

Supporting Information file

Biicosahedral Metallaboranes: Aromaticity in Metal Derivatives of Three-dimensional Analogues of Naphthalene

Amr A. A. Attia,¹ Alexandru Lupan,^{*1} and R. Bruce King^{*2}

¹ *Department of Chemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, Cluj-Napoca, Romania*

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

Table S1. Distance table for the CpNiB₂₀H₁₇ structures.

Table S2. Distance table for the CpCoB₁₉H₁₇ structures.

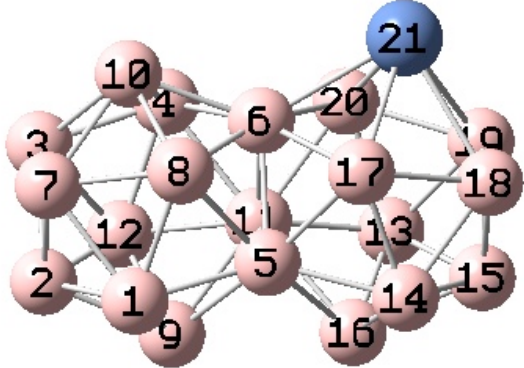
Table S3. Distance table for the CpFeB₂₀H₁₇ structures.

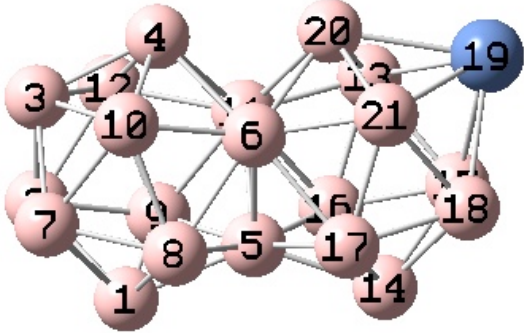
Table S4. Orbital energies and HOMO/LUMO gaps.

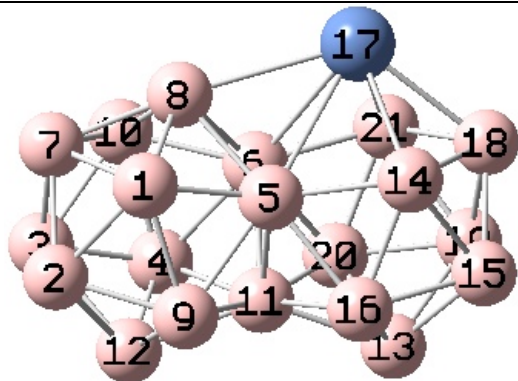
Complete Gaussian09 Reference (reference 26)

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 S1. Distance table for the CpNiB₂₀H₁₇ 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. For clarity, only the atoms forming the biicosahedral framework are presented.

 1. -2209.2534662 0.0 H/L 2.81 Cs	1	2	3	4	5
	1 B	0.000000			
	2 B	1.785945	0.000000		
	3 B	2.869169	1.737611	0.000000	
	4 B	3.418488	2.854858	1.743120	0.000000
	5 B	1.781374	2.892549	3.397907	2.966293
	6 B	2.874601	3.363281	2.869707	1.843458
	7 B	1.786085	1.737562	1.745514	2.864023
	8 B	1.772141	2.854852	2.864009	2.958571
	9 B	1.772259	1.732479	2.852818	2.949155
	10 B	2.883531	2.858356	1.786575	1.777653
	11 B	2.897296	2.892479	2.896611	1.857829
	12 B	2.888549	1.785929	1.786023	1.772119
	13 B	4.414331	4.612292	4.619281	3.260118
	14 B	3.342363	4.612503	5.134666	4.375628
	15 B	4.615712	5.416604	5.698705	4.508421
	16 B	3.259719	3.889496	4.506640	3.704408
	17 B	3.235956	4.493212	4.519643	3.731318
	18 B	4.634304	5.712593	5.730576	4.540264
	19 B	5.155103	5.712463	5.454970	3.923121
	20 B	4.382676	4.492857	3.891496	2.229720
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		6	7	8	9
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	14 B	2.913949	4.619583	3.260589	3.258970
	15 B	3.427412	5.698849	4.508893	3.891202
	16 B	2.974988	4.506705	3.704718	2.239739
	17 B	1.909943	3.891993	2.230409	3.690422
	18 B	2.966441	5.455283	3.923728	4.517818
	19 B	2.966382	5.730632	4.540734	4.517727
	20 B	1.909757	4.519448	3.731551	3.690149
	21 Ni	2.051327	4.799156	3.439123	4.738243
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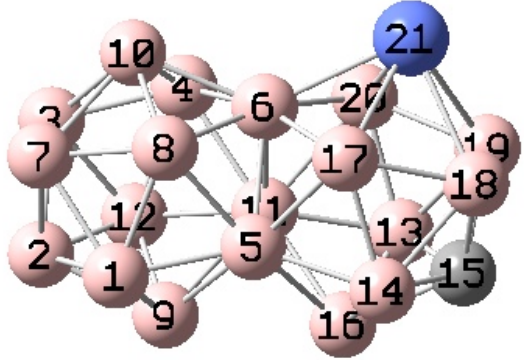
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	16 17 18 19 20 16 B 0.000000 17 B 2.942207 0.000000 18 B 2.854086 1.781323 0.000000 19 B 2.854093 2.917826 1.765335 0.000000 20 B 2.942151 3.025249 2.917835 1.781348 0.000000 21 Ni 3.837119 2.066599 2.096886 2.096863 2.066609					
 2. -2209.2381775 +9.6 H/L 2.62 C_s	1 2 3 4 5 1 B 0.000000 2 B 1.786935 0.000000 3 B 2.866693 1.740504 0.000000 4 B 3.415232 2.845968 1.723910 0.000000 5 B 1.770368 2.886497 3.394298 2.979258 0.000000 6 B 2.889700 3.383307 2.886894 1.864622 1.810463 7 B 1.786946 1.746237 1.740484 2.845966 2.886509 8 B 1.778197 2.862184 2.861361 2.960069 1.863337 9 B 1.778194 1.735314 2.861376 2.960022 1.863252 10 B 2.892323 2.870497 1.787847 1.769159 2.902358 11 B 2.889688 2.884107 2.886874 1.864601 1.810465 12 B 2.892296 1.786390 1.787841 1.769141 2.902334 13 B 4.389539 4.588087 4.611214 3.283614 2.886856 14 B 3.318619 4.597275 5.124932 4.392544 1.777245 15 B 4.582150 5.393025 5.691973 4.536301 2.882608 16 B 3.224094 3.858644 4.487774 3.714294 1.844990 17 B 3.224156 4.475972 4.487863 3.714391 1.845052 18 B 4.582179 5.675203 5.692022 4.536359 2.882639 19 Ni 5.563526 6.100317 5.792145 4.239416 3.841477 20 B 4.317773 4.443945 3.842196 2.210536 2.926739 21 B 4.389529 5.116360 4.611213 3.283629 2.886850 6 7 8 9 10 6 B 0.000000 7 B 2.884136 0.000000 8 B 1.864141 1.735274 0.000000 9 B 2.964808 2.862192 2.966879 0.000000 10 B 1.779646 1.786410 1.781359 3.427906 0.000000 11 B 1.791596 3.383290 2.964879 1.864048 2.889059 12 B 2.889053 2.870464 3.427915 1.781345 2.891036 13 B 2.903805 5.116365 4.374179 3.228410 4.422815 14 B 2.905807 4.597295 3.250327 3.250223 4.416948 15 B 3.413841 5.675173 4.497953 3.863315 5.142338					

