Supporting Information

Cyclopentadienylironphosphacarboranes: Fragility of Polyhedral Edges in the 11-Vertex System

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Complete Gaussian09 Reference (reference

22) 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 $CpFeCHPHB_5H_5$ structures, 593 in all.

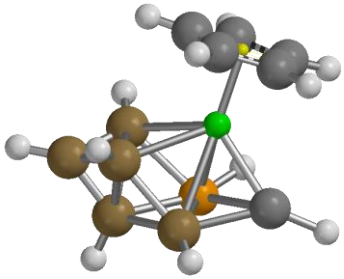
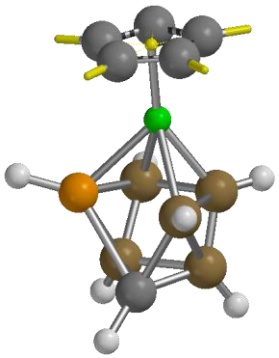
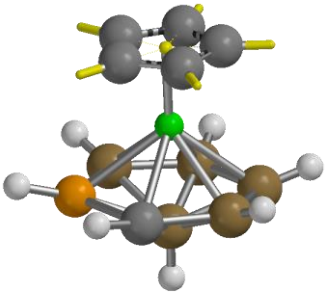
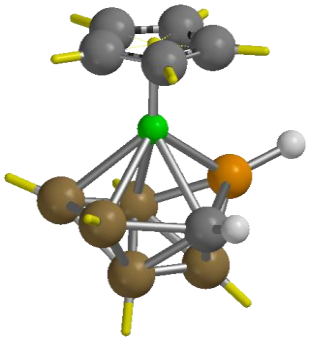
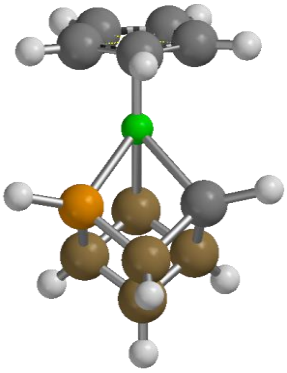
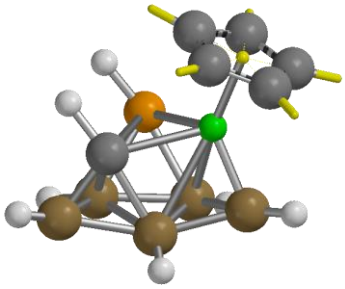
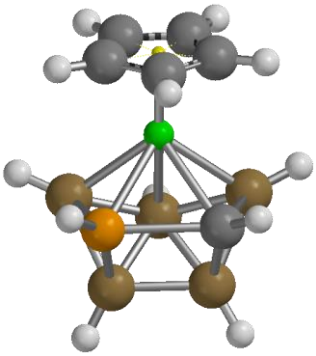
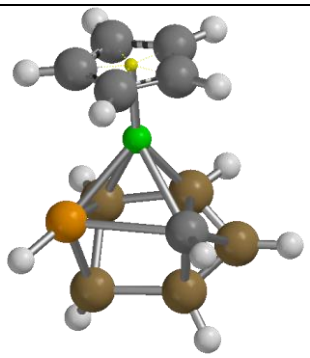
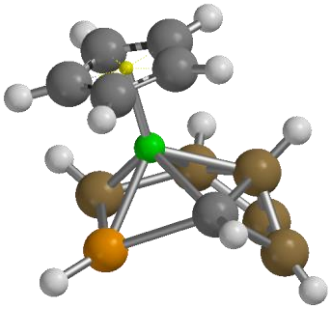
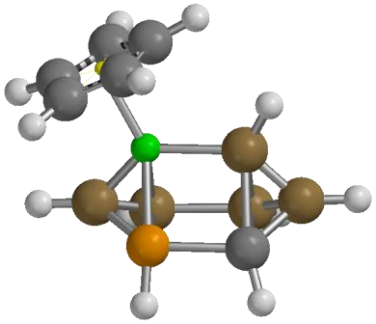
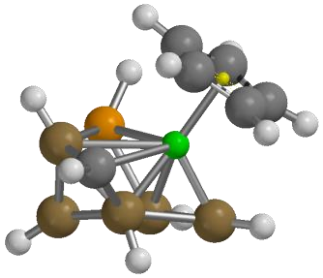
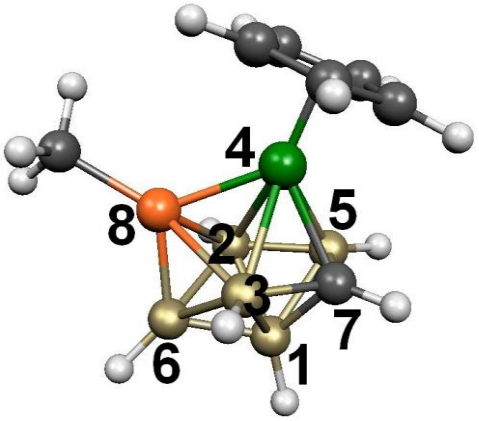
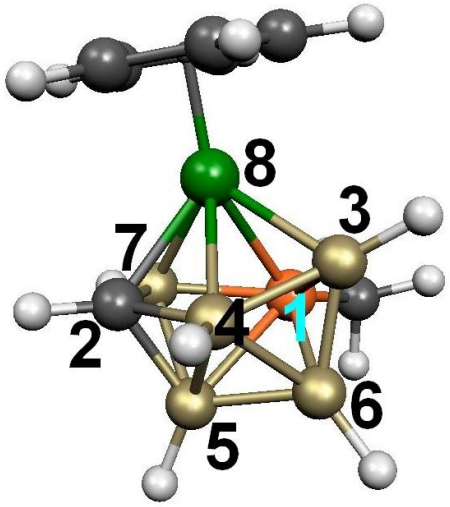
Initial structures	 Trigonal Antiprism 26	 Antiprism 22
 Hexagonal bipyramid 34	 Bisdisphenoid 52	 Cube 14
 Bicapped octahedron 74	 Bicapped trigonal prism C_{2v} 110	 Bicapped trigonal prism C_S 115
 Nido 64	 Trigonal prism 28	 Tetracapped tetrahedron 54

