

## Supporting Information

# Cyclopentadienylcobalt Azaboranes Violating the Wade-Mingos Rules: A Degree 3 Vertex For the Nitrogen Atom

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<sup>2</sup>*Department of Chemistry and Center for Computational Quantum Chemistry, University of Georgia, Athens, Georgia, 30602, USA*

Table S1A. Initial CpCoNHB<sub>6</sub>H<sub>6</sub> structures.

Table S1B. Distance table for the lowest-lying CpCoNHB<sub>6</sub>H<sub>6</sub> structures.

Table S1C. Energy ranking for all the CpCoNHB<sub>6</sub>H<sub>6</sub> structures.

Table S2A. Initial CpCoNHB<sub>7</sub>H<sub>7</sub> structures.

Table S2B. Distance table for the lowest-lying CpCoNHB<sub>7</sub>H<sub>7</sub> structures.

Table S2C. Energy ranking for all the CpCoNHB<sub>7</sub>H<sub>7</sub> structures.

Table S3A. Initial CpCoNHB<sub>8</sub>H<sub>8</sub> structures.

Table S3B. Distances table for the lowest-lying CpCoNHB<sub>8</sub>H<sub>8</sub> structures.

Table S3C. Energy ranking for all the CpCoNHB<sub>8</sub>H<sub>8</sub> structures.

Table S4A. Initial CpCoNHB<sub>9</sub>H<sub>9</sub> structures.

Table S4B. Distance table for the lowest-lying CpCoNHB<sub>9</sub>H<sub>9</sub> structures.

Table S4C. Energy ranking for all the CpCoNHB<sub>9</sub>H<sub>9</sub> structures.

Table S5A. Initial CpCoNHB<sub>10</sub>H<sub>10</sub> structures.

Table S5B. Distance table for the lowest-lying CpCoNHB<sub>10</sub>H<sub>10</sub> structures.

Table S5C. Energy ranking for all the CpCoNHB<sub>10</sub>H<sub>10</sub> structures.

Complete Gaussian09 Reference (reference 15)

Gaussian 09, Revision A.02,

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

Table S1A. Initial CpCoNHB<sub>6</sub>H<sub>6</sub> structures, 101 in all.

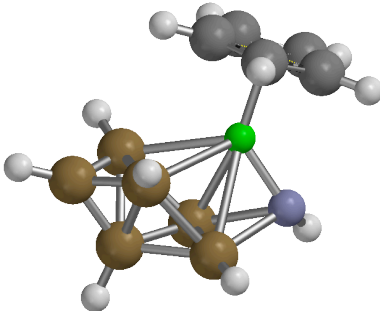
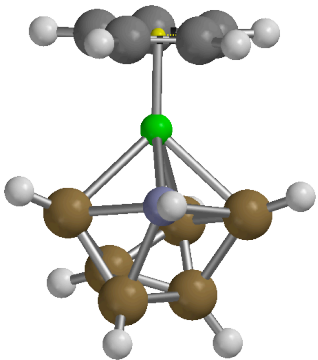
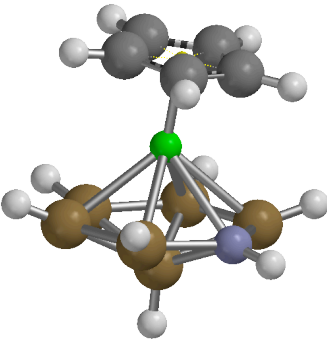
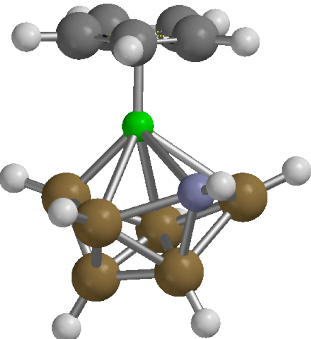
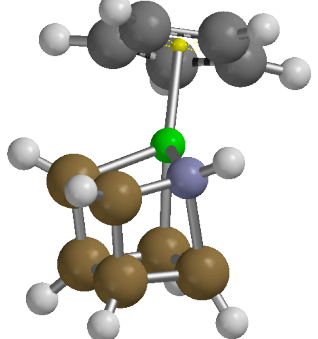
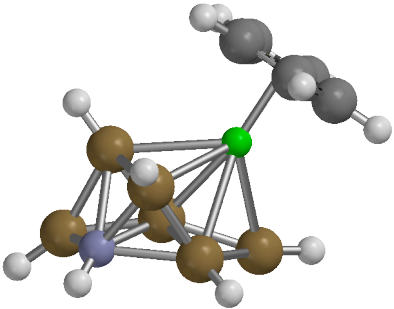
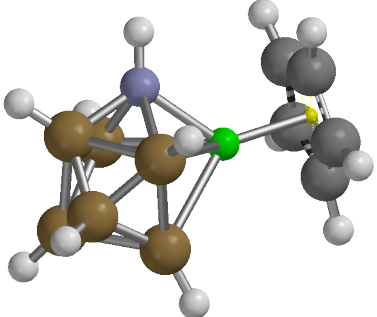
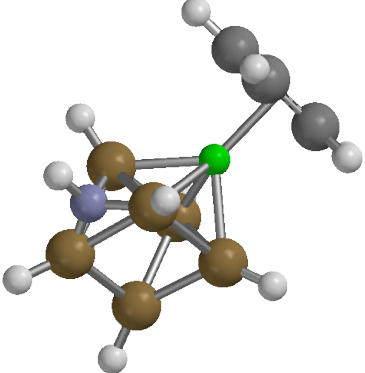
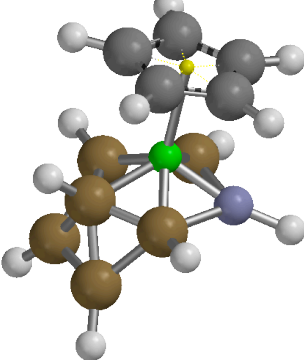
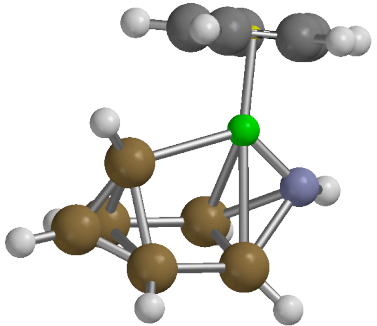
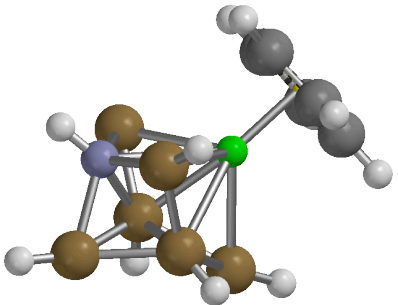
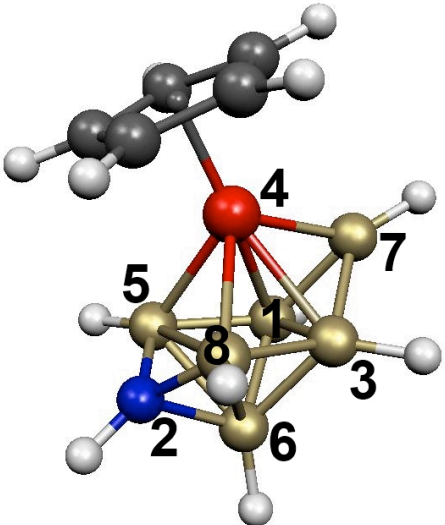
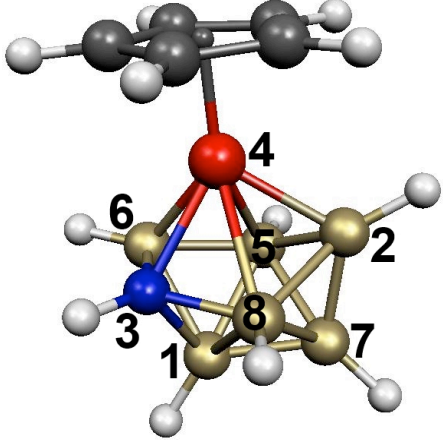
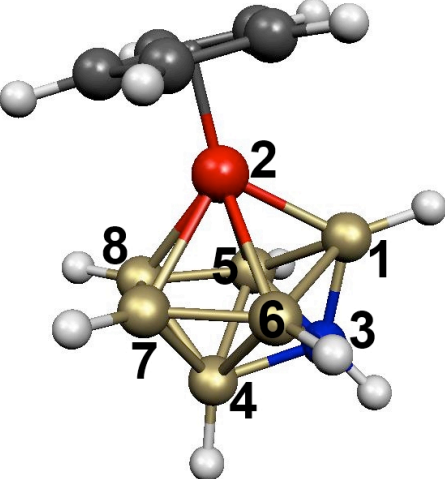
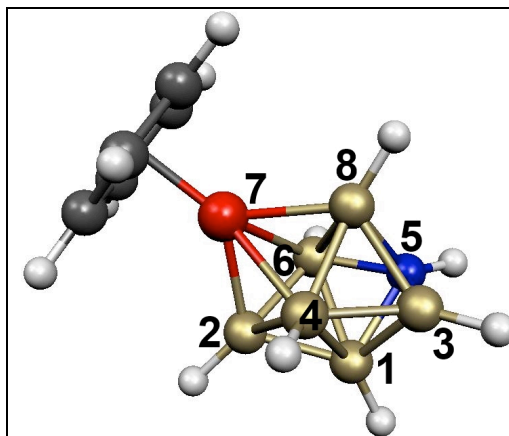
<p>Initial structures</p>	 <p>Trigonal Antiprism 6</p>	 <p>Antiprism 4</p>
 <p>Hexagonal bipyramid 8</p>	 <p>Bisdisphenoid 13</p>	 <p>Cube 3</p>
 <p>Bicapped octahedron 13</p>	 <p>Bicapped trigonal prism C<sub>2v</sub> 18</p>	 <p>Bicapped trigonal prism C<sub>s</sub> 24</p>
 <p>Nido 4</p>	 <p>Trigonal prism 5</p>	 <p>Tetracapped tetrahedron 3</p>

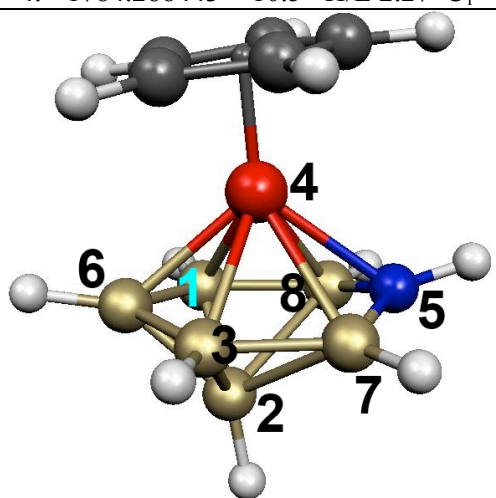
Table S1B. Distance table for the lowest-lying CpCoNHB<sub>6</sub>H<sub>6</sub> structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.

 <p>1. -1784.305162 0.0 H/L 2.90 C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 N</td><td>2.596985</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.732800</td><td>2.596985</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Co</td><td>2.108922</td><td>2.678440</td><td>2.108922</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.717723</td><td>1.500716</td><td>2.635670</td><td>2.101490</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.750527</td><td>1.567663</td><td>1.750527</td><td>2.875961</td><td>1.886243</td></tr> <tr><td>7 B</td><td>1.697894</td><td>3.690543</td><td>1.697894</td><td>1.876187</td><td>3.009220</td></tr> <tr><td>8 B</td><td>2.635670</td><td>1.500716</td><td>1.717723</td><td>2.101490</td><td>2.306200</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td></td> <td></td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.981017</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.886243</td><td>3.009220</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 N	2.596985	0.000000				3 B	1.732800	2.596985	0.000000			4 Co	2.108922	2.678440	2.108922	0.000000		5 B	1.717723	1.500716	2.635670	2.101490	0.000000	6 B	1.750527	1.567663	1.750527	2.875961	1.886243	7 B	1.697894	3.690543	1.697894	1.876187	3.009220	8 B	2.635670	1.500716	1.717723	2.101490	2.306200		6	7	8			6 B	0.000000					7 B	2.981017	0.000000				8 B	1.886243	3.009220	0.000000		
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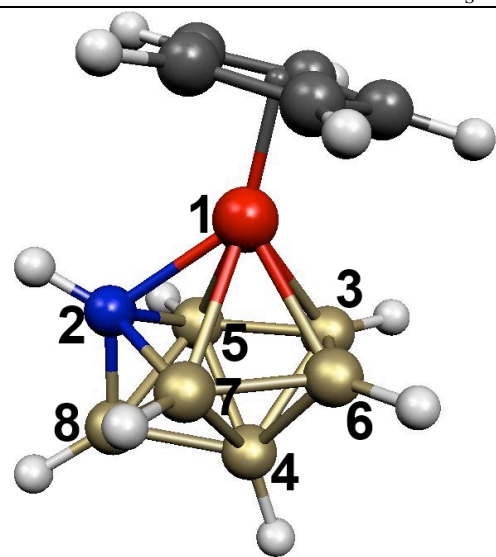
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3 B	1.797241	2.865678	0.000000		
4 B	1.914251	1.825545	1.672761	0.000000	
5 N	1.626761	2.668260	1.500285	2.415669	0.000000
6 B	1.878071	1.771267	2.624455	2.487454	1.580143
7 Co	3.010911	1.885997	3.220518	2.099504	3.028487
8 B	2.545880	2.653140	1.793725	1.825221	1.727743
		6	7	8	
6 B	0.000000				
7 Co	2.037312	0.000000			
8 B	1.936111	1.937272	0.000000		



