521077</td><td>3.526840</td><td>2.452458</td><td>0.000000</td><td></td></tr><tr><td>10 B</td><td>2.522228</td><td>2.535327</td><td>2.487981</td><td>2.460826</td><td>0.000000</td></tr></table>		1	2	3	4	5	1 C	0.000000					2 C	2.745315	0.000000				3 C	2.743510	2.739537	0.000000			4 C	2.739519	2.732976	2.741230	0.000000		5 B	1.581052	3.061926	3.062470	1.591348	0.000000	6 B	3.059415	1.584083	3.074506	1.585412	2.500048	7 B	3.035920	3.080529	1.588967	1.585872	2.473698	8 B	1.587319	3.053408	1.590321	3.073900	2.511056	9 B	1.587528	1.586035	3.026084	3.078998	2.526723	10 B	3.062921	1.588937	1.586718	3.067018	3.541714		6	7	8	9	10	6 B	0.000000					7 B	2.538631	0.000000				8 B	3.544402	2.488934	0.000000			9 B	2.521077	3.526840	2.452458	0.000000		10 B	2.522228	2.535327	2.487981	2.460826	0.000000
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9 B	2.521077	3.526840	2.452458	0.000000																																																																																																			
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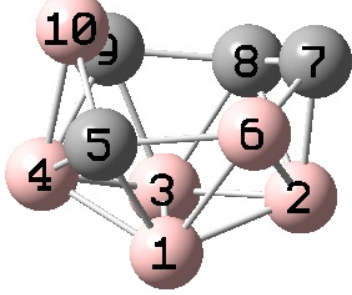
5. -935.663785 +8.7 C₂ (from B6C4-5)	<pre> 8 C 1.515363 2.693099 3.410791 2.735664 1.454050 9 B 1.864557 2.984071 2.990181 2.857108 1.751473 10 C 2.685910 1.513352 1.708003 1.461790 2.742036 6 7 8 9 10 6 B 0.000000 7 B 1.845712 0.000000 8 C 2.661983 2.703017 0.000000 9 B 1.800376 1.775516 1.712334 0.000000 10 C 2.703686 2.674959 2.924713 3.418239 0.000000 </pre>
 6. -935.657671 +12.6 C (from B6C4-3)	<pre> 1 2 3 4 5 1 B 0.000000 2 B 1.799904 0.000000 3 B 1.822117 1.805713 0.000000 4 B 1.768792 2.932676 1.750496 0.000000 5 C 1.696047 2.856670 2.733458 1.695399 0.000000 6 B 1.922771 1.906842 2.887115 2.896060 1.736420 7 C 2.742175 1.649733 2.711987 3.370201 2.803234 8 C 2.747397 1.777752 1.759220 2.776962 3.010146 9 C 2.732567 2.805031 1.748939 1.745622 2.475959 10 B 2.757631 3.334803 2.802989 1.864792 1.538562 6 7 8 9 10 6 B 0.000000 7 C 1.530236 0.000000 8 C 2.500567 1.472663 0.000000 9 C 2.964578 2.623932 1.598081 0.000000 10 B 2.495855 2.786675 2.572593 1.567056 0.000000 </pre>

Table S14. Orbital energies and HOMO/LUMO gaps.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO Gap (Hartree)	HOMO/LUMO Gap Gap (eV)
B2C4-1	-0.307627	0.051796	-0.359423	9.78
B2C4-2	-0.327170	-0.095576	-0.231594	6.30
B2C4-3	-0.313655	0.046717	-0.360372	9.81
B3C4-1	-0.325320	-0.006526	-0.318794	8.67
B3C4-2	-0.307194	-0.015642	-0.291552	7.93
B3C4-3	-0.315700	-0.035427	-0.280273	7.63
B3C4-4	-0.320786	-0.020930	-0.299856	8.16
B3C4-5	-0.315701	-0.021085	-0.294616	8.02
B3C4-6	-0.294780	0.012408	-0.307188	8.36
B4C4-1	-0.298092	0.022540	-0.320632	8.72
B4C4-2	-0.326801	-0.037576	-0.289225	7.87
B4C4-3	-0.305172	-0.016623	-0.288549	7.85
B4C4-4	-0.284500	0.002480	-0.286980	7.81
B4C4-5	-0.307459	0.002967	-0.310426	8.45
B4C4-6	-0.295411	-0.008697	-0.286714	7.80
B4C4-7	-0.297301	-0.021632	-0.275669	7.50
B5C4-1	-0.273720	0.032800	-0.306520	8.34
B5C4-2	-0.288305	-0.000236	-0.288069	7.84
B5C4-3	-0.309628	-0.034625	-0.275003	7.48
B5C4-4	-0.259711	-0.005283	-0.254428	6.92
B5C4-5	-0.315350	0.024691	-0.340041	9.25
B5C4-6	-0.302057	0.008763	-0.310820	8.46
B5C4-7	-0.290632	-0.042904	-0.247728	6.74
B5C4-8	-0.300985	-0.004845	-0.296140	8.06
B6C4-1	-0.307212	-0.004851	-0.302361	8.23
B6C4-2	-0.292429	0.021276	-0.313705	8.54
B6C4-3	-0.298783	-0.019784	-0.278999	7.59
B6C4-4	-0.337951	-0.027450	-0.310501	8.45
B6C4-5	-0.311228	-0.043704	-0.267524	7.28
B6C4-6	-0.281918	0.012659	-0.294577	8.02
B6C4-7	-0.307963	-0.031429	-0.276534	7.52
B6C4-8	-0.313394	-0.042625	-0.270769	7.37
B7C4-1	-0.292606	0.022919	-0.315525	8.59
B7C4-2	-0.310352	0.021711	-0.332063	9.04
B7C4-3	-0.290849	0.021688	-0.312537	8.50
B7C4-4	-0.299613	0.019071	-0.318684	8.67
B7C4-5	-0.294364	0.023060	-0.317424	8.64
B7C4-6	-0.283569	0.018941	-0.302510	8.23