Table S1B. Distance table for the lowest-lying $CpFeCHPCH_3B_5H_5$ 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.



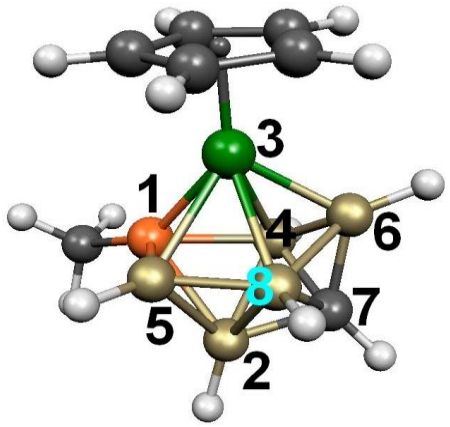
1. -2004.2092626 0.0
C_1 H/L 2.39

		1	2	3	4	5
1	B	0.000000				
2	B	1.852901	0.000000			
3	B	1.827009	2.596586	0.000000		
4	Fe	2.882392	2.289299	2.217385	0.000000	
5	B	1.789983	1.699279	2.613492	2.058878	0.000000
6	B	1.699546	1.916098	1.877178	3.112391	2.959930
7	C	1.657209	2.542382	1.565161	2.014429	1.539599
8	P	2.804536	1.989259	2.099293	2.094771	3.078882
		6	7	8		
6	B	0.000000				
7	C	2.804017	0.000000			
8	P	1.803674	3.020840	0.000000		



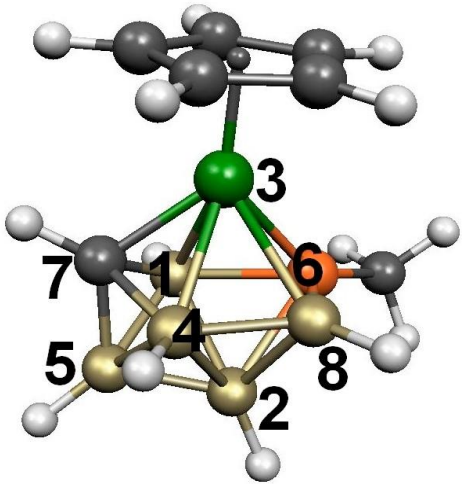
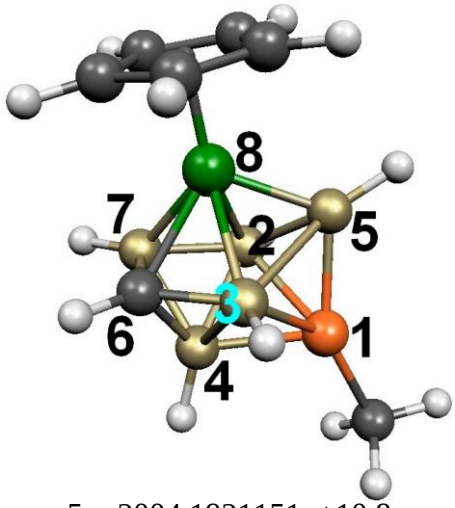
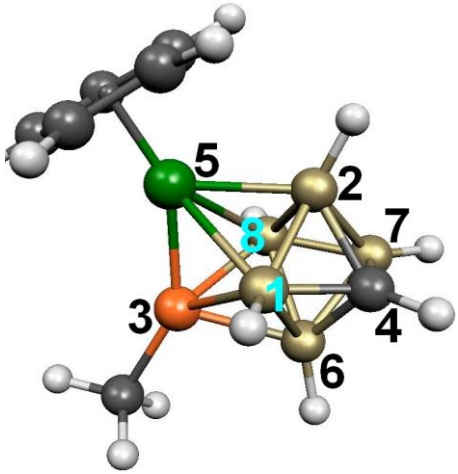
2. -2004.2092216 +0.03
C_1 H/L 2.45