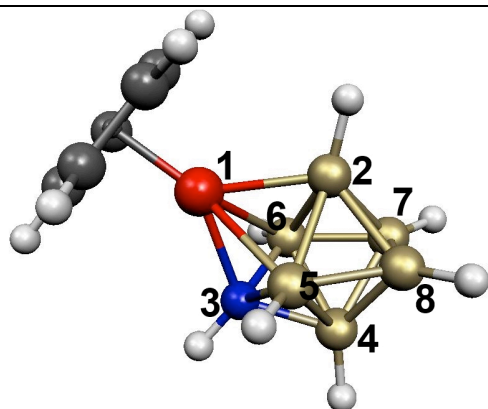
5. -1784.281127 +15.1 H/L 2.23 C<sub>s</sub>

	1	2	3	4	5
1 B	0.000000				
2 B	1.723262	0.000000			
3 B	2.668800	1.723351	0.000000		
4 Co	2.135899	2.595351	2.136503	0.000000	
5 N	2.725953	2.437015	2.725850	2.097651	0.000000
6 B	1.642240	1.724746	1.642254	2.139420	3.312089
7 B	3.074754	2.113422	1.681576	2.218835	1.446072
8 B	1.681628	2.113261	3.074679	2.218319	1.446149
		6	7	8	
6 B	0.000000				
7 B	2.909360	0.000000			
8 B	2.909346	2.482800	0.000000		



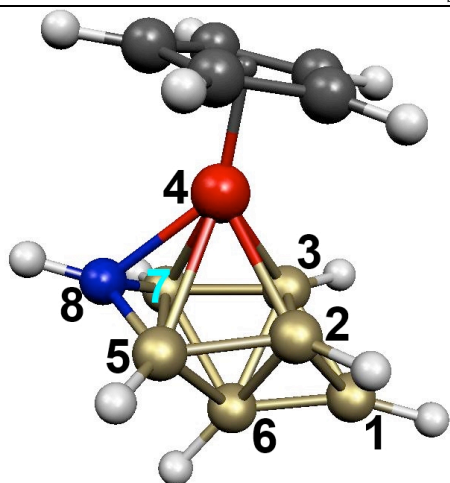
6. -1784.279751 +16.0 H/L 2.36 C<sub>s</sub>

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2 N	1.936817	0.000000			
3 B	2.073725	2.761794	0.000000		
4 B	2.887389	2.411368	1.783406	0.000000	
5 B	2.168468	1.667691	1.696322	1.893451	0.000000
6 B	2.073825	2.761815	1.629400	1.783469	2.642538
7 B	2.168540	1.667735	2.642471	1.893530	2.519600
8 B	3.030316	1.466638	2.883402	1.666867	1.836445
		6	7	8	
6 B	0.000000				
7 B	1.696254	0.000000			
8 B	2.883431	1.836548	0.000000		



1 Co	0.000000				
2 B	1.995536	0.000000			
3 N	1.866798	2.432936	0.000000		
4 B	3.093362	2.494796	1.592839	0.000000	
5 B	2.148513	1.925204	1.606548	1.861082	0.000000
6 B	2.147600	1.929340	1.606397	1.860010	2.491930
7 B	3.264160	1.785391	2.658234	1.753441	2.634951
8 B	3.265584	1.783668	2.658805	1.754064	1.706313
		6	7	8	
6 B	0.000000				
7 B	1.705737	0.000000			
8 B	2.635629	1.618919	0.000000		

7. -1784.273905 +19.6 H/L 1.56 C<sub>s</sub>



	1	2	3	4	5
1 B	0.000000				
2 B	1.728401	0.000000			
3 B	1.728783	1.725100	0.000000		
4 Co	3.363873	2.057415	2.057914	0.000000	
5 B	2.990896	1.705728	2.612007	2.191509	0.000000
6 B	1.613535	1.806792	1.806880	3.015014	1.947238
7 B	2.991455	2.611999	1.705733	2.191641	2.268300
8 N	3.693524	2.635622	2.635730	1.930533	1.470989
		6	7	8	
6 B	0.000000				
7 B	1.947769	0.000000			
8 N	2.483644	1.470980	0.000000		

8. -1784.264678 +25.4 H/L 1.63 C<sub>s</sub>

Table S1C. Energy ranking for all of the CpCoNHB<sub>6</sub>H<sub>6</sub> optimized structures:

No	Initial structure	Final energy (a.u.)	$\Delta E$ ( kcal/mol)
1	DicapTrPr-Cs-Co2-f	-1784.1558735	0.00
2	DicapTrPr-C2v-Co1-a	-1784.1558727	0.00
3	DicapTrPr-C2v-Co1-b	-1784.1558727	0.00
4	DicapTrPr-Cs-Co3-g	-1784.1558726	0.00
5	PrTrig-Co-d	-1784.1558723	0.00
6	Antipr-Co-a	-1784.1558717	0.00
7	DicapTrPr-C2v-Co1-d	-1784.1558717	0.00
8	Bisdisph-Co1-a	-1784.1558716	0.00
9	DicapOh-Co2-g	-1784.1558716	0.00
10	DicapTrPr-Cs-Co1-d	-1784.1558716	0.00
11	DicapTrPr-Cs-Co2-a	-1784.1558716	0.00
12	DicapTrPr-Cs-Co3-a	-1784.1558716	0.00
13	Nido-Co-a	-1784.1558716	0.00
14	DicapOh-Co3-c	-1784.1558715	0.00
15	Bisdisph-Co2-c_r-47	-1784.1558714	0.00
16	Tdallcap-Co-a	-1784.1558714	0.00
17	DicapTrPr-C2v-Co3-b	-1784.1558713	0.00
18	Bisdisph-Co2-d	-1784.1558712	0.00
19	DicapTrPr-C2v-Co3-c	-1784.1558706	0.00
20	Bipirhex-Co2-a_r-68	-1784.1558705	0.00
21	DicapTrPr-Cs-Co1-e	-1784.1558704	0.00
22	DicapTrPr-C2v-Co2-b_r-42	-1784.1558703	0.00
23	Antipr-Co-b	-1784.1558694	0.00
24	AntiprTrig-Co-b	-1784.1558694	0.00
25	AntiprTrig-Co-c	-1784.1558694	0.00
26	DicapTrPr-Cs-Co3-b	-1784.1558692	0.00
27	Bisdisph-Co1-b	-1784.1558684	0.00
28	DicapOh-Co3-a	-1784.1558651	0.01
29	Nido-Co-b	-1784.1558629	0.01
30	DicapTrPr-Cs-Co4-d	-1784.1558618	0.01
31	DicapOh-Co2-b	-1784.1558140	0.04
32	DicapTrPr-C2v-Co2-a	-1784.1557295	0.09
33	Nido-Co-c	-1784.1555175	0.22
34	Tdallcap-Co-b	-1784.1554390	0.27
35	Cub-Co-b	-1784.1554389	0.27
36	PrTrig-Co-e	-1784.1554380	0.27
37	DicapOh-Co2-d	-1784.1554379	0.27
38	AntiprTrig-Co-e_r-43	-1784.1554373	0.27
39	DicapOh-Co2-f	-1784.1554358	0.27
40	AntiprTrig-Co-e_i-43	-1784.1554137	0.29
41	DicapTrPr-C2v-Co2-b_i-42	-1784.1554124	0.29

42	Bisdisph-Co1-d	-1784.1475177	5.24
43	Antipr-Co-c	-1784.1475131	5.25
44	AntiprTrig-Co-d	-1784.1475131	5.25
45	DicapTrPr-Cs-Co3-c	-1784.1475130	5.25
46	DicapTrPr-Cs-Co1-c	-1784.1475121	5.25
47	DicapTrPr-C2v-Co3-d	-1784.1475110	5.25
48	DicapTrPr-C2v-Co1-f	-1784.1475100	5.25
49	Tdallcap-Co-c	-1784.1475099	5.25
50	Bisdisph-Co1-e r-497	-1784.1475009	5.25
51	DicapTrPr-Cs-Co1-b	-1784.1474983	5.26
52	Nido-Co-d	-1784.1474934	5.26
53	Cub-Co-c	-1784.1474929	5.26
54	DicapOh-Co2-c	-1784.1457371	6.36
55	Bipirhex-Co1-a	-1784.1457358	6.36
56	Antipr-Co-d	-1784.1414718	9.04
57	DicapOh-Co1-c	-1784.1414709	9.04
58	DicapTrPr-C2v-Co2-c r-180	-1784.1414705	9.04
59	DicapTrPr-Cs-Co4-b	-1784.1414704	9.04
60	DicapTrPr-C2v-Co1-c	-1784.1414701	9.04
61	DicapTrPr-Cs-Co4-e	-1784.1414701	9.04
62	Bisdisph-Co2-e	-1784.1414700	9.04
63	DicapTrPr-C2v-Co3-a r-173	-1784.1414700	9.04
64	Bisdisph-Co2-b	-1784.1414695	9.04
65	DicapTrPr-C2v-Co1-e	-1784.1414694	9.04
66	DicapTrPr-Cs-Co3-d	-1784.1414680	9.04
67	DicapTrPr-Cs-Co2-e	-1784.1414552	9.05
68	DicapTrPr-C2v-Co2-d	-1784.1414263	9.07
69	DicapTrPr-C2v-Co1-g	-1784.1382353	11.07
70	DicapTrPr-Cs-Co2-d	-1784.1382353	11.07
71	Bisdisph-Co2-a r-441	-1784.1347463	13.26
72	Bisdisph-Co1-c	-1784.1347453	13.26
73	DicapTrPr-Cs-Co1-a	-1784.1347347	13.27
74	DicapTrPr-Cs-Co2-b	-1784.1346340	13.33
75	DicapTrPr-C2v-Co3-a i-173	-1784.1331043	14.29
76	DicapTrPr-C2v-Co2-c i-180	-1784.1324933	14.67
77	Bisdisph-Co2-c i-47	-1784.1279734	17.51
78	Bipirhex-Co2-b r-45	-1784.1222004	21.13
79	Bipirhex-Co2-b i-45	-1784.1218925	21.32
80	DicapOh-Co1-b	-1784.1209862	21.89
81	PrTrig-Co-c	-1784.1209827	21.89
82	DicapTrPr-Cs-Co3-e	-1784.1209825	21.89
83	DicapTrPr-Cs-Co2-c	-1784.1209815	21.90
84	DicapOh-Co2-e	-1784.1209811	21.90
85	Bipirhex-Co2-d	-1784.1192696	22.97

86	Cub-Co-a	-1784.1183588	23.54
87	AntiprTrig-Co-a	-1784.1182961	23.58
88	PrTrig-Co-a	-1784.1182805	23.59
89	DicapOh-Co3-b	-1784.1170684	24.35
90	Bipirhex-Co2-c	-1784.1142164	26.14
91	DicapTrPr-Cs-Co3-f	-1784.1085913	29.67
92	DicapOh-Co1-a	-1784.1085536	29.69
93	DicapTrPr-Cs-Co4-c	-1784.1085493	29.70
94	DicapTrPr-Cs-Co4-a	-1784.1085212	29.71
95	Bisdisph-Co1-e i-497	-1784.1054481	31.64
96	DicapOh-Co2-a	-1784.1024619	33.52
97	PrTrig-Co-b	-1784.0917363	40.25
98	Bisdisph-Co2-a i-441	-1784.0828017	45.85
99	Bipirhex-Co1-b	-1784.0742242	51.24
100	Bipirhex-Co2-a i-68	-1784.0697028	54.07
101	DicapTrPr-Cs-Co2-g	-1784.0498135	66.55



Table S2A. Initial CpCoNHB<sub>7</sub>H<sub>7</sub> structures, 68 in all.