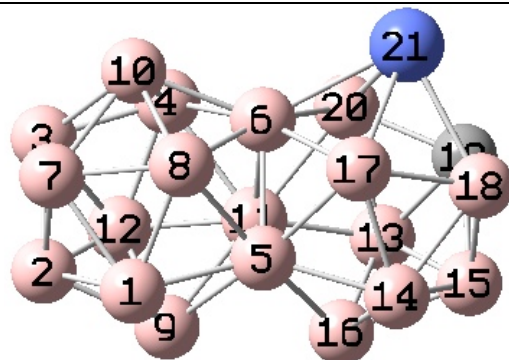
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	18 B	2.907019	5.393079	3.863444	4.497887	4.612388
	19 Ni	3.291542	6.100319	4.917692	4.917607	4.979599
	20 B	1.813062	4.443958	3.657210	3.657105	3.211718
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	16 B	1.869659	3.249815	1.765958	1.773151	1.729652
	17 B	2.962119	4.367954	3.430418	1.773159	2.874008
	18 B	3.413906	5.142368	2.913809	1.773085	1.788271
	19 Ni	3.291573	4.979602	2.090350	3.255516	2.047599
	20 B	1.813050	3.211688	1.804320	3.406285	2.895651
	21 B	2.903830	4.422809	2.935810	2.885469	2.913784
		16	17	18	19	20
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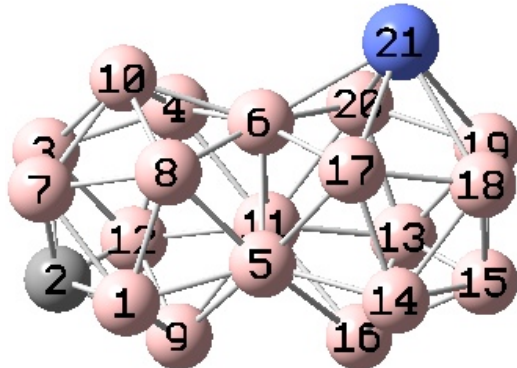
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5 B	1.768155	2.886804	3.385978	2.983517	0.000000
6 B	2.898923	3.385944	2.887076	1.877365	1.809345
7 B	1.799212	1.739500	1.739424	2.866137	2.878957
8 B	1.772122	2.826310	2.826360	2.923103	1.800612
9 B	1.773982	1.740534	2.858343	2.971421	1.876743
10 B	2.916607	2.870066	1.786438	1.774030	2.898988
11 B	2.877333	2.887758	2.887949	1.868219	1.792070
12 B	2.882334	1.785662	1.785743	1.770752	2.891610
13 B	4.392026	4.612075	4.612345	3.263245	2.881234
14 B	3.355492	4.645241	5.154801	4.420533	1.818404
15 B	4.602221	5.420088	5.692564	4.521142	2.902685
16 B	3.191425	3.853558	4.460017	3.682597	1.804764
17 Ni	3.495672	4.843087	4.843174	4.170071	2.300833
18 B	4.706822	5.783594	5.783819	4.603626	2.998816
19 B	5.126479	5.692413	5.420480	3.904503	3.404324
20 B	4.322395	4.460048	3.854071	2.214703	2.920366
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	6	7	8	9	10

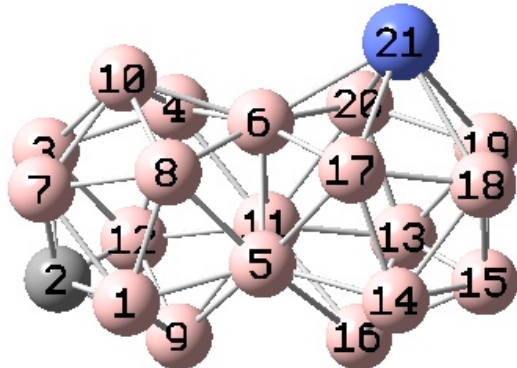
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14 B	2.920121	4.625060	3.227376	3.310913	4.435780	
15 B	3.404318	5.681358	4.443799	3.903615	5.126664	
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17 Ni	2.300713	4.061013	2.331947	4.169577	3.495687	
18 B	2.998819	5.508532	3.949520	4.602840	4.707052	
19 B	2.902781	5.681479	4.443891	4.520329	4.602605	
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21 B	1.818491	4.625282	3.227579	4.419881	3.355860	
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13 B	1.788012	3.347350	0.000000			
14 B	2.922051	4.449639	2.884040	0.000000		
15 B	2.902520	4.619255	1.770773	1.787963	0.000000	
16 B	1.833836	3.235436	1.777588	1.773802	1.753183	
17 Ni	3.509895	4.859320	3.953677	2.095736	3.301203	
18 B	3.466056	5.211798	2.863209	1.829039	1.728872	
19 B	2.902539	4.619302	1.770781	2.870833	1.748447	
20 B	1.833871	3.235546	1.777575	3.398788	2.857804	
21 B	2.922066	4.449690	2.884053	2.885397	2.870879	
	16	17	18	19	20	
16 B	0.000000					
17 Ni	3.415717	0.000000				
18 B	2.885799	2.097070	0.000000			
19 B	2.857833	3.301169	1.728850	0.000000		
20 B	2.913164	3.415652	2.885756	1.753163	0.000000	
21 B	3.398838	2.095691	1.829075	1.787985	1.773758	

Table S2. Distance table for the CpCoB₁₉H₁₇ 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. For clarity, only the atoms forming the biicosahedral framework are presented.