		1	2	3	4	5
1	P	0.000000				
2	C	2.615800	0.000000			
3	B	1.979133	2.872891	0.000000		
4	B	2.584146	1.610125	1.774933	0.000000	
5	B	2.133551	1.636322	2.757292	1.829950	0.000000
6	B	1.964582	2.769470	1.671133	1.791352	1.735271
7	B	1.888341	1.528609	3.138866	2.666408	1.928791
8	Fe	2.222265	1.999264	2.045098	2.138199	2.931459
		6	7	8		
6	B	0.000000				
7	B	3.034870	0.000000			
8	Fe	3.053345	2.097365	0.000000		



3. -2004.2090771 +0.12

		1	2	3	4	5
1	P	0.000000				
2	B	2.026207	0.000000			
3	Fe	2.165183	2.948237	0.000000		
4	B	1.934080	1.973475	2.208087	0.000000	
5	B	1.827084	1.845552	2.179937	2.800248	0.000000
6	B	3.106311	2.664014	1.968059	1.761191	3.012823
7	C	2.935269	1.578761	2.876109	1.653872	2.803758
8	B	2.781587	1.826683	2.176839	2.461117	1.704479
		6	7	8		
6	B	0.000000				
7	C	1.545781	0.000000			
8	B	1.795568	1.673490	0.000000		

C_1 H/L 2.65	
 4. -2004.2015460 +4.8 C_1 H/L 2.40	1 2 3 4 5 1 B 0.000000 2 B 1.988456 0.000000 3 Fe 2.198842 2.983595 0.000000 4 B 2.437978 1.872105 2.162936 0.000000 5 B 1.776724 1.671090 3.057091 1.791544 0.000000 6 P 1.946479 2.013606 2.173673 2.763784 3.076664 7 C 1.628841 2.523356 1.940202 1.659747 1.534575 8 B 2.811364 1.891037 2.180134 1.712380 2.959419 6 7 8 6 P 0.000000 7 C 2.975674 0.000000 8 B 1.820504 2.886201 0.000000
 5. -2004.1921151 +10.8 C_1 H/L 2.91	1 2 3 4 5 1 P 0.000000 2 B 2.024219 0.000000 3 B 2.031966 2.609734 0.000000 4 B 1.951155 1.892567 1.961285 0.000000 5 B 1.855270 1.883879 2.154071 2.886456 0.000000 6 C 2.951211 2.547886 1.574255 1.622899 3.048489 7 B 3.122932 1.710283 2.633102 1.750599 3.033470 8 Fe 3.064127 2.146570 2.053899 2.794610 1.918612 6 7 8 6 C 0.000000 7 B 1.549839 0.000000 8 Fe 2.000573 2.021890 0.000000
 6. -2004.1893969 +12.5	1 2 3 4 5 1 B 0.000000 2 B 1.836853 0.000000 3 P 2.030338 2.798771 0.000000 4 C 1.582196 1.680691 2.958672 0.000000 5 Fe 2.206775 2.065745 2.038044 3.235799 0.000000 6 B 1.937535 2.463228 1.955542 1.636829 3.203693 7 B 2.637798 1.779106 3.096759 1.534600 3.393064 8 B 2.576132 1.847673 2.014686 2.497325 2.279414 6 7 8 6 B 0.000000 7 B 1.755060 0.000000 8 B 1.940115 1.677174 0.000000