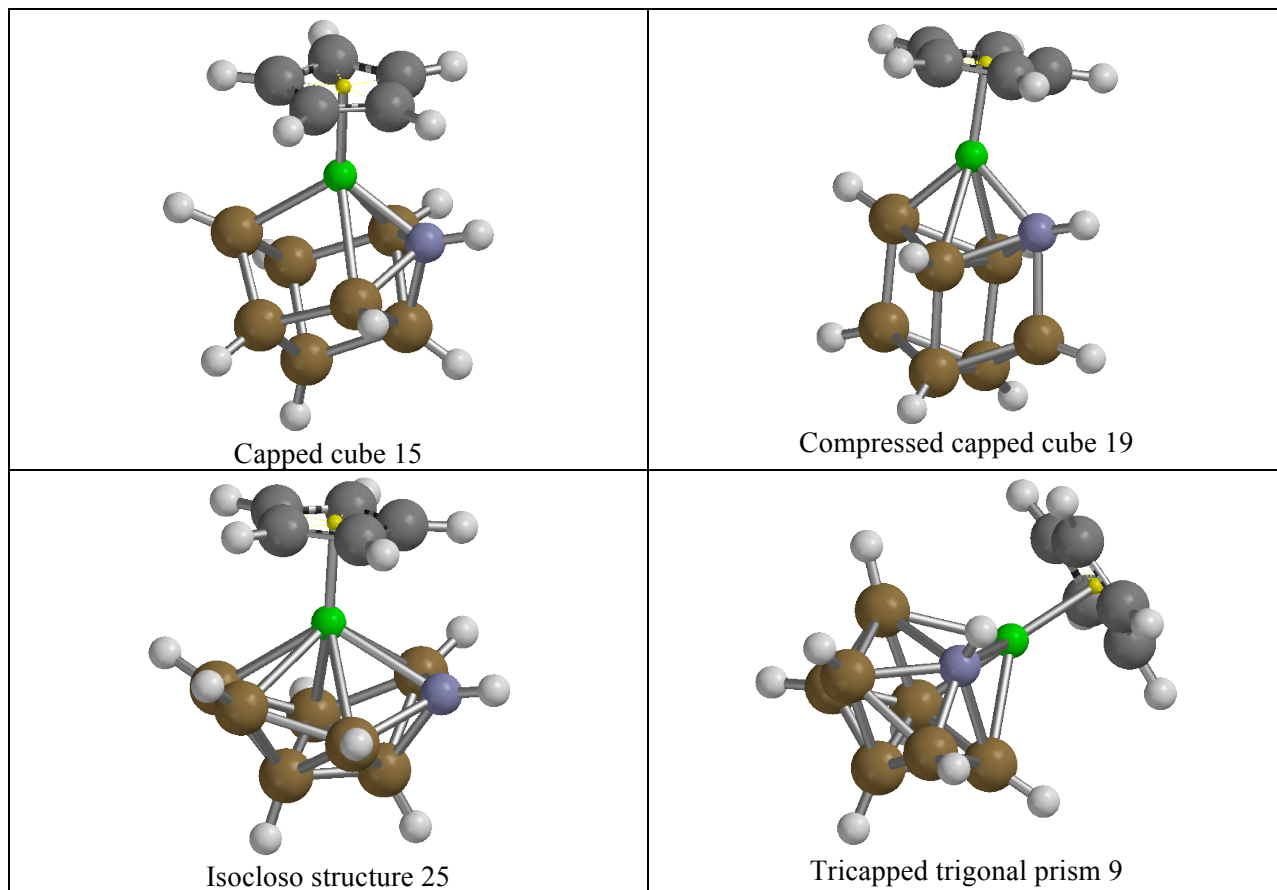
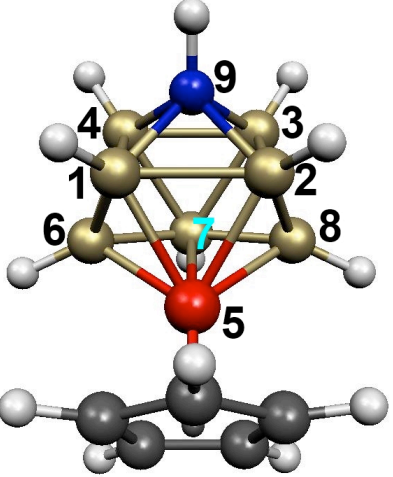
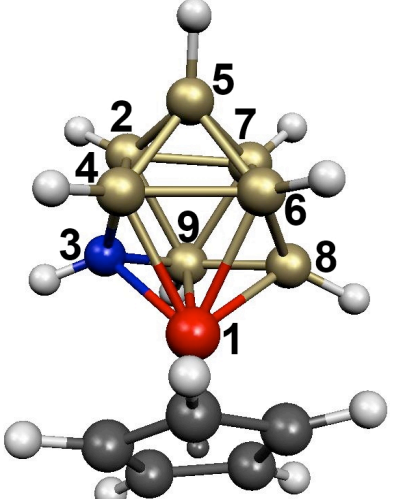
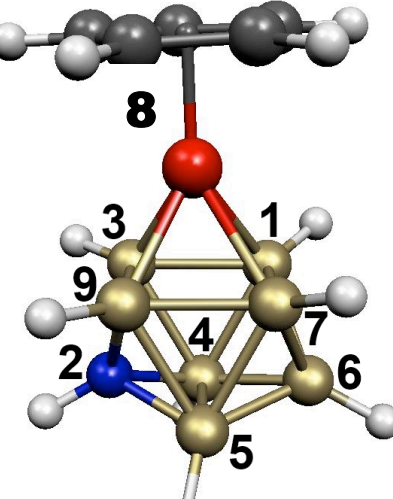


Table S2B. Distance table for the lowest-lying CpCoNHB<sub>7</sub>H<sub>7</sub> structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.

 <p>1. -1809.778116 0.0 H/L 2.35 C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.019500</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.672809</td><td>1.808398</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.808322</td><td>2.672833</td><td>1.918200</td><td>0.000000</td><td></td></tr> <tr><td>5 Co</td><td>2.087612</td><td>2.087661</td><td>2.944617</td><td>2.944606</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.703671</td><td>2.964852</td><td>2.901322</td><td>1.680895</td><td>1.975470</td></tr> <tr><td>7 B</td><td>2.616404</td><td>2.616443</td><td>1.858593</td><td>1.858652</td><td>2.140943</td></tr> <tr><td>8 B</td><td>2.964823</td><td>1.703739</td><td>1.680895</td><td>2.901342</td><td>1.975501</td></tr> <tr><td>9 N</td><td>1.581038</td><td>1.581102</td><td>1.592346</td><td>1.592266</td><td>2.905443</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</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>1.717794</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.915400</td><td>1.717747</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 N</td><td>2.643145</td><td>2.623408</td><td>2.643204</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.019500	0.000000				3 B	2.672809	1.808398	0.000000			4 B	1.808322	2.672833	1.918200	0.000000		5 Co	2.087612	2.087661	2.944617	2.944606	0.000000	6 B	1.703671	2.964852	2.901322	1.680895	1.975470	7 B	2.616404	2.616443	1.858593	1.858652	2.140943	8 B	2.964823	1.703739	1.680895	2.901342	1.975501	9 N	1.581038	1.581102	1.592346	1.592266	2.905443		6	7	8	9		6 B	0.000000					7 B	1.717794	0.000000				8 B	2.915400	1.717747	0.000000			9 N	2.643145	2.623408	2.643204	0.000000	
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 <p>2. -1809.772039 +3.8 H/L 2.08 C<sub>1</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Co</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.090197</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 N</td><td>1.915342</td><td>1.610626</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.223328</td><td>1.816863</td><td>1.569376</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.268454</td><td>1.657586</td><td>2.625250</td><td>1.685147</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.195187</td><td>2.613207</td><td>2.683913</td><td>1.905213</td><td>1.686947</td></tr> <tr><td>7 B</td><td>2.983407</td><td>1.857106</td><td>2.623512</td><td>2.606960</td><td>1.732621</td></tr> <tr><td>8 B</td><td>1.956952</td><td>2.941918</td><td>2.709988</td><td>2.928989</td><td>2.868832</td></tr> <tr><td>9 B</td><td>2.102358</td><td>1.946531</td><td>1.541249</td><td>2.601528</td><td>2.883249</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</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>1.806516</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.735071</td><td>1.696629</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Co	0.000000					2 B	3.090197	0.000000				3 N	1.915342	1.610626	0.000000			4 B	2.223328	1.816863	1.569376	0.000000		5 B	3.268454	1.657586	2.625250	1.685147	0.000000	6 B	2.195187	2.613207	2.683913	1.905213	1.686947	7 B	2.983407	1.857106	2.623512	2.606960	1.732621	8 B	1.956952	2.941918	2.709988	2.928989	2.868832	9 B	2.102358	1.946531	1.541249	2.601528	2.883249		6	7	8	9		6 B	0.000000					7 B	1.806516	0.000000				8 B	1.735071	1.696629	0.000000								
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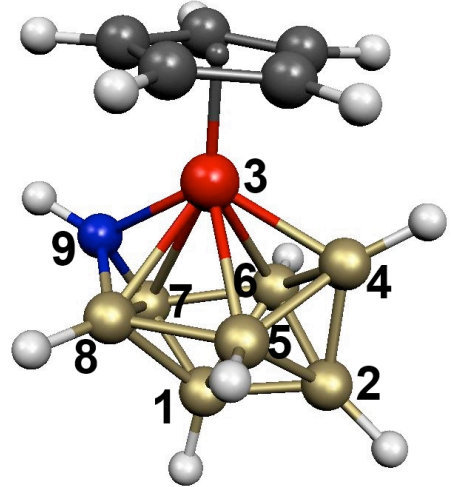
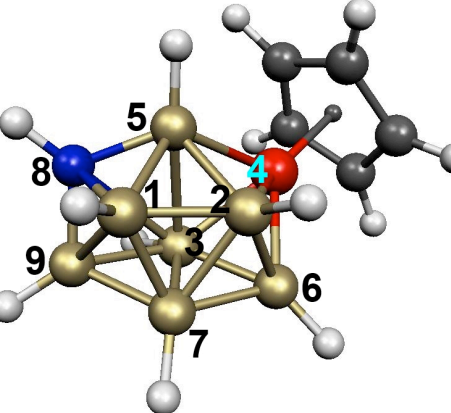
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6 B	0.000000																																																																																										
7 B	1.738926	0.000000																																																																																									
8 N	3.496857	2.547003	0.000000																																																																																								
9 B	3.041024	1.715695	1.461636	0.000000																																																																																							

Table S2C. Energy ranking for all of the CpCoNHB<sub>7</sub>H<sub>7</sub> optimized structures:

No	Initial structure	Final energy (a.u.)	$\Delta E$ ( kcal/mol)
1	CapCube-Co3-b	-1809.6156676	0.00
2	TI99-Co1-b	-1809.6156661	0.00
3	CapCube-Co2-c	-1809.6156635	0.00
4	TI99-Co2-b	-1809.6156634	0.00
5	TrTrPr-Co2-b	-1809.6156614	0.00
6	TI99-Co3-h	-1809.6156509	0.01
7	TI99-Co2-a_r-44	-1809.6156499	0.01
8	PressCapCube-Co2-c	-1809.6156480	0.01
9	TI99-Co2-a_i-44	-1809.6144250	0.78
10	PressCapCube-Co1-a_r-352	-1809.6120369	2.28
11	TI99-Co2-e	-1809.6120362	2.28
12	TrTrPr-Co2-a	-1809.6120359	2.28
13	TI99-Co4-b	-1809.6120356	2.28
14	TI99-Co3-c	-1809.6120353	2.28
15	TI99-Co3-d	-1809.6120350	2.28
16	TI99-Co3-a	-1809.6120343	2.28
17	CapCube-Co3-e	-1809.6120316	2.28
18	TrTrPr-Co2-c	-1809.5958986	12.41
19	PressCapCube-Co2-f	-1809.5958921	12.41
20	TI99-Co3-b	-1809.5958715	12.42
21	TI99-Co4-c_i-77	-1809.5957878	12.47
22	TrTrPr-Co1-b_i-78	-1809.5957788	12.48
23	TI99-Co4-a	-1809.5957727	12.48
24	TI99-Co4-e_r-97	-1809.5957677	12.49
25	TI99-Co3-e	-1809.5956708	12.55
26	TrTrPr-Co1-b_r-78	-1809.5956690	12.55
27	PressCapCube-Co3-a	-1809.5956631	12.55
28	TI99-Co4-c_r-77	-1809.5956624	12.55
29	TrTrPr-Co2-e	-1809.5956594	12.56
30	CapCube-Co3-a	-1809.5956593	12.56
31	PressCapCube-Co2-d	-1809.5956593	12.56
32	TI99-Co1-a	-1809.5956591	12.56
33	CapCube-Co2-a	-1809.5956583	12.56
34	CapCube-Co2-e	-1809.5956582	12.56
35	TI99-Co4-e_i-97	-1809.5956342	12.57
36	PressCapCube-Co2-e	-1809.5945850	13.23
37	CapCube-Co2-f	-1809.5944998	13.28
38	CapCube-Co3-d	-1809.5920827	14.80
39	TI99-Co3-f	-1809.5912331	15.33
40	CapCube-Co2-b	-1809.5907671	15.63
41	TI99-Co2-d	-1809.5907605	15.63

42	TrTrPr-Co1-c	-1809.5906371	15.71
43	TI99-Co4-d	-1809.5899055	16.17
44	PressCapCube-Co2-a	-1809.5887971	16.86
45	PressCapCube-Co3-d_r-65	-1809.5887634	16.88
46	PressCapCube-Co3-f	-1809.5874013	17.74
47	CapCube-Co3-f_r-49	-1809.5874009	17.74
48	PressCapCube-Co1-b	-1809.5874009	17.74
49	TI99-Co3-g	-1809.5874000	17.74
50	CapCube-Co1-b	-1809.5873981	17.74
51	CapCube-Co2-d	-1809.5871349	17.90
52	TI99-Co2-c	-1809.5871349	17.90
53	PressCapCube-Co3-d_i-65	-1809.5857842	18.75
54	CapCube-Co3-f_i-49	-1809.5857838	18.75
55	TrTrPr-Co2-d	-1809.5804705	22.09
56	TI99-Co1-c_r-206	-1809.5804693	22.09
57	CapCube-Co3-c	-1809.5757819	25.03
58	PressCapCube-Co3-b	-1809.5670794	30.49
59	PressCapCube-Co1-d	-1809.5670179	30.53
60	PressCapCube-Co3-e	-1809.5580330	36.17
61	TrTrPr-Co1-a	-1809.5564064	37.19
62	CapCube-Co1-a	-1809.5557844	37.58
63	PressCapCube-Co3-c_r-57	-1809.5513529	40.36
64	PressCapCube-Co3-c_i-57	-1809.5496516	41.43
65	PressCapCube-Co2-b	-1809.5360779	49.94
66	PressCapCube-Co1-c	-1809.5322828	52.33
67	TI99-Co1-c_i-206	-1809.5170176	61.90
68	PressCapCube-Co1-a_i-352	-1809.5009237	72.00

Table S3A. Initial CpCoNHB<sub>8</sub>H<sub>8</sub> structures, 97 in all.