 1. -2096.9837691 0.0 H/L 3.41 C_s	1 2 3 4 5					
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	2 B	1.790710	0.000000			
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	4 B	3.419872	2.862107	1.738210	0.000000	
	5 B	1.779024	2.890571	3.380510	2.952398	0.000000
	6 B	2.911617	3.411631	2.900132	1.861856	1.810941
	7 B	1.783215	1.739742	1.746332	2.859164	2.880881
	8 B	1.778469	2.862105	2.859168	2.951016	1.852084
	9 B	1.767470	1.725829	2.839865	2.947754	1.861201
	10 B	2.882347	2.862859	1.785910	1.768545	2.875112
	11 B	2.888695	2.890588	2.880905	1.852111	1.791377
	12 B	2.891396	1.790714	1.783217	1.778467	2.888686
	13 B	4.402376	4.604280	4.598603	3.247963	2.884168
	14 B	3.328720	4.604255	5.114690	4.361265	1.782095
	15 C	4.465663	5.267222	5.521564	4.340640	2.747533
	16 B	3.225743	3.857621	4.463271	3.673179	1.839489
	17 B	3.279057	4.533252	4.531632	3.731920	1.886939
	18 B	4.625549	5.709496	5.715876	4.529847	2.911297
	19 B	5.146999	5.709526	5.440039	3.913958	3.410685
	20 B	4.407496	4.533328	3.911268	2.252897	2.989031
	21 Co	4.734345	5.444753	4.837300	3.472305	3.261309
	6 7 8 9 10					
	6 B	0.000000				
	7 B	2.900139	0.000000			
	8 B	1.861879	1.738211	0.000000		
	9 B	2.981625	2.839864	2.947748	0.000000	
	10 B	1.771944	1.785906	1.768546	3.398369	0.000000
	11 B	1.810924	3.380521	2.952395	1.861207	2.875126
	12 B	2.911595	2.868657	3.419866	1.767470	2.882346
	13 B	2.898080	5.114708	4.361256	3.254061	4.397026
	14 B	2.898080	4.598551	3.247893	3.254058	4.396990
	15 C	3.239882	5.521543	4.340594	3.763419	4.953586
	16 B	2.957001	4.463255	3.673141	2.214924	4.334092
	17 B	1.892369	3.911163	2.252783	3.732097	3.279107
	18 B	2.932119	5.439980	3.913879	4.514726	4.643861
	19 B	2.932137	5.715896	4.529839	4.514741	4.643904
	20 B	1.892412	4.531718	3.731982	3.732135	3.279211
	21 Co	2.046192	4.837295	3.472296	4.755691	3.478716
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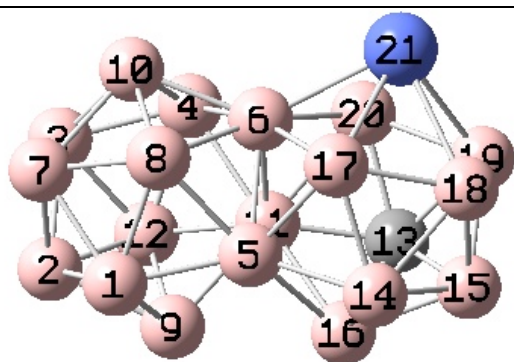
	<table><tr><td>14</td><td>B</td><td>2.884172</td><td>4.402379</td><td>2.870725</td><td>0.000000</td><td></td></tr><tr><td>15</td><td>C</td><td>2.747546</td><td>4.465694</td><td>1.694647</td><td>1.694641</td><td>0.000000</td></tr><tr><td>16</td><td>B</td><td>1.839506</td><td>3.225773</td><td>1.767702</td><td>1.767699</td><td>1.653614</td></tr><tr><td>17</td><td>B</td><td>2.988993</td><td>4.407436</td><td>3.428273</td><td>1.772506</td><td>2.733262</td></tr><tr><td>18</td><td>B</td><td>3.410679</td><td>5.146998</td><td>2.864720</td><td>1.774074</td><td>1.662367</td></tr><tr><td>19</td><td>B</td><td>2.911321</td><td>4.625600</td><td>1.774089</td><td>2.864709</td><td>1.662356</td></tr><tr><td>20</td><td>B</td><td>1.886969</td><td>3.279122</td><td>1.772486</td><td>3.428275</td><td>2.733243</td></tr><tr><td>21</td><td>Co</td><td>3.261301</td><td>4.734342</td><td>3.229787</td><td>3.229785</td><td>3.086607</td></tr><tr><td></td><td></td><td>16</td><td>17</td><td>18</td><td>19</td><td>20</td></tr><tr><td>16</td><td>B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>17</td><td>B</td><td>2.958443</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>18</td><td>B</td><td>2.853301</td><td>1.756686</td><td>0.000000</td><td></td><td></td></tr><tr><td>19</td><td>B</td><td>2.853304</td><td>2.893527</td><td>1.762350</td><td>0.000000</td><td></td></tr><tr><td>20</td><td>B</td><td>2.958449</td><td>2.999702</td><td>2.893510</td><td>1.756673</td><td>0.000000</td></tr><tr><td>21</td><td>Co</td><td>3.812844</td><td>2.026917</td><td>2.050173</td><td>2.050184</td><td>2.026915</td></tr></table>	14	B	2.884172	4.402379	2.870725	0.000000		15	C	2.747546	4.465694	1.694647	1.694641	0.000000	16	B	1.839506	3.225773	1.767702	1.767699	1.653614	17	B	2.988993	4.407436	3.428273	1.772506	2.733262	18	B	3.410679	5.146998	2.864720	1.774074	1.662367	19	B	2.911321	4.625600	1.774089	2.864709	1.662356	20	B	1.886969	3.279122	1.772486	3.428275	2.733243	21	Co	3.261301	4.734342	3.229787	3.229785	3.086607			16	17	18	19	20	16	B	0.000000					17	B	2.958443	0.000000				18	B	2.853301	1.756686	0.000000			19	B	2.853304	2.893527	1.762350	0.000000		20	B	2.958449	2.999702	2.893510	1.756673	0.000000	21	Co	3.812844	2.026917	2.050173	2.050184	2.026915																																																																																																																														
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C₁	<table><tr><td></td><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td></tr><tr><td>1</td><td>B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>2</td><td>B</td><td>1.788615</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>3</td><td>B</td><td>2.871911</td><td>1.739308</td><td>0.000000</td><td></td><td></td></tr><tr><td>4</td><td>B</td><td>3.413496</td><td>2.844740</td><td>1.731845</td><td>0.000000</td><td></td></tr><tr><td>5</td><td>B</td><td>1.782078</td><td>2.895652</td><td>3.402820</td><td>2.969907</td><td>0.000000</td></tr><tr><td>6</td><td>B</td><td>2.895859</td><td>3.387941</td><td>2.893651</td><td>1.860261</td><td>1.810869</td></tr><tr><td>7</td><td>B</td><td>1.783717</td><td>1.740572</td><td>1.745796</td><td>2.850479</td><td>2.892483</td></tr><tr><td>8</td><td>B</td><td>1.770536</td><td>2.855697</td><td>2.865026</td><td>2.952405</td><td>1.852175</td></tr><tr><td>9</td><td>B</td><td>1.772391</td><td>1.732714</td><td>2.858118</td><td>2.949399</td><td>1.864888</td></tr><tr><td>10</td><td>B</td><td>2.881832</td><td>2.857280</td><td>1.785542</td><td>1.764344</td><td>2.890252</td></tr><tr><td>11</td><td>B</td><td>2.890022</td><td>2.884268</td><td>2.890803</td><td>1.856735</td><td>1.805134</td></tr><tr><td>12</td><td>B</td><td>2.893480</td><td>1.786736</td><td>1.787787</td><td>1.765593</td><td>2.904376</td></tr><tr><td>13</td><td>B</td><td>4.394235</td><td>4.589343</td><td>4.613129</td><td>3.272219</td><td>2.884072</td></tr><tr><td>14</td><td>B</td><td>3.343039</td><td>4.613390</td><td>5.137291</td><td>4.380165</td><td>1.784513</td></tr><tr><td>15</td><td>B</td><td>4.592534</td><td>5.387293</td><td>5.681411</td><td>4.503669</td><td>2.883219</td></tr><tr><td>16</td><td>B</td><td>3.226925</td><td>3.860304</td><td>4.494476</td><td>3.710239</td><td>1.847347</td></tr><tr><td>17</td><td>B</td><td>3.262557</td><td>4.509687</td><td>4.521628</td><td>3.723359</td><td>1.864164</td></tr><tr><td>18</td><td>B</td><td>4.624872</td><td>5.691676</td><td>5.703714</td><td>4.511917</td><td>2.901340</td></tr><tr><td>19</td><td>C</td><td>4.994542</td><td>5.557000</td><td>5.327413</td><td>3.824776</td><td>3.259127</td></tr><tr><td>20</td><td>B</td><td>4.381692</td><td>4.507372</td><td>3.915765</td><td>2.268983</td><td>2.966876</td></tr><tr><td>21</td><td>Co</td><td>4.733387</td><td>5.427177</td><td>4.825433</td><td>3.460007</td><td>3.266730</td></tr><tr><td></td><td></td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td></tr><tr><td>6</td><td>B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr><tr><td>7</td><td>B</td><td>2.887775</td><td>0.000000</td><td></td><td></td><td></td></tr><tr><td>8</td><td>B</td><td>1.856418</td><td>1.739461</td><td>0.000000</td><td></td><td></td></tr><tr><td>9</td><td>B</td><td>2.966469</td><td>2.851412</td><td>2.946621</td><td>0.000000</td><td></td></tr><tr><td>10</td><td>B</td><td>1.768239</td><td>1.784732</td><td>1.777125</td><td>3.406107</td><td>0.000000</td></tr><tr><td>11</td><td>B</td><td>1.800216</td><td>3.383312</td><td>2.952393</td><td>1.860453</td><td>2.877212</td></tr><tr><td>12</td><td>B</td><td>2.894181</td><td>2.869272</td><td>3.418392</td><td>1.779749</td><td>2.878102</td></tr><tr><td>13</td><td>B</td><td>2.913109</td><td>5.118389</td><td>4.365670</td><td>3.230830</td><td>4.413216</td></tr><tr><td>14</td><td>B</td><td>2.908653</td><td>4.614787</td><td>3.256520</td><td>3.258808</td><td>4.413454</td></tr><tr><td>15</td><td>B</td><td>3.413436</td><td>5.676279</td><td>4.496276</td><td>3.856937</td><td>5.125881</td></tr></table>			1	2	3	4	5	1	B	0.000000					2	B	1.788615	0.000000				3	B	2.871911	1.739308	0.000000			4	B	3.413496	2.844740	1.731845	0.000000		5	B	1.782078	2.895652	3.402820	2.969907	0.000000	6	B	2.895859	3.387941	2.893651	1.860261	1.810869	7	B	1.783717	1.740572	1.745796	2.850479	2.892483	8	B	1.770536	2.855697	2.865026	2.952405	1.852175	9	B	1.772391	1.732714	2.858118	2.949399	1.864888	10	B	2.881832	2.857280	1.785542	1.764344	2.890252	11	B	2.890022	2.884268	2.890803	1.856735	1.805134	12	B	2.893480	1.786736	1.787787	1.765593	2.904376	13	B	4.394235	4.589343	4.613129	3.272219	2.884072	14	B	3.343039	4.613390	5.137291	4.380165	1.784513	15	B	4.592534	5.387293	5.681411	4.503669	2.883219	16	B	3.226925	3.860304	4.494476	3.710239	1.847347	17	B	3.262557	4.509687	4.521628	3.723359	1.864164	18	B	4.624872	5.691676	5.703714	4.511917	2.901340	19	C	4.994542	5.557000	5.327413	3.824776	3.259127	20	B	4.381692	4.507372	3.915765	2.268983	2.966876	21	Co	4.733387	5.427177	4.825433	3.460007	3.266730			6	7	8	9	10	6	B	0.000000					7	B	2.887775	0.000000				8	B	1.856418	1.739461	0.000000			9	B	2.966469	2.851412	2.946621	0.000000		10	B	1.768239	1.784732	1.777125	3.406107	0.000000	11	B	1.800216	3.383312	2.952393	1.860453	2.877212	12	B	2.894181	2.869272	3.418392	1.779749	2.878102	13	B	2.913109	5.118389	4.365670	3.230830	4.413216	14	B	2.908653	4.614787	3.256520	3.258808	4.413454	15	B	3.413436	5.676279	4.496276	3.856937	5.125881
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16	B	3.226925	3.860304	4.494476	3.710239	1.847347																																																																																																																																																																																																																																		
17	B	3.262557	4.509687	4.521628	3.723359	1.864164																																																																																																																																																																																																																																		
18	B	4.624872	5.691676	5.703714	4.511917	2.901340																																																																																																																																																																																																																																		
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20	B	4.381692	4.507372	3.915765	2.268983	2.966876																																																																																																																																																																																																																																		
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	16 B	2.979003	4.478381	3.682470	2.207605	4.361775
	17 B	1.884139	3.897301	2.238936	3.710459	3.269616
	18 B	2.918880	5.432368	3.908810	4.498372	4.628762
	19 C	2.823014	5.581751	4.399235	4.356475	4.538351
	20 B	1.886648	4.521474	3.718763	3.700223	3.282337
	21 Co	2.051042	4.830192	3.476312	4.746679	3.467092
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	12 B	1.779242	0.000000			
	13 B	1.781384	3.324888	0.000000		
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	16 B	1.872660	3.249874	1.775544	1.769921	1.729417
	17 B	2.972880	4.388912	3.427687	1.773439	2.876929
	18 B	3.387234	5.125025	2.847895	1.784188	1.747964
	19 C	2.772124	4.496418	1.696513	2.734865	1.655499
	20 B	1.856461	3.261179	1.771353	3.400495	2.838954
	21 Co	3.247230	4.713694	3.247597	3.248936	3.240166
	16	17	18	19	20	
	16 B	0.000000				
	17 B	2.959840	0.000000			
18 B	2.859821	1.765884	0.000000			
19 C	2.736886	2.782169	1.665729	0.000000		
20 B	2.956566	2.969301	2.832794	1.670401	0.000000	
21 Co	3.842749	2.048297	2.043133	2.025447	2.006592	