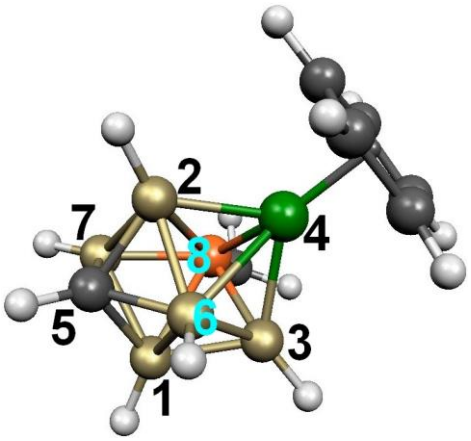
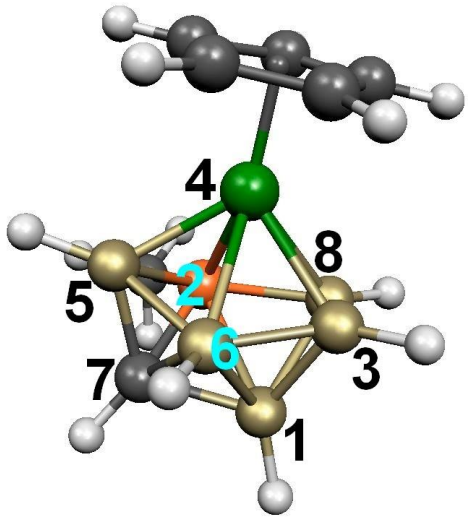
C_1 H/L 1.72	
 7. -2004.1838728 +15.9 C_1 H/L 1.71	1 2 3 4 5 1 B 0.000000 2 B 2.634533 0.000000 3 B 1.775145 2.793354 0.000000 4 Fe 3.050986 1.977127 1.953075 0.000000 5 C 1.644837 1.617407 2.771978 3.066387 0.000000 6 B 1.812625 1.784833 1.740447 2.143135 1.642172 7 B 1.888298 2.089608 3.014378 3.219828 1.543627 8 P 2.094095 2.415253 1.968741 2.129597 2.655587 6 7 8 6 B 0.000000 7 B 2.707391 0.000000 8 P 2.687006 1.859935 0.000000
 8. -2004.1820758 +17.1 C_1 H/L 2.61	1 2 3 4 5 1 B 0.000000 2 P 2.199029 0.000000 3 B 1.719695 2.737727 0.000000 4 Fe 2.920725 2.176297 2.059902 0.000000 5 B 2.741188 2.021945 2.941053 1.980141 0.000000 6 B 1.796336 2.646279 1.704558 2.173626 1.763244 7 C 1.654705 1.866617 2.753922 2.855705 1.576578 8 B 1.901926 1.837040 1.650978 2.199652 3.153570 6 7 8 6 B 0.000000 7 C 1.700494 0.000000 8 B 2.732300 2.845502 0.000000

Table S1C. Energy ranking for all of the $CpFeCHPHB_5H_5$ optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	09b-DicapTrPr-Fe1P2C5	-1964.9367924	0.00
2	07b-Tdallcap-Fe1P1C1	-1964.9367913	0.00
3	10b-DicapTrPrism-Fe3P1C4	-1964.9367840	0.01
4	10b-DicapTrPrism-Fe2P2C1_r-12	-1964.9367755	0.01
5	06b-Bipirhex-Fe2P1C1	-1964.9367630	0.02
6	09a-DicapTrPr-Fe2C4P2	-1964.9367622	0.02
7	08a-Nido-Fe2C4P1	-1964.9367468	0.03
8	10b-DicapTrPrism-Fe2P2C1_i-12	-1964.9367436	0.03
9	07b-Tdallcap-Fe2P1C4	-1964.9367383	0.03
10	10a-DicapTrPrism-Fe2C1P2	-1964.9367318	0.04
11	05b-Bisdisph-Fe1P4C2	-1964.9367224	0.04
12	08a-Nido-Fe1C1P6_r-15	-1964.9367125	0.05
13	09a-DicapTrPr-Fe1C1P6	-1964.9367114	0.05
14	09b-DicapTrPr-Fe1P1C6	-1964.9367056	0.05
15	08b-Nido-Fe1P1C4_i-28	-1964.9367050	0.05
16	09a-DicapTrPr-Fe1C1P2	-1964.9367041	0.06
17	10b-DicapTrPrism-Fe1P1C1	-1964.9366996	0.06
18	09b-DicapTrPr-Fe3P1C4_r-10	-1964.9366991	0.06
19	02a-Antipr-FeC1P4	-1964.9366975	0.06
20	04a-AntiprTrig-FeC3P2	-1964.9366975	0.06
21	04b-AntiprTriP-FeP3C2	-1964.9366975	0.06
22	10b-DicapTrPrism-Fe3P3C2	-1964.9366935	0.06
23	06b-Bipirhex-Fe2P1C2	-1964.9366924	0.06
24	10b-DicapTrPrism-Fe2P1C3	-1964.9366911	0.06
25	06b-Bipirhex-Fe2P2C1	-1964.9366892	0.06
26	08b-Nido-Fe1P2C1	-1964.9366840	0.07
27	11b-DicapOh-Fe1P1C5	-1964.9366828	0.07
28	05b-Bisdisph-Fe1P1C2	-1964.9366780	0.07
29	10b-DicapTrPrism-Fe3P1C3	-1964.9366748	0.07
30	09b-DicapTrPr-Fe1P1C2	-1964.9366674	0.08
31	09b-DicapTrPr-Fe1P2C4	-1964.9366673	0.08
32	08a-Nido-Fe1C1P6_i-15	-1964.9366627	0.08
33	10b-DicapTrPrism-Fe3P3C3	-1964.9366587	0.08
34	09a-DicapTrPr-Fe1C2P4	-1964.9366577	0.08
35	06a-Bipirhex-Fe2C2P1	-1964.9366487	0.09
36	09a-DicapTrPr-Fe1C2P5	-1964.9366397	0.10
37	09b-DicapTrPr-Fe3P1C4_i-10	-1964.9366396	0.10
38	04b-AntiprTriP-FeP1C2	-1964.9366394	0.10
39	10a-DicapTrPrism-Fe3C5P2	-1964.9366277	0.10