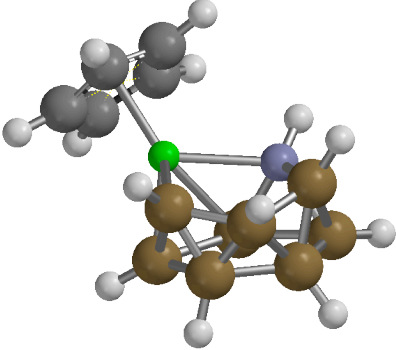
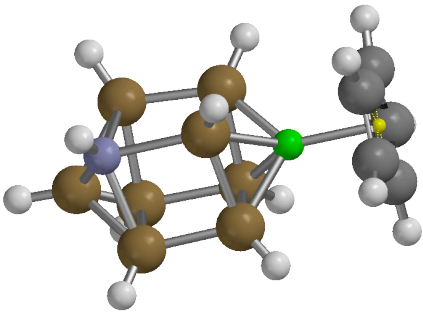
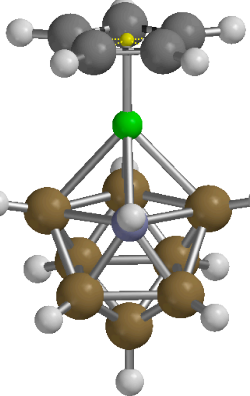
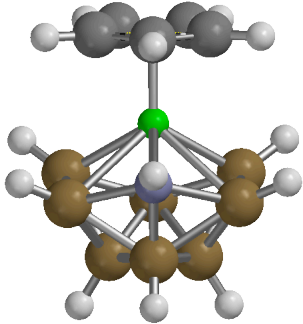
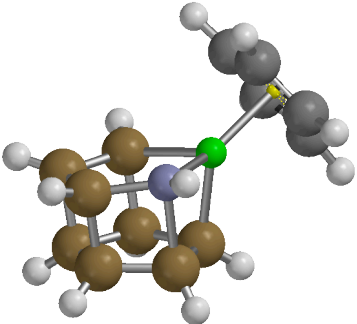
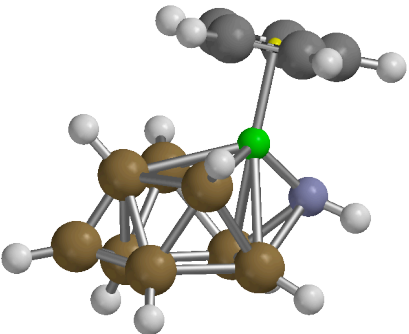
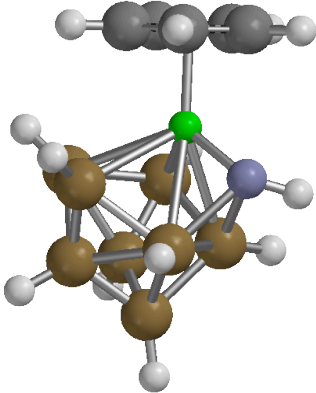
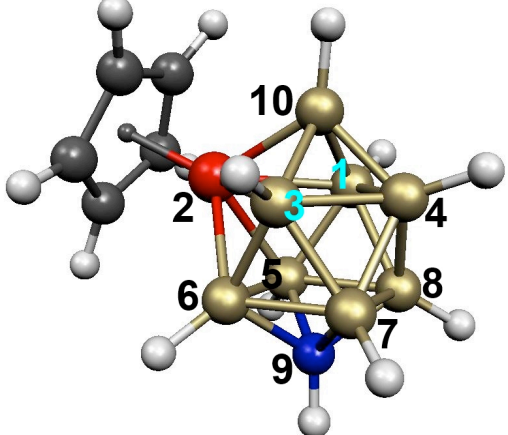
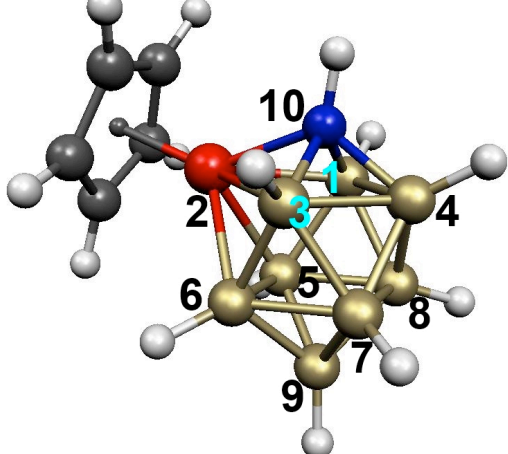
<p><b>Initial structures</b></p>	 <p>Pentagonal antiprism</p>
 <p>Bicapped cube</p>	 <p>Bicapped square antiprism</p>
 <p>Isocloso</p>	 <p>Pentagonal prism</p>
 <p>Tetracapped trigonal prism <math>C_{2v}</math></p>	 <p>Tetracapped trigonal prism <math>C_{3v}</math></p>

Table S3B. Distance table for the lowest-lying CpCoNHB<sub>8</sub>H<sub>8</sub> structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.

 <p><b>1. -1835.277003 0.0 H/L 3.07 C<sub>s</sub></b></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Co</td><td>2.117208</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.601600</td><td>2.117208</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.823917</td><td>2.945390</td><td>1.823917</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.746670</td><td>2.017560</td><td>2.849163</td><td>2.811547</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.849163</td><td>2.017560</td><td>1.746670</td><td>2.811547</td><td>1.947600</td></tr> <tr><td>7 B</td><td>2.805982</td><td>3.170344</td><td>1.751828</td><td>1.762857</td><td>2.637259</td></tr> <tr><td>8 B</td><td>1.751828</td><td>3.170344</td><td>2.805982</td><td>1.762857</td><td>1.832569</td></tr> <tr><td>9 N</td><td>2.663242</td><td>2.974071</td><td>2.663242</td><td>2.669600</td><td>1.589183</td></tr> <tr><td>10 B</td><td>1.736968</td><td>1.959672</td><td>1.736968</td><td>1.696151</td><td>2.931801</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>1.832569</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.637259</td><td>1.846800</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 N</td><td>1.589183</td><td>1.577560</td><td>1.577560</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.931801</td><td>2.896730</td><td>2.896730</td><td>3.474972</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Co	2.117208	0.000000				3 B	2.601600	2.117208	0.000000			4 B	1.823917	2.945390	1.823917	0.000000		5 B	1.746670	2.017560	2.849163	2.811547	0.000000	6 B	2.849163	2.017560	1.746670	2.811547	1.947600	7 B	2.805982	3.170344	1.751828	1.762857	2.637259	8 B	1.751828	3.170344	2.805982	1.762857	1.832569	9 N	2.663242	2.974071	2.663242	2.669600	1.589183	10 B	1.736968	1.959672	1.736968	1.696151	2.931801		6	7	8	9	10	6 B	0.000000					7 B	1.832569	0.000000				8 B	2.637259	1.846800	0.000000			9 N	1.589183	1.577560	1.577560	0.000000		10 B	2.931801	2.896730	2.896730	3.474972	0.000000
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 <p><b>2. -1835.265024 +7.5 H/L 2.54 C<sub>s</sub></b></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Co</td><td>2.128232</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.562400</td><td>2.128232</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.857835</td><td>3.042327</td><td>1.857835</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.812605</td><td>2.093789</td><td>2.816324</td><td>2.842213</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.816324</td><td>2.093789</td><td>1.812605</td><td>2.842213</td><td>1.813200</td></tr> <tr><td>7 B</td><td>2.796944</td><td>3.230088</td><td>1.778026</td><td>1.743407</td><td>2.580265</td></tr> <tr><td>8 B</td><td>1.778026</td><td>3.230088</td><td>2.796944</td><td>1.743407</td><td>1.832810</td></tr> <tr><td>9 B</td><td>2.902712</td><td>3.290949</td><td>2.902712</td><td>2.870661</td><td>1.700816</td></tr> <tr><td>10 N</td><td>1.565663</td><td>1.902040</td><td>1.565663</td><td>1.577282</td><td>2.766426</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>1.832810</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.580265</td><td>1.819200</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.700816</td><td>1.698748</td><td>1.698748</td><td>0.000000</td><td></td></tr> <tr><td>10 N</td><td>2.766426</td><td>2.674536</td><td>2.674536</td><td>3.500876</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Co	2.128232	0.000000				3 B	2.562400	2.128232	0.000000			4 B	1.857835	3.042327	1.857835	0.000000		5 B	1.812605	2.093789	2.816324	2.842213	0.000000	6 B	2.816324	2.093789	1.812605	2.842213	1.813200	7 B	2.796944	3.230088	1.778026	1.743407	2.580265	8 B	1.778026	3.230088	2.796944	1.743407	1.832810	9 B	2.902712	3.290949	2.902712	2.870661	1.700816	10 N	1.565663	1.902040	1.565663	1.577282	2.766426		6	7	8	9	10	6 B	0.000000					7 B	1.832810	0.000000				8 B	2.580265	1.819200	0.000000			9 B	1.700816	1.698748	1.698748	0.000000		10 N	2.766426	2.674536	2.674536	3.500876	0.000000
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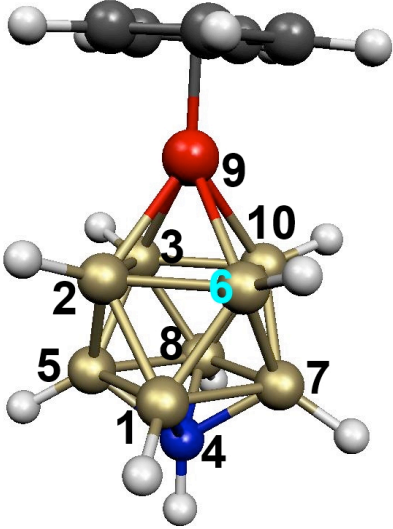
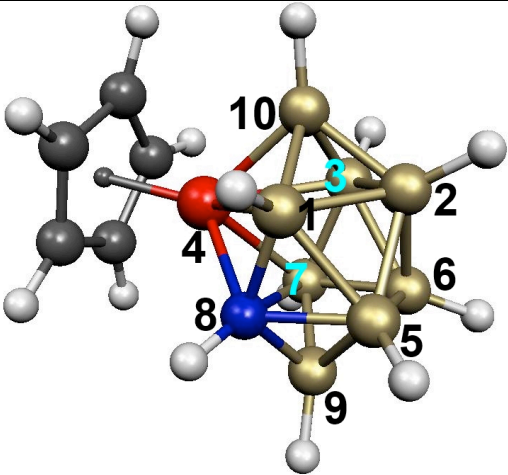
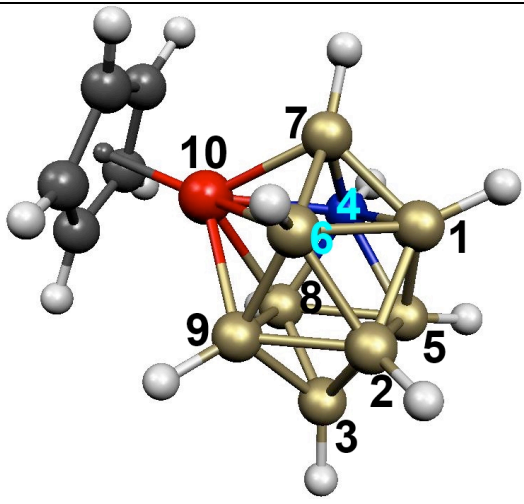
 <p>3. -1835.246686 +19.0 H/L 2.25 C<sub>4v</sub>-C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.770364</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.814519</td><td>1.824338</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 N</td><td>1.575503</td><td>2.670698</td><td>2.672198</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.853802</td><td>1.770559</td><td>1.771019</td><td>1.575583</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.770449</td><td>1.823456</td><td>2.579980</td><td>2.671022</td><td>2.813364</td></tr> <tr><td>7 B</td><td>1.853730</td><td>2.812999</td><td>2.813699</td><td>1.575539</td><td>2.620619</td></tr> <tr><td>8 B</td><td>2.620842</td><td>2.812762</td><td>1.770977</td><td>1.575742</td><td>1.852593</td></tr> <tr><td>9 Co</td><td>3.287339</td><td>2.016630</td><td>2.018580</td><td>3.890544</td><td>3.288286</td></tr> <tr><td>10 B</td><td>2.814426</td><td>2.579664</td><td>1.824267</td><td>2.672022</td><td>2.813680</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>1.770858</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.813149</td><td>1.852421</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 Co</td><td>2.016123</td><td>3.287708</td><td>3.288842</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>1.824778</td><td>1.770811</td><td>1.770708</td><td>2.018177</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.770364	0.000000				3 B	2.814519	1.824338	0.000000			4 N	1.575503	2.670698	2.672198	0.000000		5 B	1.853802	1.770559	1.771019	1.575583	0.000000	6 B	1.770449	1.823456	2.579980	2.671022	2.813364	7 B	1.853730	2.812999	2.813699	1.575539	2.620619	8 B	2.620842	2.812762	1.770977	1.575742	1.852593	9 Co	3.287339	2.016630	2.018580	3.890544	3.288286	10 B	2.814426	2.579664	1.824267	2.672022	2.813680		6	7	8	9	10	6 B	0.000000					7 B	1.770858	0.000000				8 B	2.813149	1.852421	0.000000			9 Co	2.016123	3.287708	3.288842	0.000000		10 B	1.824778	1.770811	1.770708	2.018177	0.000000
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Table S3C. Energy ranking for all of the CpCoNHB<sub>8</sub>H<sub>8</sub> optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE( kcal/mol)
1	BicapSqAntipr-Co2-c	-1835.10111050	0.00
2	Isocloso-Co3-d	-1835.10111040	0.00
3	Isocloso-Co4-d	-1835.10111030	0.00
4	TetrTriPri2-Co2-d	-1835.10110950	0.00
5	TetrTriPri1-Co2-d	-1835.10110850	0.00
6	TetrTriPri2-Co1-e	-1835.10110850	0.00
7	TetrTriPri2-Co3-d	-1835.10110840	0.00
8	BicapCub-Co2-d_r-48	-1835.10110830	0.00
9	TetrTriPri1-Co3-i	-1835.10110830	0.00
10	TetrTriPri2-Co3-c	-1835.10110820	0.00
11	TetrTriPri2-Co2-c_r-48	-1835.10110750	0.00
12	TetrTriPri2-Co1-a	-1835.10110640	0.00
13	Isocloso-Co4-c	-1835.10110530	0.00
14	PentagPrism-Co-e	-1835.10110510	0.00
15	Isocloso-Co1-b	-1835.10110330	0.00
16	TetrTriPri2-Co1-d	-1835.10110230	0.01
17	BicapCub-Co2-d_i-48	-1835.09936420	1.10
18	TetrTriPri2-Co2-c_i-48	-1835.09936190	1.10
19	BicapSqAntipr-Co2-a	-1835.08944600	7.32
20	BicapCub-Co2-a	-1835.08944400	7.32
21	TetrTriPri2-Co3-f	-1835.08944180	7.32
22	TetrTriPri2-Co3-a	-1835.08943970	7.32
23	Isocloso-Co4-e	-1835.08943930	7.32
24	TetrTriPri1-Co3-a	-1835.08943930	7.32
25	TetrTriPri2-Co2-e	-1835.08943800	7.32
26	Isocloso-Co2-d	-1835.08940600	7.34
27	Isocloso-Co3-b	-1835.07101450	18.89
28	BicapSqAntipr-Co1-d	-1835.07097170	18.91
29	BicapCub-Co1-c_r-391	-1835.07092800	18.94
30	TetrTriPri2-Co1-c	-1835.07086830	18.98
31	Isocloso-Co2-b	-1835.07085920	18.98
32	TetrTriPri2-Co2-b	-1835.07082270	19.01
33	Isocloso-Co1-a_r-196	-1835.05896870	26.44
34	BicapCub-Co2-g	-1835.05896860	26.44
35	Isocloso-Co4-f	-1835.05896860	26.44
36	TetrTriPri1-Co2-b	-1835.05896850	26.44
37	TetrTriPri2-Co1-b	-1835.05896780	26.45
38	TetrTriPri2-Co2-f	-1835.05896780	26.45
39	BicapSqAntipr-Co2-e	-1835.05896770	26.45
40	PenPr-Co-d	-1835.05896640	26.45
41	BicapCub-Co2-e	-1835.05896500	26.45