B7C4-7	-0.292237	0.014528	-0.306765	8.35
B8C4-1	-0.287133	-0.008617	-0.278516	7.58
B8C4-2	-0.322697	-0.035045	-0.287652	7.83
B8C4-3	-0.287349	-0.003667	-0.283682	7.72
B8C4-4	-0.296488	-0.012108	-0.284380	7.74
B8C4-5	-0.310526	-0.048737	-0.261789	7.12
B8C4-6	-0.291541	0.003565	-0.295106	8.03
B8C4-7	-0.292254	0.007680	-0.299934	8.16
B8C4-8	-0.300427	-0.024149	-0.276278	7.52
B8C4-9	-0.297835	-0.035945	-0.261890	7.13
B8C4-10	-0.291823	-0.030599	-0.261224	7.11
B8C4-11	-0.304585	-0.048985	-0.255600	6.96
B8C4-12	-0.293433	-0.044735	-0.248698	6.77
B8C4-13	-0.310228	-0.042127	-0.268101	7.30
B8C4-14	-0.307270	-0.020746	-0.286524	7.80
B8C4-15	-0.320574	-0.046911	-0.273663	7.45
B8C4-1_Me	-0.271945	-0.008702	-0.263243	7.16
B8C4-2_Me	-0.307072	-0.041314	-0.265758	7.23
B8C4-3_Me	-0.293248	-0.042486	-0.250762	6.82
B8C4-4_Me	-0.275599	-0.000340	-0.275259	7.49
B8C4-5_Me	-0.279092	-0.006675	-0.272417	7.41
B8C4-6_Me	-0.271146	0.010771	-0.281917	7.67
B8C4-7_Me	-0.269273	0.012533	-0.281806	7.67
B8C4-8_Me	-0.283710	-0.042725	-0.240985	6.56
B8C4-9_Me	-0.287172	-0.011692	-0.275480	7.50
B8C4-10_Me	-0.297331	-0.030625	-0.266706	7.26
B8C4-11_Me	-0.281733	-0.018930	-0.262803	7.15
B8C4-12_Me	-0.286842	-0.016546	-0.270296	7.36
B8C4-13_Me	-0.277210	-0.040222	-0.236988	6.45
B8C4-14_Me	-0.273935	-0.028759	-0.245176	6.67
B8C4-15_Me	-0.294800	-0.034604	-0.260196	7.08
B8C4-1_Et	-0.268320	-0.005402	-0.262918	7.15
B8C4-2_Et	-0.271676	0.003563	-0.275239	7.49
B8C4-3_Et	-0.268450	0.013626	-0.282076	7.68
B8C4-4_Et	-0.290503	-0.040718	-0.249785	6.80
B8C4-5_Et	-0.304132	-0.040737	-0.263395	7.17
B8C4-6_Et	-0.266996	0.012539	-0.279535	7.61
B8C4-7_Et	-0.279801	-0.008047	-0.271754	7.39
B8C4-8_Et	-0.282933	-0.014919	-0.268014	7.29
B8C4-9_Et	-0.278186	-0.006902	-0.271284	7.38
B8C4-10_Et	-0.296129	-0.032398	-0.263731	7.18
B8C4-11_Et	-0.276342	-0.012866	-0.263476	7.17

B8C4-12_Et	-0.280096	-0.040652	-0.239444	6.52
B8C4-13_Et	-0.277317	0.003891	-0.281208	7.65
B8C4-14_Et	-0.273272	-0.037981	-0.235291	6.40
B8C4-15_Et	-0.290554	-0.031137	-0.259417	7.06
B9C4-1	-0.321305	-0.026641	-0.294664	8.02
B9C4-2	-0.326236	-0.028889	-0.297347	8.09
B9C4-3	-0.324831	-0.033394	-0.291437	7.93
B9C4-4	-0.291919	-0.026486	-0.265433	7.22
B9C4-5	-0.272859	0.015200	-0.288059	7.84
B9C4-6	-0.291502	-0.032037	-0.259465	7.06
B9C4-7	-0.305385	-0.015311	-0.290074	7.89
B9C4-8	-0.322023	-0.007504	-0.314519	8.56
B9C4-9	-0.307913	-0.059396	-0.248517	6.76
B9C4-10	-0.319454	-0.047739	-0.271715	7.39
B9C4-11	-0.295942	-0.060819	-0.235123	6.40