40	08b-Nido-Fe1P1C4_r-28	-1964.9366081	0.12
41	09a-DicapTrPr-Fe3C1P4	-1964.9365875	0.13
42	07a-Tdallcap-Fe1C1P1	-1964.9336389	1.98
43	02a-Antipr-FeC1P2	-1964.9336191	1.99
44	10a-DicapTrPrism-Fe3C1P3	-1964.9335778	2.02
45	10a-DicapTrPrism-Fe1C1P1_i-30	-1964.9335708	2.02
46	09b-DicapTrPr-Fe2P4C2	-1964.9335644	2.03
47	05b-Bisdisph-Fe2P1C4	-1964.9335582	2.03
48	10a-DicapTrPrism-Fe3C1P4	-1964.9335535	2.03
49	11b-DicapOh-Fe3P1C4	-1964.9335530	2.03
50	10a-DicapTrPrism-Fe1C1P1_r-30	-1964.9335525	2.03
51	11b-DicapOh-Fe3P2C5	-1964.9335515	2.03
52	09b-DicapTrPr-Fe2P1C5	-1964.9335487	2.04
53	06a-Bipirhex-Fe2C1P1_i-30	-1964.9335462	2.04
54	02b-Antipr-FeP1C2	-1964.9335455	2.04
55	07a-Tdallcap-Fe2C1P4	-1964.9335412	2.04
56	05a-Bisdisph-Fe1C1P2	-1964.9335395	2.04
57	10a-DicapTrPrism-Fe2C2P2_i-27	-1964.9335383	2.04
58	09a-DicapTrPr-Fe3C3P3_i-16	-1964.9335350	2.04
59	07a-Tdallcap-Fe2C1P6	-1964.9335345	2.04
60	08a-Nido-Fe2C1P5	-1964.9335250	2.05
61	08b-Nido-Fe2P4C2	-1964.9335228	2.05
62	09b-DicapTrPr-Fe3P2C4	-1964.9335221	2.05
63	11a-DicapOh-Fe3C1P4	-1964.9335176	2.06
64	10b-DicapTrPrism-Fe2P2C2	-1964.9335150	2.06
65	08b-Nido-Fe1P2C2	-1964.9335144	2.06
66	02b-Antipr-FeP1C4	-1964.9335102	2.06
67	08a-Nido-Fe1C1P4	-1964.9335092	2.06
68	09a-DicapTrPr-Fe3C3P3_r-16	-1964.9335081	2.06
69	10a-DicapTrPrism-Fe2C2P2_r-27	-1964.9335035	2.06
70	10b-DicapTrPrism-Fe1P2C2	-1964.9334875	2.07
71	08a-Nido-Fe1C2P1_r-20	-1964.9334847	2.08
72	10a-DicapTrPrism-Fe1C1P5	-1964.9334826	2.08
73	10b-DicapTrPrism-Fe2P1C2	-1964.9334736	2.08
74	08a-Nido-Fe1C2P1_i-20	-1964.9334727	2.08
75	10a-DicapTrPrism-Fe2C2P1	-1964.9334720	2.08
76	10a-DicapTrPrism-Fe1C2P1	-1964.9334691	2.09
77	05a-Bisdisph-Fe2C1P1	-1964.9334681	2.09
78	10b-DicapTrPrism-Fe1P2C1	-1964.9334520	2.10
79	06a-Bipirhex-Fe2C1P1_r-30	-1964.9334176	2.12
80	10b-DicapTrPrism-Fe3P2C2	-1964.9303766	4.03
81	03b-TriPyr-FeP1C6	-1964.9303750	4.03