42	Isocloso-Co1-a_i-196	-1835.05525500	28.78
43	TetrTriPri2-Co3-e	-1835.05155790	31.10
44	PentagPrism-Co-a	-1835.05155700	31.10
45	TetrTriPri1-Co3-b	-1835.05155590	31.10
46	TetrTriPri1-Co3-c	-1835.04853870	32.99
47	Isocloso-Co2-e	-1835.04486280	35.30
48	Isocloso-Co4-a_r-150	-1835.04485850	35.30
49	TetrTriPri1-Co3-e	-1835.04484740	35.31
50	BicapSqAntipr-Co2-d	-1835.04484420	35.31
51	PenPr-Co-c	-1835.04372260	36.01
52	BicapCub-Co2-f	-1835.04372150	36.01
53	PenPr-Co-e	-1835.04253130	36.76
54	PentagPrism-Co-b	-1835.04125570	37.56
55	Isocloso-Co2-f	-1835.04125500	37.56
56	BicapSqAntipr-Co2-f	-1835.04125320	37.56
57	BicapCub-Co2-c	-1835.04125310	37.56
58	Isocloso-Co1-c_r-356	-1835.04125280	37.56
59	Isocloso-Co4-b_r-283	-1835.04125210	37.56
60	Isocloso-Co4-a_i-150	-1835.04090100	37.78
61	TetrTriPri1-Co2-a	-1835.03952670	38.65
62	TetrTriPri1-Co1-c	-1835.03875290	39.13
63	TetrTriPri1-Co3-h	-1835.03874290	39.14
64	TetrTriPri1-Co1-a	-1835.03767100	39.81
65	TetrTriPri1-Co1-f	-1835.03757470	39.87
66	TetrTriPri2-Co3-b	-1835.03523150	41.34
67	TetrTriPri1-Co3-d	-1835.03523140	41.34
68	BicapSqAntipr-Co2-b	-1835.03523040	41.34
69	BicapCub-Co2-b	-1835.03522790	41.34
70	TetrTriPri2-Co1-f	-1835.03479850	41.61
71	Isocloso-Co3-f	-1835.03479740	41.61
72	Isocloso-Co2-a	-1835.03307270	42.70
73	Isocloso-Co3-e	-1835.03306960	42.70
74	BicapCub-Co1-a	-1835.03305190	42.71
75	Isocloso-Co2-c	-1835.03271620	42.92
76	BicapSqAntipr-Co1-a	-1835.03270510	42.93
77	Isocloso-Co3-c	-1835.02940710	45.00
78	TetrTriPri2-Co2-a	-1835.02940430	45.00
79	BicapSqAntipr-Co1-c	-1835.02908330	45.20
80	Isocloso-Co3-a	-1835.02908170	45.20
81	BicapSqAntipr-Co1-b	-1835.02907990	45.20
82	BicapCub-Co1-b	-1835.02878910	45.38
83	PentagPrism-Co-c_r-213	-1835.02639040	46.89
84	Isocloso-Co4-b_i-283	-1835.02482070	47.87
85	TetrTriPri1-Co2-e	-1835.02075700	50.42

86	PenPr-Co-b	-1835.02046270	50.61
87	TetrTriPri1-Co2-c	-1835.01796320	52.18
88	TetrTriPri1-Co1-e	-1835.01040110	56.92
89	TetrTriPri1-Co1-d	-1835.00859600	58.05
90	TetrTriPri1-Co3-g	-1835.00343130	61.30
91	TetrTriPri1-Co1-b	-1835.00257610	61.83
92	TetrTriPri1-Co3-f	-1835.00090390	62.88
93	PenPr-Co-a	-1834.99155820	68.75
94	Isocloso-Co1-c_i-356	-1834.98352280	73.79
95	PentagPrism-Co-d	-1834.97908320	76.57
96	PentagPrism-Co-c_i-213	-1834.97220300	80.89
97	BicapCub-Co1-c_i-391	-1834.92356330	111.41

Table S4A. Initial CpCoNHB<sub>9</sub>H<sub>9</sub> structures, 140 in all.

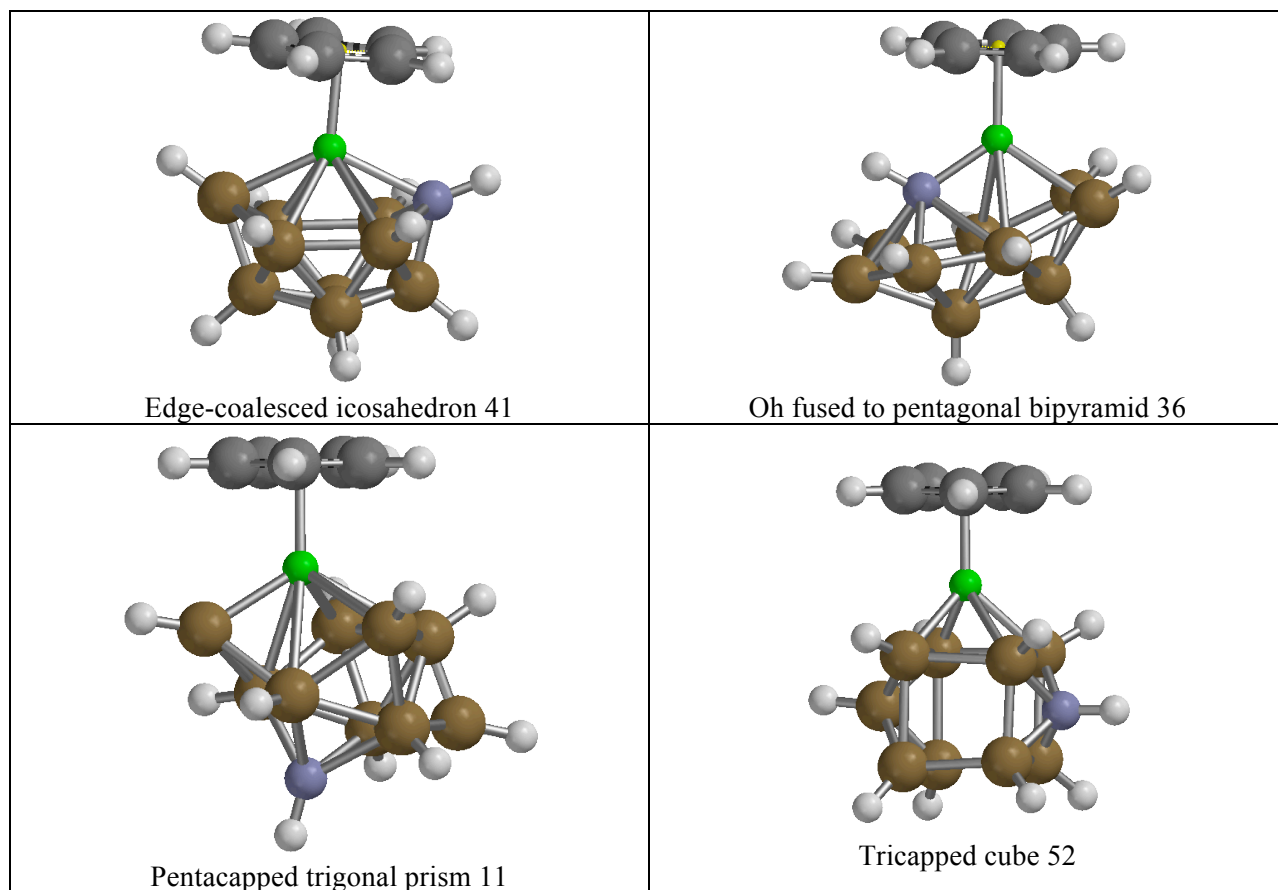
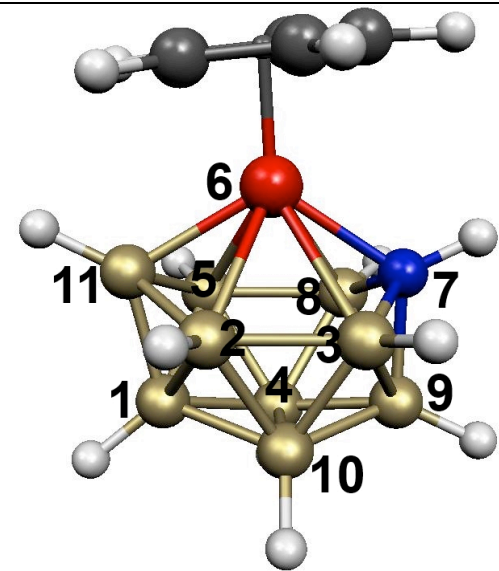
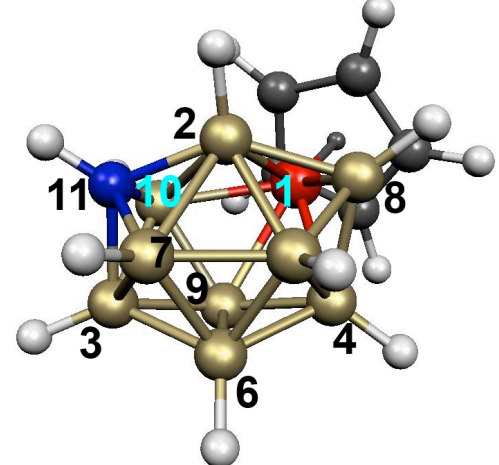
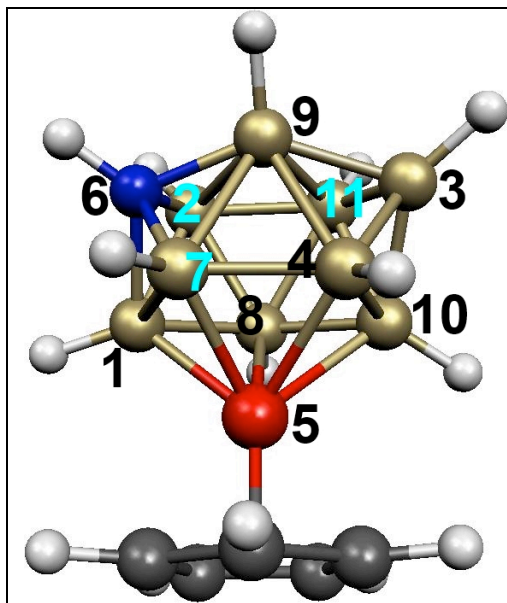