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	1 B	0.000000				
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	7 B	1.768485	1.661730	1.748751	2.856231	2.886850
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	9 B	1.767983	1.662027	2.842445	2.925813	1.832139
	10 B	2.868034	2.713418	1.772254	1.771171	2.892391
	11 B	2.888050	2.750160	2.887132	1.851578	1.792046
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	16 B	3.273598	3.785604	4.514499	3.715861	1.881522
	17 B	3.293298	4.392013	4.554286	3.743386	1.892499
	18 B	4.634979	5.557948	5.725952	4.531757	2.911947
	19 B	5.150003	5.558169	5.452015	3.923155	3.408895
	20 B	4.417334	4.392628	3.934071	2.272629	2.997271
21 Co	4.701409	5.242252	4.802596	3.435093	3.236937	

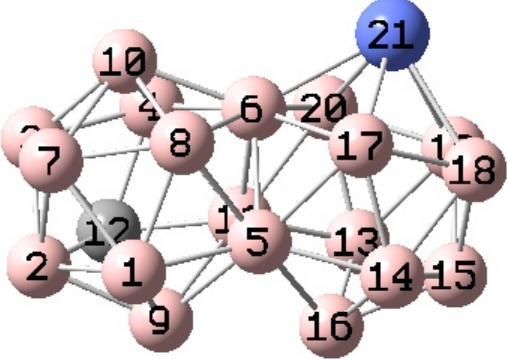
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	11 B	1.810552	3.386504	2.947511	1.832167	2.892411
	12 B	2.896303	2.855705	3.402438	1.768002	2.868080
	13 B	2.917082	5.115902	4.360866	3.209477	4.422232
	14 B	2.917026	4.596026	3.247103	3.209272	4.422060
	15 B	3.432458	5.688430	4.503515	3.847394	5.155695
	16 B	3.007219	4.514330	3.715198	2.223108	4.400567
	17 B	1.919641	3.933129	2.271324	3.708223	3.323925
	18 B	2.955156	5.451436	3.922035	4.479611	4.679595
	19 B	2.955236	5.725854	4.530911	4.479754	4.679756
	20 B	1.919930	4.554675	3.743006	3.708645	3.324409
	21 Co	2.024065	4.802276	3.434226	4.695682	3.465166
	11 12 13 14 15					
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	15 B	2.894796	4.609048	1.793971	1.793948	0.000000
	16 B	1.881524	3.273779	1.763584	1.763593	1.712352
	17 B	2.997019	4.417091	3.442432	1.776150	2.870310
	18 B	3.408931	5.150212	2.879377	1.798248	1.737971
	19 B	2.912195	4.635565	1.798343	2.879313	1.737928
	20 B	1.892905	3.294113	1.776143	3.442469	2.870248
	21 Co	3.237030	4.701736	3.251609	3.251540	3.245188
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	17 B	2.983224	0.000000			
	18 B	2.851421	1.751814	0.000000		
	19 B	2.851432	2.889665	1.752483	0.000000	
	20 B	2.983306	3.013626	2.889615	1.751722	0.000000
	21 Co	3.831974	2.018459	2.080395	2.080449	2.018487
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	1 B	0.000000				
	2 B	1.775773	0.000000			
4. -2096.9792804 +2.8 H/L 3.34 C ₁	3 C	2.723038	1.660779	0.000000		
	4 B	3.399598	2.843860	1.661978	0.000000	
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	7 B	1.769976	1.743376	1.668125	2.847976	2.879059
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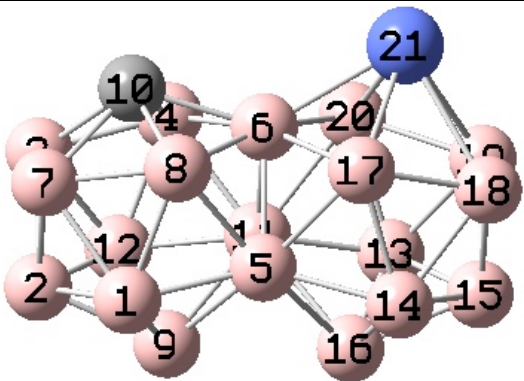
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	15 B	4.618648	5.393539	5.528712	4.478195	2.899074
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	17 B	3.308454	4.543502	4.401561	3.728308	1.894928
	18 B	4.653968	5.708924	5.572998	4.514204	2.922622
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	11 B	1.801670	3.386340	2.947169	1.858733	2.875860
	12 B	2.898897	2.855993	3.401531	1.771810	2.864922
	13 B	2.904529	5.115207	4.360935	3.229289	4.405595
	14 B	2.903907	4.593009	3.238361	3.219161	4.400735
	15 B	3.414038	5.681365	4.495507	3.854458	5.132094
	16 B	2.995334	4.503767	3.703080	2.220259	4.377426
	17 B	1.916355	3.933041	2.272080	3.723430	3.310569
	18 B	2.944463	5.451943	3.923565	4.497641	4.663785
	19 B	2.951818	5.733733	4.541479	4.507753	4.673507
	20 B	1.918822	4.564585	3.755256	3.738009	3.324169
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	16 B	1.879430	3.258111	1.775862	1.766756	1.719568
	17 B	2.995704	4.415199	3.442252	1.767829	2.864878
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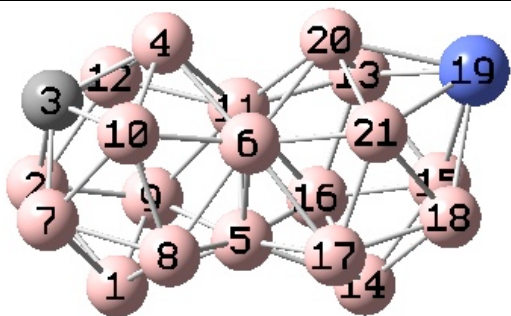
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8 B	1.771489	2.857412	2.861089	2.952794	1.851910
9 B	1.770412	1.730786	2.853502	2.962292	1.867514
10 B	2.878640	2.859072	1.787368	1.767919	2.884263
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13 C	4.267924	4.487347	4.493512	3.158500	2.747394
14 B	3.345514	4.607320	5.128242	4.372431	1.786572
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16 B	3.222903	3.845814	4.465946	3.686146	1.846065
17 B	3.298533	4.543729	4.550818	3.736804	1.879825
18 B	4.654738	5.720719	5.732832	4.536481	2.928979
19 B	5.151613	5.698472	5.438848	3.912900	3.419391
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21 Co	4.734931	5.426289	4.820662	3.442579	3.261101
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12 B	2.911315	2.874063	3.424124	1.782742	2.886979
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14 B	2.916237	4.621180	3.276735	3.243861	4.419348
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16 B	2.971193	4.464361	3.678359	2.198026	4.343217
17 B	1.898257	3.943840	2.292323	3.728383	3.306150
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19 B	2.948900	5.723191	4.547689	4.504845	4.656047
20 B	1.885852	4.508413	3.720425	3.705738	3.265554
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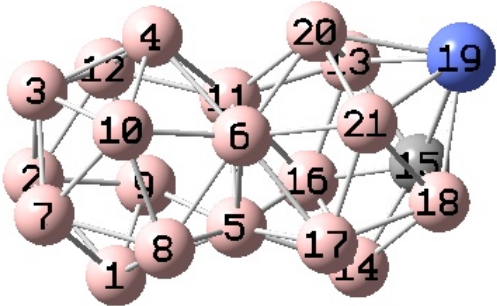
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 6. -2096.9725931 +7.0 H/L 3.39 C₁		1	2	3	4	5
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	15 B	4.614188	5.387558	5.672469	4.472126	2.897393
	16 B	3.263544	3.875838	4.499579	3.695037	1.883311
	17 B	3.322832	4.556970	4.564911	3.728425	1.892547
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	17 B	1.914979	3.968862	2.304944	3.712676	3.335452
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		21 Co	3.841501	2.021829	2.079676	2.080480
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		17 B	3.295582	4.553171	4.550421	3.733922
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		19 B	5.161023	5.722671	5.442303	3.897172
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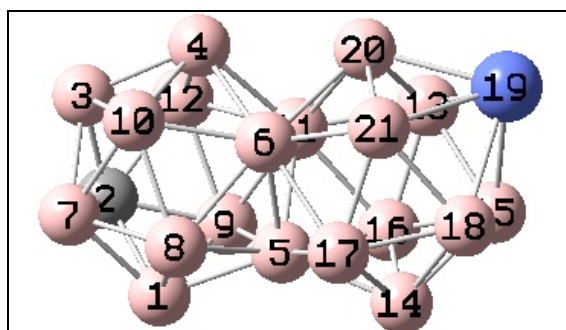
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		13 B	1.773520	3.339916	0.000000		
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		15 B	2.892690	4.620226	1.789765	1.789765	0.000000
		16 B	1.876893	3.284712	1.769394	1.769398	1.720645
		17 B	3.012975	4.431773	3.447459	1.767153	2.864813
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		20 B	2.985284	3.037283	2.895185	1.751030	0.000000
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		2 B	1.769938	0.000000			
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		8 B	1.780782	2.858783	2.727693	2.935284	1.845867
		9 B	1.780784	1.737675	2.727707	2.935272	1.845836
		10 B	2.875071	2.854823	1.698151	1.765007	2.887338
		11 B	2.904911	2.887025	2.752225	1.835341	1.811474
		12 B	2.875068	1.770160	1.698144	1.765011	2.887349
		13 B	4.414788	4.590331	4.483300	3.253109	2.903073
		14 B	3.318967	4.572090	4.941960	4.342991	1.764100
		15 B	4.612473	5.394785	5.537004	4.493384	2.897607
		16 B	3.260237	3.872524	4.353373	3.697566	1.866912
		17 B	3.260281	4.491219	4.353363	3.697540	1.866956
		18 B	4.612501	5.673302	5.537014	4.493390	2.897639
		19 Co	5.582450	6.096454	5.662528	4.209595	3.850741