82	05a-Bisdisph-Fe1C1P4	-1964.9303698	4.03
83	02b-Antipr-FeP1C5	-1964.9303690	4.03
84	03b-TriPyr-FeP1C1	-1964.9303677	4.03
85	03a-TrigPyr-FeC2P3	-1964.9303676	4.03
86	04b-AntiprTriP-FeP2C5	-1964.9303676	4.03
87	01b-Cube-FeP1C4	-1964.9303668	4.03
88	10a-DicapTrPrism-Fe2C3P2_i-22	-1964.9303660	4.03
89	10b-DicapTrPrism-Fe2P3C1	-1964.9303649	4.03
90	10a-DicapTrPrism-Fe2C3P2_r-22	-1964.9303619	4.04
91	09b-DicapTrPr-Fe2P1C2	-1964.9303571	4.04
92	09a-DicapTrPr-Fe2C2P3	-1964.9303532	4.04
93	09b-DicapTrPr-Fe1P1C3	-1964.9303517	4.04
94	07a-Tdallcap-Fe1C2P3	-1964.9303468	4.04
95	07a-Tdallcap-Fe2C2P3	-1964.9303464	4.04
96	10b-DicapTrPrism-Fe3P2C3	-1964.9303452	4.05
97	07b-Tdallcap-Fe2P3C1	-1964.9303440	4.05
98	10a-DicapTrPrism-Fe2C2P4	-1964.9303320	4.05
99	07a-Tdallcap-Fe1C1P2	-1964.9303317	4.05
100	11a-DicapOh-Fe3C3P1	-1964.9303310	4.05
101	05a-Bisdisph-Fe1C2P2	-1964.9303306	4.05
102	07a-Tdallcap-Fe2C1P3	-1964.9303280	4.06
103	05a-Bisdisph-Fe1C3P2	-1964.9303214	4.06
104	10a-DicapTrPrism-Fe2C1P5	-1964.9303179	4.06
105	08b-Nido-Fe1P1C3	-1964.9303140	4.07
106	09a-DicapTrPr-Fe2C2P1	-1964.9303127	4.07
107	11a-DicapOh-Fe3C3P2	-1964.9303062	4.07
108	05a-Bisdisph-Fe1C2P3	-1964.9302997	4.07
109	08b-Nido-Fe1P3C3	-1964.9302992	4.07
110	09a-DicapTrPr-Fe2C2P2	-1964.9302910	4.08
111	08b-Nido-Fe1P3C2	-1964.9302905	4.08
112	09b-DicapTrPr-Fe3P4C2	-1964.9302815	4.09
113	10a-DicapTrPrism-Fe3C1P6	-1964.9302740	4.09
114	05a-Bisdisph-Fe2C1P3	-1964.9301437	4.17
115	06a-Bipirhex-Fe2C2P4	-1964.9299117	4.32
116	10b-DicapTrPrism-Fe2P1C5	-1964.9240661	7.99
117	05b-Bisdisph-Fe1P3C2	-1964.9240233	8.01
118	10a-DicapTrPrism-Fe3C2P3	-1964.9240184	8.02
119	09a-DicapTrPr-Fe2C1P2	-1964.9240113	8.02
120	10a-DicapTrPrism-Fe3C2P2	-1964.9240092	8.02
121	07b-Tdallcap-Fe2P2C3	-1964.9239893	8.03
122	03b-TriPyr-FeP1C5	-1964.9239868	8.04
123	05b-Bisdisph-Fe1P2C2	-1964.9239841	8.04

124	07b-Tdallcap-Fe2P1C3	-1964.9239817	8.04
125	08a-Nido-Fe1C3P3	-1964.9239784	8.04
126	07b-Tdallcap-Fe2P3C2	-1964.9239777	8.04
127	07a-Tdallcap-Fe2C3P1	-1964.9239741	8.04
128	09a-DicapTrPr-Fe2C3P3	-1964.9239699	8.05
129	11a-DicapOh-Fe3C2P3	-1964.9239686	8.05
130	02a-Antipr-FeC3P3	-1964.9239540	8.06
131	08a-Nido-Fe1C2P3	-1964.9239515	8.06
132	09a-DicapTrPr-Fe2C3P2	-1964.9239472	8.06
133	09b-DicapTrPr-Fe2P2C3	-1964.9239406	8.06
134	09b-DicapTrPr-Fe3P5C2	-1964.9238864	8.10
135	10a-DicapTrPrism-Fe2C3P1	-1964.9227790	8.79
136	04a-AntiprTrig-FeC2P1	-1964.9213406	9.70
137	04b-AntiprTriP-FeP2C1	-1964.9213399	9.70
138	01a-Cube-FeC2P1	-1964.9213385	9.70
139	01b-Cube-FeP2C1_r-13	-1964.9213344	9.70
140	11a-DicapOh-Fe1C1P6	-1964.9213163	9.71
141	11a-DicapOh-Fe3C2P5	-1964.9212929	9.73
142	06a-Bipirhex-Fe1C1P2	-1964.9212688	9.74
143	11b-DicapOh-Fe3P5C2	-1964.9212554	9.75
144	11b-DicapOh-Fe1P1C6	-1964.9212528	9.75
145	06b-Bipirhex-Fe1P1C2	-1964.9212227	9.77
146	08a-Nido-Fe1C1P2	-1964.9211972	9.79
147	01b-Cube-FeP2C1_i-13	-1964.9210319	9.89
148	10a-DicapTrPrism-Fe1C2P3	-1964.9209008	9.97
149	10b-DicapTrPrism-Fe3P1C2	-1964.9207742	10.05
150	08b-Nido-Fe1P1C5	-1964.9207525	10.07
151	08a-Nido-Fe1C1P5	-1964.9206679	10.12
152	09a-DicapTrPr-Fe3C4P3	-1964.9206341	10.14
153	09a-DicapTrPr-Fe3C2P2	-1964.9206319	10.14
154	09a-DicapTrPr-Fe3C4P1	-1964.9205373	10.20
155	10a-DicapTrPrism-Fe1C3P4	-1964.9205196	10.21
156	11b-DicapOh-Fe3P2C3	-1964.9204864	10.23
157	09a-DicapTrPr-Fe2C6P1	-1964.9139735	14.32
158	10b-DicapTrPrism-Fe1P2C4	-1964.9139722	14.32
159	09b-DicapTrPr-Fe1P2C2	-1964.9139663	14.32
160	09b-DicapTrPr-Fe2P3C2	-1964.9139578	14.33
161	05b-Bisdisph-Fe2P2C2	-1964.9139502	14.33
162	02a-Antipr-FeC1P5	-1964.9137789	14.44
163	09b-DicapTrPr-Fe2P2C2	-1964.9137601	14.45
164	09a-DicapTrPr-Fe1C1P3	-1964.9137424	14.46
165	10b-DicapTrPrism-Fe1P3C4	-1964.9137379	14.47