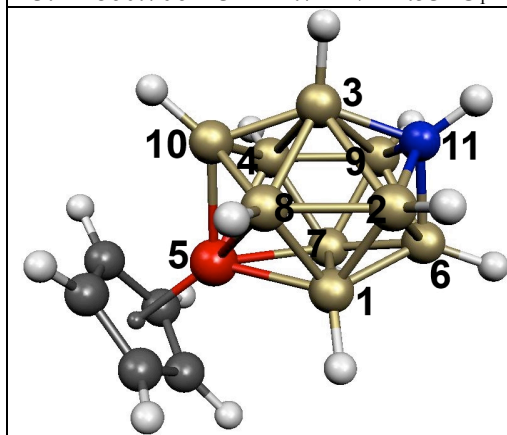
Table S4B. Distance table for the lowest-lying CpCoNHB<sub>9</sub>H<sub>9</sub> structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.

 <p>1. -1860.724989 0.0 H/L 1.96 C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>1.803912</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.905940</td><td>1.804882</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.763288</td><td>2.814197</td><td>2.792082</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.803937</td><td>2.621800</td><td>3.187004</td><td>1.778091</td><td>0.000000</td></tr> <tr><td>6 Co</td><td>3.002670</td><td>2.197352</td><td>2.305158</td><td>3.175543</td><td>2.197325</td></tr> <tr><td>7 N</td><td>3.361617</td><td>2.785386</td><td>1.536271</td><td>2.617789</td><td>2.785463</td></tr> <tr><td>8 B</td><td>2.905971</td><td>3.186938</td><td>2.631400</td><td>1.737816</td><td>1.804982</td></tr> <tr><td>9 B</td><td>2.904821</td><td>2.933797</td><td>1.819855</td><td>1.725776</td><td>2.933830</td></tr> <tr><td>10 B</td><td>1.763293</td><td>1.778136</td><td>1.737806</td><td>1.814800</td><td>2.814206</td></tr> <tr><td>11 B</td><td>1.694478</td><td>1.704902</td><td>3.103849</td><td>2.886076</td><td>1.704967</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 Co</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 N</td><td>1.945973</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.305086</td><td>1.536241</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.145527</td><td>1.644534</td><td>1.819774</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>3.175579</td><td>2.617728</td><td>2.791985</td><td>1.725704</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.030754</td><td>3.359079</td><td>3.103909</td><td>3.713531</td><td>2.886083</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	1.803912	0.000000				3 B	2.905940	1.804882	0.000000			4 B	1.763288	2.814197	2.792082	0.000000		5 B	1.803937	2.621800	3.187004	1.778091	0.000000	6 Co	3.002670	2.197352	2.305158	3.175543	2.197325	7 N	3.361617	2.785386	1.536271	2.617789	2.785463	8 B	2.905971	3.186938	2.631400	1.737816	1.804982	9 B	2.904821	2.933797	1.819855	1.725776	2.933830	10 B	1.763293	1.778136	1.737806	1.814800	2.814206	11 B	1.694478	1.704902	3.103849	2.886076	1.704967		6	7	8	9	10	6 Co	0.000000					7 N	1.945973	0.000000				8 B	2.305086	1.536241	0.000000			9 B	3.145527	1.644534	1.819774	0.000000		10 B	3.175579	2.617728	2.791985	1.725704	0.000000	11 B	2.030754	3.359079	3.103909	3.713531	2.886083
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 <p>2. -1860.715708 +5.8 H/L 2.78 C<sub>1</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Co</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.166042</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>3.252153</td><td>2.722195</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>2.101193</td><td>2.633171</td><td>2.918521</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.985859</td><td>1.945378</td><td>2.910998</td><td>1.799268</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.195966</td><td>2.772656</td><td>1.746075</td><td>1.759451</td><td>1.768874</td></tr> <tr><td>7 B</td><td>3.525438</td><td>1.982715</td><td>1.800925</td><td>2.873433</td><td>1.756139</td></tr> <tr><td>8 B</td><td>1.918150</td><td>1.769480</td><td>3.665005</td><td>1.756117</td><td>1.671915</td></tr> <tr><td>9 B</td><td>2.085062</td><td>2.795918</td><td>1.759170</td><td>1.771178</td><td>2.828043</td></tr> <tr><td>10 B</td><td>2.010548</td><td>2.104489</td><td>1.796719</td><td>2.937048</td><td>3.264572</td></tr> <tr><td>11 N</td><td>2.974904</td><td>1.615259</td><td>1.637645</td><td>3.307199</td><td>2.743727</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.743079</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.881647</td><td>2.981919</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.803875</td><td>2.799046</td><td>2.936478</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.822502</td><td>2.688934</td><td>3.139561</td><td>1.750990</td><td>0.000000</td></tr> <tr><td>11 N</td><td>2.629844</td><td>1.558270</td><td>3.190107</td><td>2.621586</td><td>1.555155</td></tr> </tbody> </table>		1	2	3	4	5	1 Co	0.000000					2 B	2.166042	0.000000				3 B	3.252153	2.722195	0.000000			4 B	2.101193	2.633171	2.918521	0.000000		5 B	2.985859	1.945378	2.910998	1.799268	0.000000	6 B	3.195966	2.772656	1.746075	1.759451	1.768874	7 B	3.525438	1.982715	1.800925	2.873433	1.756139	8 B	1.918150	1.769480	3.665005	1.756117	1.671915	9 B	2.085062	2.795918	1.759170	1.771178	2.828043	10 B	2.010548	2.104489	1.796719	2.937048	3.264572	11 N	2.974904	1.615259	1.637645	3.307199	2.743727		6	7	8	9	10	6 B	0.000000					7 B	1.743079	0.000000				8 B	2.881647	2.981919	0.000000			9 B	1.803875	2.799046	2.936478	0.000000		10 B	2.822502	2.688934	3.139561	1.750990	0.000000	11 N	2.629844	1.558270	3.190107	2.621586	1.555155
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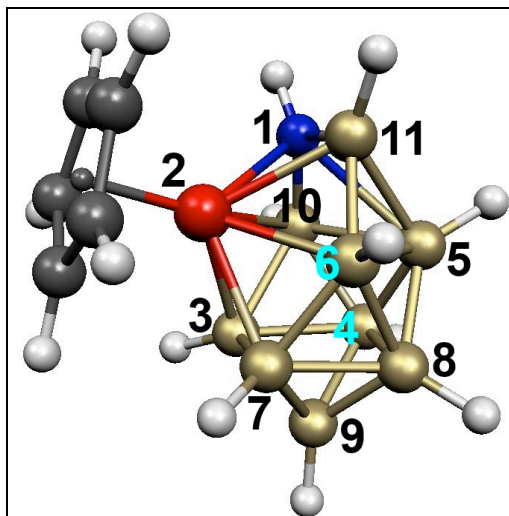
3. -1860.706413 +11.7 H/L 2.53 C<sub>1</sub>

	1	2	3	4	5
1 B	0.000000				
2 B	1.783560	0.000000			
3 B	3.642304	3.000211	0.000000		
4 B	3.013705	3.251783	1.671601	0.000000	
5 Co	2.003427	3.176755	3.224218	2.066829	0.000000
6 N	1.653995	1.561734	3.137193	2.777509	2.956590
7 B	1.886874	2.683100	2.968263	1.807907	1.990577
8 B	1.747054	1.732589	2.865132	2.853140	2.099343
9 B	2.730152	2.003061	1.744858	2.004961	3.186658
10 B	2.968241	2.910197	1.726216	1.806283	2.058688
11 B	2.918812	1.774785	1.662778	2.655015	3.217087
	6	7	8	9	10
6 N	0.000000				
7 B	1.547115	0.000000			
8 B	2.623413	2.821055	0.000000		
9 B	1.590685	2.000968	2.764793	0.000000	
10 B	3.326825	2.910523	1.786555	2.650740	0.000000
11 B	2.708484	3.175700	1.789990	1.902276	1.809807



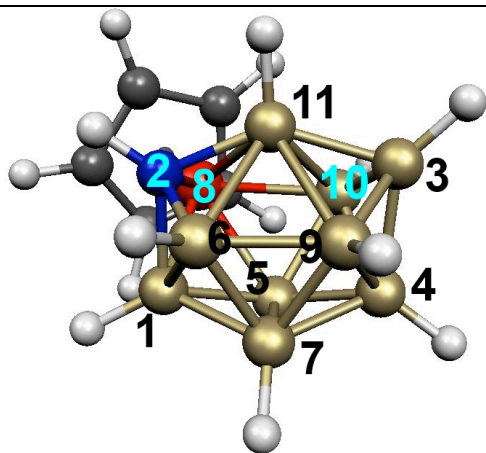
4. -1860.700713 +15.2 H/L 2.11 C<sub>s</sub>

	1	2	3	4	5
1 B	0.000000				
2 B	1.732259	0.000000			
3 B	2.794526	2.047392	0.000000		
4 B	2.841493	3.208750	1.934693	0.000000	
5 Co	2.045546	3.273235	3.024188	2.090076	0.000000
6 B	1.762554	1.796157	2.734837	2.924635	3.283307
7 B	1.837900	2.814946	2.794616	1.788859	2.045589
8 B	1.788881	1.786755	1.934660	2.652100	2.090022
9 B	2.814968	2.678800	2.047765	1.786771	3.273325
10 B	2.896367	3.011537	1.705694	1.688302	1.985117
11 N	2.622780	1.551875	1.612217	2.710547	3.719104
	6	7	8	9	10
6 B	0.000000				
7 B	1.762553	0.000000			
8 B	2.924737	2.841588	0.000000		
9 B	1.796104	1.732198	3.209028	0.000000	
10 B	3.631198	2.896420	1.688253	3.011766	0.000000
11 N	1.639231	2.622745	2.710738	1.551897	3.122841



5. -1860.697318 +17.4 H/L 2.45 C<sub>1</sub>

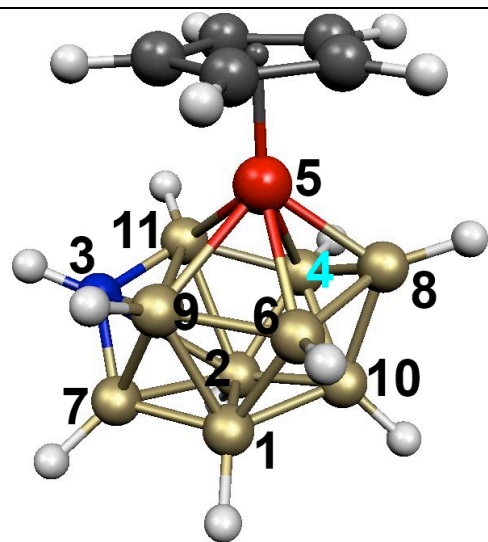
	1	2	3	4	5
1 N	0.000000				
2 Co	1.993387	0.000000			
3 B	2.914533	2.124200	0.000000		
4 B	2.933040	3.204918	1.882330	0.000000	
5 B	2.295795	2.972064	2.881533	1.748213	0.000000
6 B	2.674765	2.171784	2.813422	2.740472	1.749760
7 B	3.459164	2.179165	1.792548	2.562343	2.764258
8 B	3.577636	3.279653	2.588426	1.809103	1.731654
9 B	4.004481	3.342200	1.674303	1.704448	2.861946
10 B	1.476144	2.264776	1.871357	1.771541	2.122618
11 B	1.449613	2.153730	3.387273	3.204375	1.875564
	6	7	8	9	10
6 B	0.000000				
7 B	1.771047	0.000000			
8 B	1.762706	1.804472	0.000000		
9 B	2.881751	1.713973	1.688956	0.000000	
10 B	2.864213	2.998107	3.012749	2.948468	0.000000
11 B	1.720838	3.143007	3.072264	4.030834	2.456600