8. -2096.9624576 +13.4 H/L 2.77 C_s

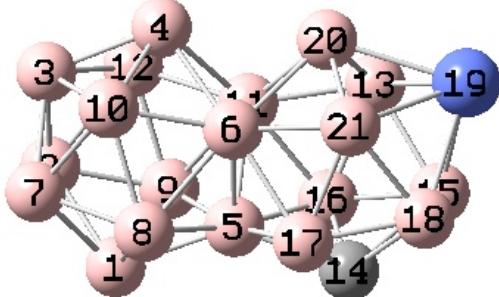
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	7 B	2.887044	0.000000			
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	11 B	1.785166	3.384159	2.955301	1.861663	2.883169
	12 B	2.883135	2.854798	3.409195	1.773784	2.872530
	13 B	2.899742	5.118345	4.369056	3.228998	4.420540
	14 B	2.888959	4.572077	3.219102	3.219099	4.392089
	15 B	3.398523	5.673273	4.486022	3.862109	5.130945
	16 B	2.972018	4.491190	3.694225	2.214493	4.376246
	17 B	1.882444	3.872537	2.214536	3.694231	3.261926
	18 B	2.898144	5.394800	3.862152	4.486024	4.610479
	19 Co	3.283889	6.096454	4.907368	4.907329	4.980196
	20 B	1.871439	4.520332	3.714323	3.714206	3.287371
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	17 B	2.972076	4.376264	3.443379	1.766665	2.868692
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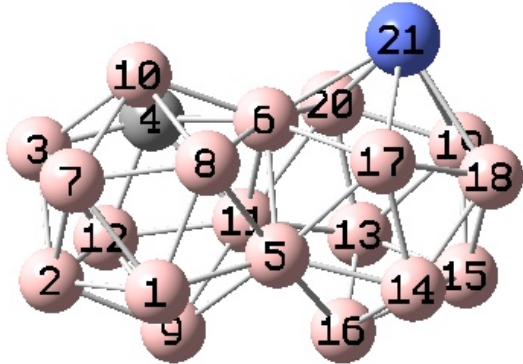
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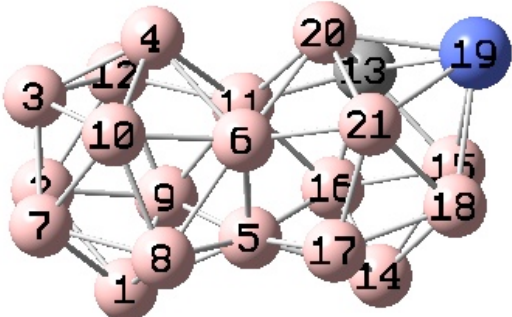
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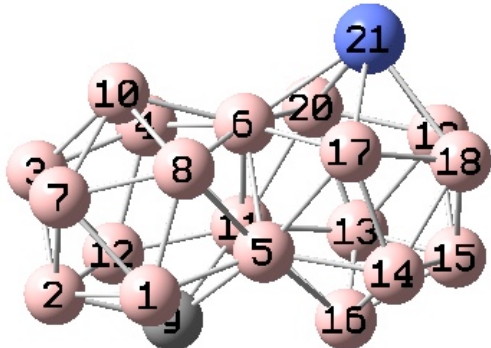
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	9 B 1.790078 1.735225 2.854611 2.961154 1.851669
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	17 B	3.312918	4.565771	4.590426	3.673595	1.898288
	18 B	4.660989	5.727464	5.752174	4.491488	2.927809