166	05b-Bisdisph-Fe2P1C3	-1964.9137199	14.48
167	10b-DicapTrPrism-Fe3P1C6	-1964.9136775	14.51
168	05b-Bisdisph-Fe1P1C4	-1964.9136451	14.53
169	10b-DicapTrPrism-Fe2P3C2	-1964.9135873	14.56
170	07b-Tdallcap-Fe2P1C6	-1964.9124554	15.27
171	10b-DicapTrPrism-Fe1P1C5	-1964.9124059	15.30
172	08a-Nido-Fe1C2P2	-1964.9122981	15.37
173	08a-Nido-Fe1C3P2	-1964.9121430	15.47
174	10b-DicapTrPrism-Fe2P2C4	-1964.9121015	15.49
175	01b-Cube-FeP1C3_i-15	-1964.9120890	15.50
176	09b-DicapTrPr-Fe2P6C1	-1964.9120829	15.51
177	11b-DicapOh-Fe3P2C4_r-14	-1964.9120595	15.52
178	06b-Bipirhex-Fe1P1C3	-1964.9120115	15.55
179	01b-Cube-FeP1C3_r-15	-1964.9120042	15.56
180	06a-Bipirhex-Fe1C1P3	-1964.9119989	15.56
181	07b-Tdallcap-Fe1P1C4	-1964.9119955	15.56
182	09b-DicapTrPr-Fe2P1C3	-1964.9119574	15.58
183	01a-Cube-FeC1P3	-1964.9119419	15.59
184	11b-DicapOh-Fe3P4C3	-1964.9116778	15.76
185	07b-Tdallcap-Fe1P2C3	-1964.9116396	15.78
186	10b-DicapTrPrism-Fe1P3C3	-1964.9095971	17.07
187	11b-DicapOh-Fe1P2C3	-1964.9095851	17.07
188	09a-DicapTrPr-Fe2C2P4	-1964.9095758	17.08
189	05a-Bisdisph-Fe2C1P2	-1964.9095729	17.08
190	08b-Nido-Fe2P1C2	-1964.9095639	17.09
191	05a-Bisdisph-Fe2C2P4	-1964.9095526	17.09
192	02b-Antipr-FeP3C3	-1964.9095477	17.10
193	08a-Nido-Fe2C3P4	-1964.9095454	17.10
194	10a-DicapTrPrism-Fe3C3P2	-1964.9095428	17.10
195	10a-DicapTrPrism-Fe3C4P3	-1964.9095427	17.10
196	10a-DicapTrPrism-Fe3C3P3	-1964.9095404	17.10
197	02a-Antipr-FeC2P2	-1964.9095386	17.10
198	05a-Bisdisph-Fe2C4P1	-1964.9095366	17.10
199	10b-DicapTrPrism-Fe1P1C4_r-32	-1964.9095323	17.11
200	08b-Nido-Fe2P1C3	-1964.9095289	17.11
201	11b-DicapOh-Fe1P1C3	-1964.9094989	17.13
202	09b-DicapTrPr-Fe1P2C3	-1964.9094969	17.13
203	10b-DicapTrPrism-Fe1P1C3	-1964.9094947	17.13
204	08b-Nido-Fe1P3C1	-1964.9094534	17.16
205	11a-DicapOh-Fe3C4P3	-1964.9094122	17.18
206	11a-DicapOh-Fe2C2P3	-1964.9094089	17.18
207	11b-DicapOh-Fe3P3C3	-1964.9094069	17.18