6. -1860.694856 +18.9 H/L 1.77 C<sub>1</sub>

	1	2	3	4	5
1 B	0.000000				
2 N	1.626052	0.000000			
3 B	3.579210	3.114997	0.000000		
4 B	2.933030	3.343156	1.757434	0.000000	
5 B	1.783619	2.691301	2.864049	1.766750	0.000000
6 B	1.824536	1.536509	2.923037	2.873529	2.826901
7 B	1.771393	2.627142	2.844628	1.755431	1.809818
8 Co	2.072331	1.908443	3.390102	3.342713	2.077876
9 B	2.948669	2.776125	1.660149	1.769262	2.833245
10 B	2.926145	2.800509	1.671653	1.797764	1.782873
11 B	2.662473	1.575749	1.727883	2.665175	2.766968
	6	7	8	9	10
6 B	0.000000				
7 B	1.736284	0.000000			
8 Co	3.112779	3.246668	0.000000		
9 B	1.788855	1.770937	3.733262	0.000000	
10 B	3.203399	2.813796	2.121600	2.661284	0.000000
11 B	2.018394	2.785395	2.343388	2.055860	1.940647





7. -1860.686559 +24.1 H/L 2.16 C<sub>1</sub>

	1	2	3	4	5
1 B	0.000000				
2 B	1.747319	0.000000			
3 N	2.611461	2.359893	0.000000		
4 B	2.752879	1.732137	2.906003	0.000000	
5 Co	3.192750	3.208205	2.836054	2.170164	0.000000
6 B	1.763176	2.737068	3.176988	2.564855	2.054691
7 B	1.686765	1.915639	1.447774	3.192806	3.564108
8 B	2.920006	2.893910	3.880236	1.746079	1.924975
9 B	1.895095	2.660247	1.703292	2.914670	2.103614
10 B	1.741252	1.752797	3.515726	1.821480	2.948479
11 B	2.939356	2.064577	1.499350	1.720526	2.088295
	6	7	8	9	10
6 B	0.000000				
7 B	2.992521	0.000000			
8 B	1.757798	4.004451	0.000000		
9 B	1.782042	1.900990	3.036694	0.000000	
10 B	1.805896	3.056907	1.710599	2.891794	0.000000
11 B	3.026132	2.467361	2.991067	2.261355	3.015826

Table S4C. Energy ranking for all of the CpCoNHB<sub>9</sub>H<sub>9</sub> optimized structures:

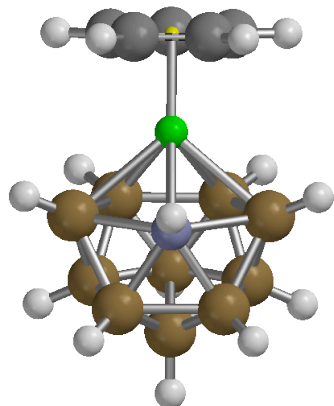
No	Initial structure	Final energy (a.u.)	$\Delta E$ ( kcal/mol)
1	TricapCubeA-Co3-h	-1860.5406611	0.00
2	Icos-1vx-Co4-a	-1860.5406607	0.00
3	TricapCubeB-Co5-d	-1860.5406601	0.00
4	Icos-1vx-Co1-a_r-50	-1860.5406600	0.00
5	Icos-1vx-Co2-a	-1860.5406600	0.00
6	Icos-1vx-Co5-g	-1860.5406600	0.00
7	TricapCubeA-Co3-b	-1860.5406600	0.00
8	Icos-1vx-Co3-f	-1860.5406597	0.00
9	TricapCubeB-Co5-a	-1860.5406588	0.00
10	TricapCubeA-Co1-a	-1860.5406575	0.00
11	TricapCubeB-Co3-a	-1860.5406506	0.01
12	Icos-1vx-Co1-a_i-50	-1860.5391627	0.94
13	TricapCubeB-Co1-b	-1860.5310072	6.06
14	TricapCubeB-Co4-e	-1860.5310024	6.06
15	TricapCubeB-Co5-f	-1860.5310013	6.06
16	TricapCubeA-Co3-f	-1860.5310006	6.06
17	Icos-1vx-Co1-c	-1860.5310003	6.06
18	TricapCubeA-Co3-i	-1860.5310000	6.06
19	TricapCubeB-Co3-d	-1860.5309995	6.06
20	TricapCubeA-Co2-h	-1860.5309989	6.06
21	TricapCubeA-Co3-j	-1860.5309973	6.06
22	Icos-1vx-Co4-b_r-71	-1860.5309970	6.06
23	TricapCubeA-Co2-g	-1860.5309967	6.06
24	OhfusettoPentBipyr-Co4-h	-1860.5309965	6.06
25	TricapCubeA-Co3-a	-1860.5309949	6.07
26	Icos-1vx-Co4-e	-1860.5309948	6.07
27	TricapCubeB-Co5-g	-1860.5309947	6.07
28	Icos-1vx-Co5-e	-1860.5309942	6.07
29	Icos-1vx-Co2-f	-1860.5309940	6.07
30	TricapCubeA-Co2-e	-1860.5309935	6.07
31	Icos-1vx-Co2-b	-1860.5309932	6.07
32	TricapCubeB-Co3-b	-1860.5309919	6.07
33	PentaCapTrPr-Co2-b	-1860.5309912	6.07
34	TricapCubeB-Co2-a	-1860.5309657	6.08
35	TricapCubeB-Co4-a	-1860.5309657	6.08
36	Icos-1vx-Co4-f	-1860.5309649	6.08
37	Icos-1vx-Co5-f	-1860.5309643	6.08
38	PentaCapTrPr-Co1-a	-1860.5309639	6.09
39	TricapCubeB-Co1-d	-1860.5309639	6.09
40	TricapCubeB-Co4-g	-1860.5309639	6.09
41	Icos-1vx-Co5-a	-1860.5309635	6.09

42	TricapCubeA-Co3-c	-1860.5309618	6.09
43	TricapCubeB-Co2-g	-1860.5309618	6.09
44	TricapCubeA-Co2-a	-1860.5309602	6.09
45	TricapCubeB-Co1-a	-1860.5309601	6.09
46	Icos-1vx-Co2-g_r-45	-1860.5285598	7.59
47	Icos-1vx-Co2-g_i-45	-1860.5280759	7.90
48	Icos-1vx-Co3-d	-1860.5219858	11.72
49	TricapCubeA-Co3-d	-1860.5219838	11.72
50	TricapCubeA-Co2-c	-1860.5219833	11.72
51	TricapCubeA-Co1-b	-1860.5219832	11.72
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53	TricapCubeA-Co1-c	-1860.5219827	11.72
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56	Icos-1vx-Co5-d_r-42	-1860.5219816	11.72
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71	TricapCubeA-Co2-b	-1860.5138657	16.81
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74	OhfusettoPentBipyr-Co1-e	-1860.5134715	17.06
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78	OhfusettoPentBipyr-Co2-g	-1860.5075895	20.75
79	PentaCapTrPr-Co1-c	-1860.5068186	21.24
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81	Icos-1vx-Co4-b_i-71	-1860.5067825	21.26
82	PentaCapTrPr-Co2-c	-1860.5030906	23.58
83	TricapCubeB-Co5-c	-1860.5027503	23.79
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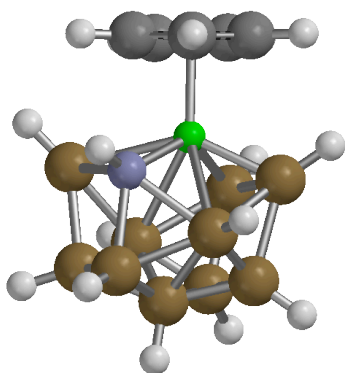
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88	TricapCubeB-Co1-c	-1860.4936402	29.51
89	TricapCubeB-Co3-c	-1860.4936272	29.51
90	PentaCapTrPr-Co2-a	-1860.4921287	30.46
91	Icos-1vx-Co1-b_r-230	-1860.4882015	32.92
92	TricapCubeA-Co2-i	-1860.4881999	32.92
93	PentaCapTrPr-Co1-d	-1860.4881994	32.92
94	OhfusetopentBipyr-Co3-d_r-91	-1860.4826198	36.42
95	OhfusetopentBipyr-Co2-b_r-240	-1860.4761814	40.46
96	Icos-1vx-Co4-d	-1860.4745088	41.51
97	Icos-1vx-Co2-j	-1860.4745073	41.51
98	OhfusetopentBipyr-Co4-c_r-76	-1860.4740844	41.78
99	Icos-1vx-Co3-a	-1860.4722010	42.96
100	PentaCapTrPr-Co2-d	-1860.4718086	43.21
101	Icos-1vx-Co1-d	-1860.4718076	43.21
102	PentaCapTrPr-Co1-g	-1860.4716112	43.33
103	TricapCubeB-Co2-d	-1860.4693993	44.72
104	TricapCubeB-Co4-d	-1860.4693991	44.72
105	Icos-1vx-Co3-b_i-227	-1860.4690599	44.93
106	OhfusetopentBipyr-Co2-d	-1860.4687048	45.15
107	TricapCubeB-Co2-b	-1860.4683952	45.35
108	TricapCubeB-Co4-b	-1860.4683950	45.35
109	TricapCubeB-Co5-e	-1860.4683925	45.35
110	Icos-1vx-Co2-i	-1860.4683912	45.35
111	Icos-1vx-Co2-h	-1860.4680749	45.55
112	Icos-1vx-Co4-g	-1860.4646284	47.71
113	Icos-1vx-Co5-d_i-42	-1860.4631972	48.61
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118	PentaCapTrPr-Co1-f	-1860.4556611	53.34
119	Icos-1vx-Co4-c	-1860.4544672	54.09
120	OhfusetopentBipyr-Co3-h	-1860.4499662	56.91
121	OhfusetopentBipyr-Co1-b_r-228	-1860.4440236	60.64
122	OhfusetopentBipyr-Co1-c	-1860.4381062	64.36
123	OhfusetopentBipyr-Co4-d	-1860.4323636	67.96
124	PentaCapTrPr-Co1-b	-1860.4282043	70.57
125	OhfusetopentBipyr-Co1-g	-1860.4276778	70.90
126	OhfusetopentBipyr-Co2-f	-1860.4229047	73.89
127	OhfusetopentBipyr-Co3-d_i-91	-1860.4204911	75.41
128	OhfusetopentBipyr-Co2-b_i-240	-1860.4204338	75.45
129	OhfusetopentBipyr-Co4-e	-1860.4127011	80.30

130	OhfusettoPentBipyr-Co3-e	-1860.4121568	80.64
131	OhfusettoPentBipyr-Co3-c	-1860.4093826	82.38
132	OhfusettoPentBipyr-Co4-f_r-71	-1860.4051838	85.01
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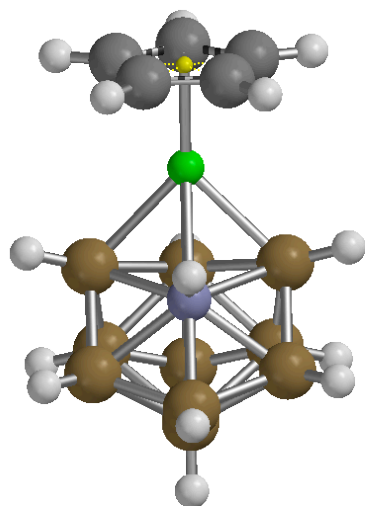
Table S5A. Initial CpCoNHB<sub>10</sub>H<sub>10</sub> structures, 35 in all.



Icosahedron 3

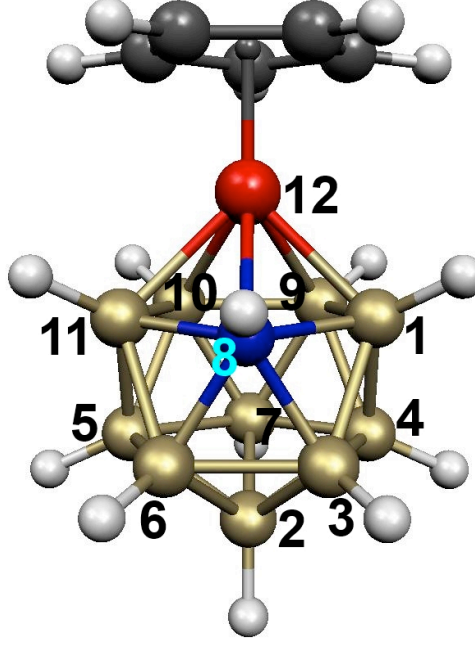
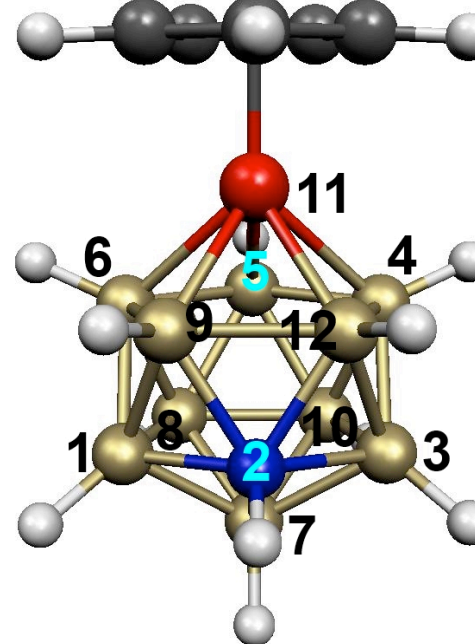


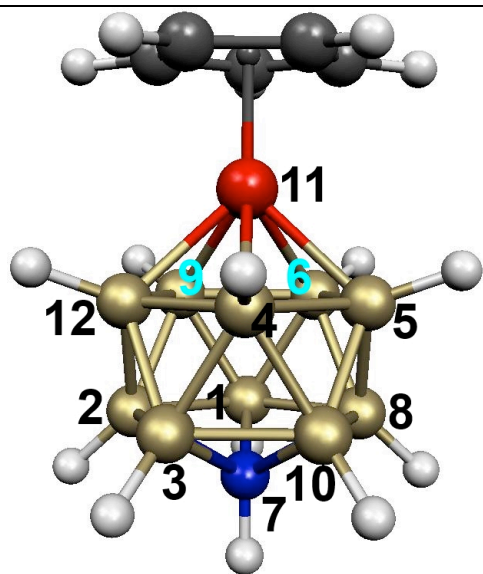
Cubeoctahedron 20



Anticubeoctahedron 12

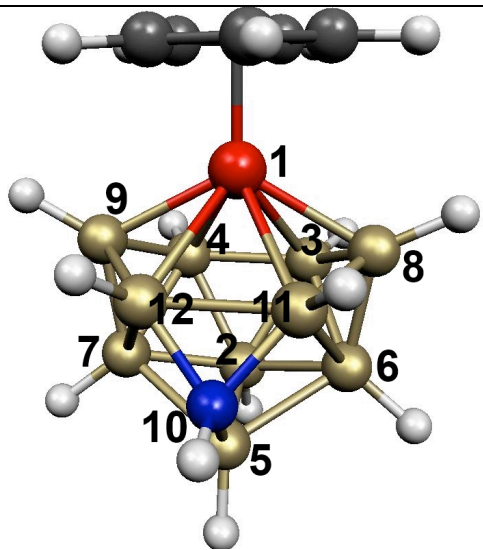
Table S5B. Distance table for the lowest-lying CpCoNHB<sub>10</sub>H<sub>10</sub> structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.