	19 B 5.201514 5.757506 5.512061 3.979291 3.454660 20 B 4.490789 4.625600 4.029255 2.403415 3.054085 21 Co 4.716441 5.415442 4.819398 3.443371 3.246065 6 7 8 9 10 6 B 0.000000 7 B 2.910491 0.000000 8 B 1.853507 1.749983 0.000000 9 B 2.938148 2.855478 2.916722 0.000000 10 B 1.785225 1.785446 1.776725 3.381395 0.000000 11 B 1.757906 3.386371 2.917019 1.857856 2.848616 12 B 2.877155 2.863241 3.390745 1.781035 2.846034 13 B 2.883580 5.126915 4.351310 3.227864 4.391162 14 B 2.897045 4.613474 3.240828 3.213083 4.409982 15 B 3.402940 5.697798 4.492253 3.846155 5.131564 16 B 2.985972 4.522754 3.700130 2.217944 4.383709 17 B 1.937210 3.959093 2.279797 3.718058 3.336154 18 B 2.946755 5.473293 3.925791 4.491561 4.672179 19 B 2.973712 5.776457 4.559017 4.522766 4.697980 20 B 1.954535 4.633530 3.789285 3.778093 3.366594 21 Co 2.021872 4.812352 3.434249 4.702143 3.450389 11 12 13 14 15 11 B 0.000000 12 B 1.788736 0.000000 13 B 1.777418 3.314094 0.000000 14 B 2.874431 4.394296 2.894357 0.000000 15 B 2.884683 4.593014 1.796603 1.792175 0.000000 16 B 1.897454 3.269259 1.798929 1.760702 1.718113 17 B 2.987239 4.424660 3.451240 1.760386 2.866755 18 B 3.397454 5.147395 2.881906 1.799067 1.741228 19 B 2.938235 4.663985 1.814409 2.887682 1.733780 20 B 1.933950 3.354491 1.749827 3.440724 2.834676 21 Co 3.206647 4.688080 3.235217 3.246652 3.240353 16 17 18 19 20 16 B 0.000000 17 B 2.983275 0.000000 18 B 2.863318 1.754240 0.000000 19 B 2.888481 2.918149 1.747839 0.000000 20 B 3.013023 3.039304 2.857631 1.726370 0.000000 21 Co 3.838783 2.037900 2.082173 2.096267 1.989808					
	1 B 0.000000 2 B 1.786993 0.000000 3 B 2.864207 1.737400 0.000000 4 B 3.421804 2.852551 1.725253 0.000000 5 B 1.769802 2.885730 3.391781 2.986242 0.000000 6 B 2.895798 3.392329 2.895209 1.874015 1.813810 7 B 1.784839 1.744071 1.739100 2.847556 2.884602 8 B 1.779596 2.862478 2.859440 2.960116 1.862981					
						

14. -2096.9563331 +17.22 H/L 2.76 C ₁	9 B	1.776472	1.734369	2.859945	2.973363	1.863773
	10 B	2.889098	2.869491	1.790346	1.765623	2.897885
	11 B	2.868327	2.861565	2.861527	1.858008	1.798047
	12 B	2.898280	1.792565	1.789413	1.777853	2.905122
	13 C	4.269218	4.485762	4.498168	3.181382	2.758791
	14 B	3.327721	4.590329	5.117051	4.384895	1.777454
	15 B	4.594413	5.381749	5.662954	4.500739	2.892801
	16 B	3.216044	3.833505	4.455146	3.690940	1.841870
	17 B	3.245045	4.494210	4.509027	3.728476	1.849145
	18 B	4.610524	5.687844	5.698950	4.533984	2.903667
	19 Co	5.576482	6.095890	5.785611	4.230978	3.858156
	20 B	4.348751	4.483128	3.885726	2.256446	2.947080
	21 B	4.413608	5.137810	4.633863	3.299340	2.904710
		6	7	8	9	10
	6 B	0.000000				
	7 B	2.890693	0.000000			
	8 B	1.864031	1.735727	0.000000		
	9 B	2.975481	2.859706	2.967471	0.000000	
	10 B	1.780666	1.786623	1.775305	3.427078	0.000000
	11 B	1.783852	3.355332	2.940999	1.855405	2.862840
	12 B	2.900125	2.874837	3.431771	1.787992	2.893627
	13 C	2.761393	4.983748	4.229579	3.145138	4.283354
	14 B	2.903507	4.606679	3.272346	3.231314	4.419520
	15 B	3.390454	5.669472	4.503866	3.858223	5.118463
	16 B	2.948602	4.456308	3.682639	2.185548	4.343055
	17 B	1.876265	3.890148	2.243249	3.694395	3.275044
	18 B	2.910571	5.419419	3.899185	4.504145	4.626697
	19 Co	3.302804	6.110899	4.941603	4.914029	4.988379
	20 B	1.840515	4.482547	3.683879	3.690293	3.247796
	21 B	1.797170	4.617430	3.257695	4.390581	3.353684
		11	12	13	14	15
	11 B	0.000000				
	12 B	1.764574	0.000000			
	13 C	1.689415	3.244969	0.000000		
	14 B	2.880786	4.395523	2.752894	0.000000	
	15 B	2.887888	4.576591	1.721902	1.780230	0.000000
	16 B	1.847814	3.213098	1.687618	1.756241	1.746541
	17 B	2.950081	4.376859	3.275200	1.772785	2.854180
	18 B	3.408618	5.135690	2.793703	1.796242	1.766999
	19 Co	3.296137	4.957698	2.047054	3.257736	1.999755
	20 B	1.852352	3.248364	1.695976	3.378801	2.817147
	21 B	2.912002	4.435702	2.809890	2.889473	2.875493
		16	17	18	19	20
	16 B	0.000000				
	17 B	2.932837	0.000000			
	18 B	2.877586	1.735557	0.000000		
	19 Co	3.248059	3.265000	2.041608	0.000000	
	20 B	2.922373	2.930485	2.843797	1.992526	0.000000
	21 B	3.425889	1.772823	1.784957	2.099415	1.783986

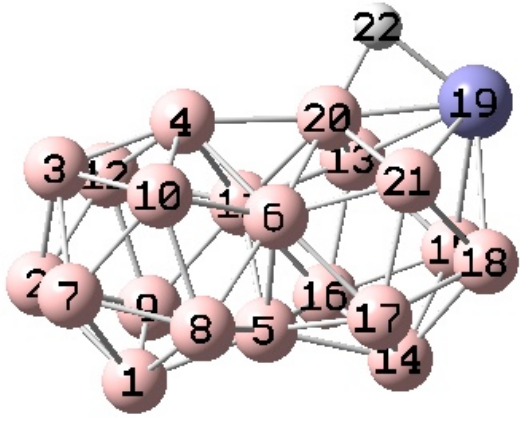


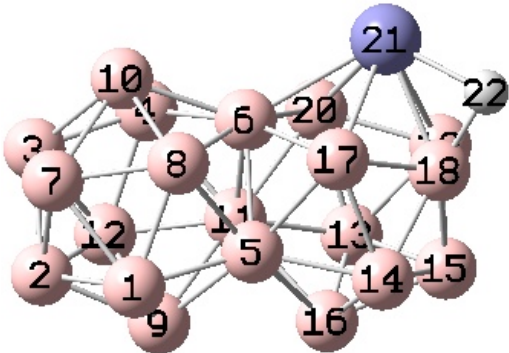
15. -2096.9552761 +17.9 H/L 3.13 Cs

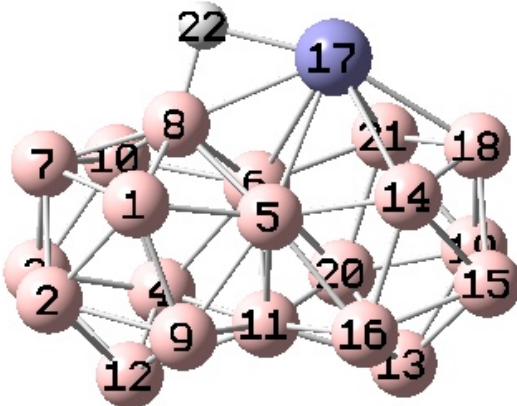
	1	2	3	4	5
1 B	0.000000				
2 B	1.784414	0.000000			
3 B	2.864005	1.742906	0.000000		
4 B	3.392346	2.865554	1.751206	0.000000	
5 B	1.790739	2.907450	3.390826	2.921417	0.000000
6 B	2.898434	3.413886	2.900465	1.835878	1.804008
7 B	1.784868	1.742900	1.756739	2.863097	2.902755
8 B	1.779832	2.865551	2.863093	2.920523	1.851508
9 C	1.659412	1.646864	2.690996	2.776468	1.762358
10 B	2.869238	2.851813	1.775024	1.766736	2.885701
11 B	2.863577	2.907445	2.902748	1.851495	1.748538
12 B	2.855721	1.784413	1.784866	1.779830	2.863574
13 B	4.388875	4.612838	4.613241	3.246693	2.863007
14 B	3.324012	4.612877	5.131759	4.352126	1.779861
15 B	4.630956	5.457684	5.728642	4.516035	2.912438
16 B	3.325177	3.988917	4.592262	3.757747	1.920188
17 B	3.307968	4.573046	4.569426	3.732829	1.913153
18 B	4.635672	5.733777	5.740068	4.521859	2.912010
19 B	5.148160	5.733752	5.464748	3.913944	3.398518
20 B	4.420519	4.572982	3.948346	2.267113	2.987456
21 Co	4.708891	5.431791	4.820388	3.432607	3.235128
	6	7	8	9	10
6 B	0.000000				
7 B	2.900474	0.000000			
8 B	1.835903	1.751202	0.000000		
9 C	2.818484	2.690991	2.776469	0.000000	
10 B	1.780544	1.775026	1.766732	3.207001	0.000000
11 B	1.804002	3.390823	2.921426	1.762357	2.885700
12 B	2.898420	2.863998	3.392343	1.659415	2.869235
13 B	2.925021	5.131728	4.352118	3.224927	4.426166
14 B	2.925046	4.613282	3.246738	3.224960	4.426191
15 B	3.454149	5.728649	4.516060	3.918825	5.175864
16 B	3.051913	4.592259	3.757752	2.364337	4.453604
17 B	1.919420	3.948418	2.267191	3.650086	3.321333
18 B	2.957422	5.464786	3.913999	4.461624	4.679788
19 B	2.957401	5.740055	4.521871	4.461604	4.679767
20 B	1.919359	4.569366	3.732792	3.650034	3.321277
21 Co	2.030256	4.820396	3.432629	4.609620	3.474450
	11	12	13	14	15
11 B	0.000000				
12 B	1.790730	0.000000			
13 B	1.779829	3.323967	0.000000		
14 B	2.863029	4.388899	2.876130	0.000000	
15 B	2.912431	4.630941	1.804915	1.804915	0.000000
16 B	1.920198	3.325180	1.745820	1.745818	1.690273
17 B	2.987500	4.420568	3.450835	1.802222	2.890730
18 B	3.398524	5.148161	2.882073	1.804502	1.733748

	19 B	2.911982	4.635628	1.804496	2.882077	1.733753
	20 B	1.913103	3.307901	1.802221	3.450824	2.890730
	21 Co	3.235126	4.708879	3.258088	3.258087	3.243766
		16	17	18	19	20
	16 B	0.000000				
	17 B	3.012657	0.000000			
	18 B	2.831281	1.752535	0.000000		
	19 B	2.831281	2.891101	1.755881	0.000000	
	20 B	3.012647	3.011068	2.891099	1.752536	0.000000
	21 Co	3.839928	2.008648	2.075272	2.075271	2.008650

Table S3. Distance table for the CpFeB₂₀H₁₇ 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. For clarity, only the atoms forming the biicosahedral framework are presented.

 1. -1964.6503266 0.0 H/L 2.08 C_s	1 2 3 4 5					
	1 B	0.000000				
	2 B	1.802860	0.000000			
	3 B	2.905478	1.767913	0.000000		
	4 B	3.345819	2.822256	1.737694	0.000000	
	5 B	1.808014	2.935505	3.441283	2.883087	0.000000
	6 B	2.840785	3.354868	2.855137	1.781079	1.794207
	7 B	1.802808	1.745188	1.767926	2.822284	2.935453
	8 B	1.763661	2.863745	2.889943	2.906112	1.893196
	9 B	1.763579	1.739291	2.889880	2.906001	1.893149
	10 B	2.886229	2.861831	1.783086	1.781819	2.934602
	11 B	2.840915	2.826612	2.855352	1.781142	1.794197
	12 B	2.886192	1.760665	1.783172	1.781739	2.934529
	13 B	4.415938	4.531234	4.494456	3.076530	2.943680
	14 B	3.463876	4.686897	5.133048	4.183711	1.802335
	15 B	4.696682	5.412237	5.585336	4.233211	2.941447
	16 B	3.324897	3.940474	4.521769	3.587250	1.892240
	17 B	3.324622	4.551443	4.521327	3.586943	1.892135
	18 B	4.696510	5.691156	5.585041	4.232956	2.941329
	19 Fe	5.620205	5.991860	5.500400	3.811952	3.942343
	20 B	4.154409	4.240029	3.592889	1.903543	2.808694
	21 B	4.415980	5.090632	4.494198	3.076321	2.943849
		6	7	8	9	10
	6 B	0.000000				
	7 B	2.826364	0.000000			
	8 B	1.813557	1.739311	0.000000		
	9 B	2.973158	2.863612	2.965574	0.000000	
	10 B	1.751229	1.760651	1.790142	3.442950	0.000000
	11 B	1.871774	3.355015	2.973304	1.813683	2.920087
	12 B	2.919928	2.861843	3.443016	1.790042	2.916704
	13 B	2.981239	5.090685	4.427905	3.233951	4.403766
	14 B	2.828734	4.686766	3.326073	3.326252	4.406661
	15 B	3.355821	5.691284	4.554348	3.933976	5.064555
	16 B	2.989357	4.551724	3.758255	2.302817	4.405369
	17 B	1.834930	3.939958	2.302296	3.758072	3.275337
	18 B	2.817046	5.411870	3.933597	4.554304	4.524028
	19 Fe	3.246297	5.991862	4.947660	4.947586	4.782534
	20 B	1.744484	4.239842	3.528101	3.528406	3.043215
	21 B	1.764517	4.531045	3.233876	4.427927	3.224014
		11	12	13	14	15
	11 B	0.000000				
	12 B	1.751361	0.000000			
	13 B	1.764444	3.224229	0.000000		

	14 B 2.828725 4.406713 2.874863 0.000000 15 B 2.817198 4.524357 1.736922 1.811369 0.000000 16 B 1.835186 3.275766 1.771879 1.748657 1.747844 17 B 2.989143 4.405054 3.509433 1.748731 2.887759 18 B 3.355563 5.064361 2.914658 1.811338 1.776119 19 Fe 3.246030 4.782404 2.142220 3.389811 2.144720 20 B 1.744781 3.043547 1.814009 3.225030 2.712600 21 B 2.981132 4.403606 3.084814 2.875055 2.914886 16 17 18 19 20 16 B 0.000000 17 B 2.974813 0.000000 18 B 2.887592 1.747895 0.000000 19 Fe 3.368341 3.368616 2.144848 0.000000 20 B 2.848227 2.847702 2.712144 1.911300 0.000000 21 B 3.509583 1.772074 1.736922 2.142536 1.813219 Bridging H: Fe19-H22-B20 Fe19-H22 1.604 B20-H22 1.315					
	 2. -1964.6437013 +4.2 H/L 1.91 C₁ (Cs)					
	1 2 3 4 5 1 B 0.000000 2 B 1.787653 0.000000 3 B 2.869481 1.740329 0.000000 4 B 3.418981 2.854674 1.734454 0.000000 5 B 1.773954 2.887364 3.390785 2.968003 0.000000 6 B 2.914013 3.406967 2.899549 1.862753 1.827452 7 B 1.781602 1.739906 1.745344 2.854390 2.881103 8 B 1.780918 2.860356 2.858971 2.945489 1.847510 9 B 1.769523 1.731225 2.851627 2.952164 1.856148 10 B 2.888862 2.860670 1.779486 1.761604 2.891915 11 B 2.890675 2.899362 2.900346 1.868732 1.791842 12 B 2.885881 1.789961 1.788414 1.768059 2.885203 13 B 4.417705 4.601593 4.621909 3.286177 2.920418 14 B 3.340023 4.614284 5.120014 4.363463 1.783847 15 B 4.643969 5.434704 5.710504 4.523364 2.938873 16 B 3.258397 3.903719 4.523202 3.732335 1.865740 17 B 3.201399 4.450773 4.449343 3.678752 1.845511 18 B 4.462086 5.476014 5.448964 4.239273 2.733196 19 B 5.236387 5.750803 5.482768 3.942819 3.516253 20 B 4.428770 4.544562 3.946456 2.293429 3.015231 21 Fe 4.840539 5.546666 4.933725 3.565736 3.376263 6 7 8 9 10 6 B 0.000000 7 B 2.897552 0.000000 8 B 1.854242 1.741026 0.000000 9 B 2.982579 2.845673 2.945954 0.000000 10 B 1.774702 1.787540 1.776424 3.406132 0.000000 11 B 1.803468 3.386658 2.941198 1.866414 2.881851 12 B 2.897815 2.865669 3.407077 1.768934 2.872731 13 B 2.955037 5.139693 4.394355 3.239170 4.443734					