 <p>1. -1886.206878 0.0 H/L 2.68 C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.859943</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.798982</td><td>1.747438</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.742069</td><td>1.772849</td><td>1.746139</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.354216</td><td>1.772787</td><td>2.851775</td><td>2.867700</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.883472</td><td>1.747436</td><td>1.772600</td><td>2.851715</td><td>1.746234</td></tr> <tr><td>7 B</td><td>2.841228</td><td>1.759097</td><td>2.842484</td><td>1.773133</td><td>1.773037</td></tr> <tr><td>8 N</td><td>1.693648</td><td>2.680558</td><td>1.680066</td><td>2.677772</td><td>2.677811</td></tr> <tr><td>9 B</td><td>1.777896</td><td>2.877156</td><td>2.895905</td><td>1.780958</td><td>2.874040</td></tr> <tr><td>10 B</td><td>2.871372</td><td>2.877163</td><td>3.395885</td><td>2.874092</td><td>1.780956</td></tr> <tr><td>11 B</td><td>2.865000</td><td>2.859990</td><td>2.883659</td><td>3.354261</td><td>1.742153</td></tr> <tr><td>12 Co</td><td>2.059489</td><td>3.848910</td><td>3.304458</td><td>3.275017</td><td>3.275015</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.842470</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 N</td><td>1.679951</td><td>3.157153</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.395772</td><td>1.765183</td><td>2.738788</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.895934</td><td>1.765145</td><td>2.738861</td><td>1.774400</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.799046</td><td>2.841220</td><td>1.693718</td><td>2.871309</td><td>1.777909</td></tr> <tr><td>12 Co</td><td>3.304358</td><td>3.282449</td><td>2.027482</td><td>2.088118</td><td>2.088159</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 Co</td><td>2.059418</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.859943	0.000000				3 B	1.798982	1.747438	0.000000			4 B	1.742069	1.772849	1.746139	0.000000		5 B	3.354216	1.772787	2.851775	2.867700	0.000000	6 B	2.883472	1.747436	1.772600	2.851715	1.746234	7 B	2.841228	1.759097	2.842484	1.773133	1.773037	8 N	1.693648	2.680558	1.680066	2.677772	2.677811	9 B	1.777896	2.877156	2.895905	1.780958	2.874040	10 B	2.871372	2.877163	3.395885	2.874092	1.780956	11 B	2.865000	2.859990	2.883659	3.354261	1.742153	12 Co	2.059489	3.848910	3.304458	3.275017	3.275015		6	7	8	9	10	6 B	0.000000					7 B	2.842470	0.000000				8 N	1.679951	3.157153	0.000000			9 B	3.395772	1.765183	2.738788	0.000000		10 B	2.895934	1.765145	2.738861	1.774400	0.000000	11 B	1.799046	2.841220	1.693718	2.871309	1.777909	12 Co	3.304358	3.282449	2.027482	2.088118	2.088159		11	12				11 B	0.000000					12 Co	2.059418	0.000000			
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 <p>2. -1886.205739 +0.7 H/L 3.22 C<sub>s</sub></p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 N</td><td>1.683010</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.892100</td><td>1.683065</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.387557</td><td>2.683217</td><td>1.747790</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.847344</td><td>3.134390</td><td>2.847365</td><td>1.789419</td><td>0.000000</td></tr> <tr><td>6 B</td><td>1.747736</td><td>2.683090</td><td>3.387490</td><td>2.911600</td><td>1.789407</td></tr> <tr><td>7 B</td><td>1.795134</td><td>1.699388</td><td>1.795162</td><td>2.868268</td><td>2.835071</td></tr> <tr><td>8 B</td><td>1.751300</td><td>2.670150</td><td>2.863737</td><td>2.885970</td><td>1.769960</td></tr> <tr><td>9 B</td><td>1.784552</td><td>1.707604</td><td>2.919836</td><td>2.909516</td><td>2.867844</td></tr> <tr><td>10 B</td><td>2.863715</td><td>2.670194</td><td>1.751362</td><td>1.777730</td><td>1.769944</td></tr> <tr><td>11 Co</td><td>3.233019</td><td>3.042614</td><td>3.233025</td><td>2.064937</td><td>2.075118</td></tr> <tr><td>12 B</td><td>2.919829</td><td>1.707647</td><td>1.784526</td><td>1.757321</td><td>2.867808</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>2.868211</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.777720</td><td>1.735763</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.757265</td><td>2.919761</td><td>2.873116</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.885923</td><td>1.735781</td><td>1.775100</td><td>3.396023</td><td>0.000000</td></tr> <tr><td>11 Co</td><td>2.064869</td><td>3.808696</td><td>3.267467</td><td>1.998843</td><td>3.267472</td></tr> <tr><td>12 B</td><td>2.909395</td><td>2.919751</td><td>3.395988</td><td>1.846700</td><td>2.873109</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>11 Co</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>12 B</td><td>1.998821</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 N	1.683010	0.000000				3 B	2.892100	1.683065	0.000000			4 B	3.387557	2.683217	1.747790	0.000000		5 B	2.847344	3.134390	2.847365	1.789419	0.000000	6 B	1.747736	2.683090	3.387490	2.911600	1.789407	7 B	1.795134	1.699388	1.795162	2.868268	2.835071	8 B	1.751300	2.670150	2.863737	2.885970	1.769960	9 B	1.784552	1.707604	2.919836	2.909516	2.867844	10 B	2.863715	2.670194	1.751362	1.777730	1.769944	11 Co	3.233019	3.042614	3.233025	2.064937	2.075118	12 B	2.919829	1.707647	1.784526	1.757321	2.867808		6	7	8	9	10	6 B	0.000000					7 B	2.868211	0.000000				8 B	1.777720	1.735763	0.000000			9 B	1.757265	2.919761	2.873116	0.000000		10 B	2.885923	1.735781	1.775100	3.396023	0.000000	11 Co	2.064869	3.808696	3.267467	1.998843	3.267472	12 B	2.909395	2.919751	3.395988	1.846700	2.873109		11	12				11 Co	0.000000					12 B	1.998821	0.000000			
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3. -1886.201259 +3.5 H/L 3.20  $C_{5v}$

	1	2	3	4	5
1 B	0.000000				
2 B	1.791796	0.000000			
3 B	2.898829	1.791939	0.000000		
4 B	3.390039	2.875785	1.747009	0.000000	
5 B	2.875641	3.391027	2.876233	1.800421	0.000000
6 B	1.746890	2.875824	3.389972	2.911626	1.799138
7 N	1.686321	1.686887	1.686241	2.673289	2.673559
8 B	1.791594	2.899381	2.898979	2.875837	1.747096
9 B	1.747192	1.747142	2.876290	2.912665	2.913180
10 B	2.899645	2.900143	1.792074	1.746175	1.746455
11 Co	3.220235	3.220271	3.220243	2.052174	2.052935
12 B	2.875518	1.746532	1.746473	1.799693	2.912976
	6	7	8	9	10
6 B	0.000000				
7 N	2.673025	0.000000			
8 B	1.746683	1.686128	0.000000		
9 B	1.800582	2.674051	2.876488	0.000000	
10 B	2.875090	1.687405	1.792221	3.391286	0.000000
11 Co	2.052618	3.558500	3.220733	2.052829	3.219691
12 B	2.912431	2.673088	3.390474	1.800520	2.875429
	11	12			
11 Co	0.000000				
12 B	2.052879	0.000000			



4. -1886.137805 +43.3 H/L 2.61  $C_s$

	1	2	3	4	5
1 Co	0.000000				
2 B	3.071312	0.000000			
3 B	2.135321	1.786123	0.000000		
4 B	2.130642	1.783603	1.755181	0.000000	
5 B	3.573012	1.707165	3.020987	3.016630	0.000000
6 B	3.006868	1.753789	1.807784	2.925487	1.930712
7 B	3.007389	1.754653	2.931188	1.806861	1.929850
8 B	2.052670	2.825805	1.710951	3.038869	3.168033
9 B	2.050158	2.824151	3.043884	1.713036	3.160707
10 N	3.178464	2.801403	3.492482	3.491236	1.495232
11 B	2.266559	2.946768	2.762902	3.318012	2.390057
12 B	2.266566	2.944538	3.320807	2.762931	2.382417
	6	7	8	9	10
6 B	0.000000				
7 B	3.024629	0.000000			
8 B	1.648440	3.690963	0.000000		
9 B	3.685333	1.645860	3.600233	0.000000	
10 N	2.466973	2.476366	3.008536	3.008190	0.000000
11 B	1.988239	3.134813	1.689561	3.130725	1.536633
12 B	3.124999	1.993472	3.130223	1.690966	1.533766
	11	12			
11 B	0.000000				
12 B	1.928453	0.000000			



Table S5C. Energy ranking for all of the CpCoNHB<sub>10</sub>H<sub>10</sub> optimized structures:

No	Initial structure	Final energy (a.u.)	$\Delta E$ ( kcal/mol)
1	Anticuboh-Co3-f	-1886.0120089	0.00
2	Anticuboh-Co3-a_r-267	-1886.0120083	0.00
3	Cuboctaedru-Co2-a	-1886.0120055	0.00
4	Anticuboh-Co1-d	-1886.0120052	0.00
5	Anticuboh-Co1-a	-1886.0120049	0.00
6	Anticuboh-Co3-e	-1886.0120047	0.00
7	Cuboctaedru-Co1-b	-1886.0120045	0.00
8	Cuboctaedru-Co2-e	-1886.0120036	0.00
9	Cuboctaedru-Co2-f	-1886.0120009	0.01
10	Icos-Co-a	-1886.0120005	0.01
11	Cuboctaedru-Co1-a	-1886.0119999	0.01
12	Anticuboh-Co3-d	-1886.0106949	0.82
13	Icos-Co-b	-1886.0106930	0.83
14	Cuboctaedru-Co2-d	-1886.0106913	0.83
15	Cuboctaedru-Co2-h	-1886.0106911	0.83
16	Cuboctaedru-Co2-g	-1886.0106903	0.83
17	Anticuboh-Co2-b_r-330	-1886.0106893	0.83
18	Cuboctaedru-Co2-b	-1886.0106882	0.83
19	Cuboctaedru-Co1-c	-1886.0106869	0.83
20	Icos-Co-c	-1886.0050772	4.35
21	Cuboctaedru-Co1-d	-1886.0050162	4.39
22	Cuboctaedru-Co2-c	-1886.0049887	4.41
23	Anticuboh-Co1-e	-1886.0049765	4.41
24	Anticuboh-Co2-e	-1885.9510681	38.24
25	Anticuboh-Co2-d	-1885.9457810	41.56
26	Anticuboh-Co2-c	-1885.9393122	45.62
27	Anticuboh-Co3-b	-1885.9342017	48.83
28	Anticuboh-Co3-g	-1885.9306984	51.02
29	Anticuboh-Co2-a	-1885.9305291	51.13
30	Anticuboh-Co3-c_r-332	-1885.9303060	51.27
31	Anticuboh-Co3-c_i-332	-1885.9295732	51.73
32	Anticuboh-Co1-b	-1885.9135172	61.81
33	Anticuboh-Co3-a_i-267	-1885.9062007	66.40
34	Anticuboh-Co1-c	-1885.9020220	69.02
35	Anticuboh-Co2-b_i-330	-1885.8500313	101.64