 3. -1964.6432972 +4.4 H/L 1.10 C₁ (Cs)	14 B	2.886549	4.595639	3.228405	3.270253	4.392885
	15 B	3.440370	5.715423	4.530468	3.906501	5.158224
	16 B	2.995301	4.505491	3.695119	2.254197	4.384251
	17 B	1.838049	3.808611	2.140213	3.681737	3.196497
	18 B	2.668806	5.226688	3.732061	4.299171	4.402911
	19 B	3.028920	5.798349	4.638197	4.546226	4.728324
	20 B	1.941209	4.569393	3.766680	3.725794	3.334814
	21 Fe	2.151327	4.933234	3.558685	4.859801	3.569414
	11	12	13	14	15	
	11 B	0.000000				
	12 B	1.786533	0.000000			
	13 B	1.787578	3.313988	0.000000		
	14 B	2.874859	4.404807	2.909679	0.000000	
	15 B	2.895690	4.610086	1.790987	1.834300	0.000000
	16 B	1.881423	3.275586	1.776814	1.767963	1.733582
	17 B	2.948212	4.340724	3.517201	1.790311	2.983192
	18 B	3.113783	4.859757	2.684298	1.724239	1.687414
	19 B	2.913398	4.615890	1.772202	2.967803	1.754905
	20 B	1.869434	3.268233	1.776432	3.414298	2.836153
	21 Fe	3.346086	4.821251	3.370756	3.272524	3.279963
	16	17	18	19	20	
	16 B	0.000000				
	17 B	2.980398	0.000000			
	18 B	2.674608	1.751671	0.000000		
	19 B	2.881348	3.114914	1.721029	0.000000	
	20 B	2.960657	3.040043	2.595558	1.721638	0.000000
	21 Fe	3.910974	2.135585	1.892001	2.201189	2.134888
Bridging H: Fe21-H22-B18 Fe21-H22 1.643 B18-H22 1.303						

1	2	3	4	5
1 B	0.000000			
2 B	1.758564	0.000000		
3 B	2.876941	1.753364	0.000000	
4 B	3.473183	2.886660	1.746274	0.000000
5 B	1.805121	2.894118	3.412776	3.025277
6 B	2.937126	3.412003	2.906412	1.918911
7 B	1.801814	1.765012	1.765786	2.898489
8 B	1.747303	2.732603	2.735351	2.826227
9 B	1.765760	1.750895	2.883258	3.003112
10 B	2.948210	2.873730	1.761827	1.775884
11 B	2.935134	2.937696	2.912355	1.871827
12 B	2.853154	1.788462	1.782116	1.756942
13 B	4.459939	4.676594	4.631981	3.251989
14 B	3.351230	4.613511	5.153956	4.450094
15 B	4.597550	5.408764	5.668859	4.503233
16 B	3.295446	3.898208	4.480882	3.676223
17 Fe	3.237791	4.607503	4.682070	4.150463
18 B	4.588803	5.670319	5.672365	4.546814

	19 B	5.113589	5.688094	5.391140	3.889385	3.362293
	20 B	4.374764	4.514740	3.871056	2.233466	2.959209
	21 B	4.414985	5.139027	4.623788	3.344728	2.912905
		6	7	8	9	10
	6 B	0.000000				
	7 B	2.885062	0.000000			
	8 B	1.700064	1.692121	0.000000		
	9 B	3.008747	2.889492	2.803487	0.000000	
	10 B	1.790474	1.800019	1.743696	3.451896	0.000000
	11 B	1.802699	3.416513	2.761377	1.924188	2.885031
	12 B	2.883088	2.866227	3.192487	1.769383	2.843992
	13 B	2.852727	5.137723	4.163075	3.347352	4.373480
	14 B	2.946084	4.612311	3.186667	3.257427	4.475584
	15 B	3.345891	5.640880	4.301981	3.899170	5.088860
	16 B	2.947073	4.507055	3.541758	2.250711	4.360005
	17 Fe	2.272280	3.786772	2.106116	3.983021	3.402516
	18 B	2.862294	5.337596	3.726756	4.521958	4.582998
	19 B	2.812895	5.616535	4.268639	4.540834	4.531114
	20 B	1.780576	4.446139	3.456700	3.760535	3.162652
	21 B	1.767122	4.547437	3.088290	4.432465	3.310271
		11	12	13	14	15
	11 B	0.000000				
	12 B	1.784219	0.000000			
	13 B	1.788553	3.381804	0.000000		
	14 B	2.921209	4.397989	2.906262	0.000000	
	15 B	2.872758	4.591446	1.783310	1.756194	0.000000
	16 B	1.814869	3.199650	1.759956	1.814899	1.735929
	17 Fe	3.477277	4.702307	4.024052	2.151160	3.366827
	18 B	3.408608	5.120413	2.884414	1.820182	1.766957
	19 B	2.886052	4.618623	1.777936	2.884266	1.762518
	20 B	1.868280	3.280868	1.782987	3.456971	2.866807
	21 B	2.945327	4.447949	2.912229	2.945938	2.879163
		16	17	18	19	20
	16 B	0.000000				
	17 Fe	3.462631	0.000000			
	18 B	2.903213	2.150759	0.000000		
	19 B	2.856325	3.412972	1.749207	0.000000	
	20 B	2.938220	3.512166	2.870555	1.734128	0.000000
	21 B	3.451119	2.233994	1.771562	1.772086	1.804301
	Bridging H: Fe17-H22-B8 Fe17-H22 1.649 B8-H22 1.257					

Table S4. Orbital energies and HOMO/LUMO gaps:

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO Gap (Hartree)	HOMO/LUMO Gap (eV)
01-CpCoCB19H17	-0.249649	-0.124363	-0.125286	3.41
02-CpCoCB19H17	-0.253452	-0.138229	-0.115223	3.14
03-CpCoCB19H17	-0.233598	-0.108893	-0.124705	3.39
04-CpCoCB19H17	-0.234906	-0.112032	-0.122874	3.34
05-CpCoCB19H17	-0.248942	-0.124644	-0.124298	3.38
06-CpCoCB19H17	-0.236112	-0.111686	-0.124426	3.39
07-CpCoCB19H17	-0.239690	-0.116465	-0.123225	3.35
08-CpCoCB19H17	-0.222149	-0.120497	-0.101652	2.77
09-CpCoCB19H17	-0.242168	-0.142933	-0.099235	2.70
10-CpCoCB19H17	-0.221714	-0.120931	-0.100783	2.74
11-CpCoCB19H17	-0.238728	-0.130515	-0.108213	2.94
12-CpCoCB19H17	-0.229945	-0.151009	-0.078936	2.15
13-CpCoCB19H17	-0.245568	-0.129085	-0.116483	3.17
14-CpCoCB19H17	-0.242313	-0.140918	-0.101395	2.76
15-CpCoCB19H17	-0.241195	-0.126305	-0.114890	3.13
01-CpNiB20H17	-0.263940	-0.160605	-0.103335	2.81
02-CpNiB20H17	-0.259826	-0.163587	-0.096239	2.62
03-CpNiB20H17	-0.248700	-0.188792	-0.059908	1.63
01-CpFeB20H17	-0.226645	-0.150309	-0.076336	2.08
02-CpFeB20H17	-0.236432	-0.166314	-0.070118	1.91
03-CpFeB20H17	-0.229901	-0.189450	-0.040451	1.10