208	09b-DicapTrPr-Fe3P2C3	-1964.9060765	19.27
209	11a-DicapOh-Fe3C1P3	-1964.9060710	19.28
210	11a-DicapOh-Fe2C2P2	-1964.9060644	19.28
211	11b-DicapOh-Fe2P2C2	-1964.9060333	19.30
212	09b-DicapTrPr-Fe3P1C2	-1964.9060277	19.31
213	08a-Nido-Fe1C1P3	-1964.9060212	19.31
214	10b-DicapTrPrism-Fe1P1C4_i-32	-1964.9089081	17.50
215	09b-DicapTrPr-Fe2P3C3	-1964.9031384	21.12
216	10a-DicapTrPrism-Fe3C2P4	-1964.9031287	21.12
217	10a-DicapTrPrism-Fe2C1P6	-1964.9031214	21.13
218	07b-Tdallcap-Fe2P2C1	-1964.9030876	21.15
219	10b-DicapTrPrism-Fe2P3C4	-1964.9030852	21.15
220	05a-Bisdisph-Fe1C3P1	-1964.9030840	21.15
221	08b-Nido-Fe1P3C4	-1964.9030318	21.19
222	09a-DicapTrPr-Fe2C1P5	-1964.9029907	21.21
223	03a-TrigPyr-FeC2P1	-1964.9028957	21.27
224	07a-Tdallcap-Fe2C4P2	-1964.9028761	21.28
225	10b-DicapTrPrism-Fe3P1C5	-1964.9028716	21.29
226	01a-Cube-FeC1P1	-1964.9028686	21.29
227	01b-Cube-FeP1C1	-1964.9028610	21.29
228	09a-DicapTrPr-Fe3C2P3	-1964.9027997	21.33
229	09b-DicapTrPr-Fe1P1C1	-1964.9027360	21.37
230	11b-DicapOh-Fe3P4C2	-1964.9027087	21.39
231	11a-DicapOh-Fe3C2P4	-1964.9026929	21.40
232	09a-DicapTrPr-Fe3C2P4	-1964.9026901	21.40
233	09b-DicapTrPr-Fe3P3C4	-1964.9026867	21.40
234	07b-Tdallcap-Fe2P4C1	-1964.9000527	23.05
235	07a-Tdallcap-Fe2C4P1	-1964.9000464	23.06
236	07a-Tdallcap-Fe1C1P4_r-22	-1964.9000358	23.07
237	05b-Bisdisph-Fe1P4C1	-1964.9000271	23.07
238	05a-Bisdisph-Fe1C4P1	-1964.8999963	23.09
239	08b-Nido-Fe1P1C6	-1964.8999959	23.09
240	07a-Tdallcap-Fe1C1P4_i-22	-1964.8996570	23.30
241	10a-DicapTrPrism-Fe2C2P3	-1964.8987402	23.88
242	10a-DicapTrPrism-Fe2C1P1	-1964.8987208	23.89
243	08a-Nido-Fe1C2P5	-1964.8987124	23.90
244	10b-DicapTrPrism-Fe2P1C1	-1964.8987028	23.90
245	04b-AntiprTriP-FeP1C1	-1964.8986966	23.91
246	11b-DicapOh-Fe1P1C1	-1964.8986741	23.92
247	07b-Tdallcap-Fe2P1C5	-1964.8986739	23.92
248	05b-Bisdisph-Fe1P4C3	-1964.8986736	23.92
249	08b-Nido-Fe1P2C5	-1964.8984540	24.06

250	10a-DicapTrPrism-Fe3C6P1	-1964.8983456	24.13
251	05a-Bisdisph-Fe1C4P2	-1964.8981901	24.22
252	10b-DicapTrPrism-Fe3P5C2	-1964.8981604	24.24
253	10a-DicapTrPrism-Fe2C1P3	-1964.8981354	24.26
254	10a-DicapTrPrism-Fe3C1P5	-1964.8973176	24.77
255	08b-Nido-Fe1P1C1	-1964.8973129	24.77
256	11b-DicapOh-Fe3P1C6	-1964.8973020	24.78
257	09a-DicapTrPr-Fe2C5P2	-1964.8972975	24.78
258	10b-DicapTrPrism-Fe2P1C4	-1964.8972799	24.79
259	09a-DicapTrPr-Fe1C2P1	-1964.8972788	24.80
260	09b-DicapTrPr-Fe1P2C1	-1964.8972739	24.80
261	09b-DicapTrPr-Fe1P1C5	-1964.8972674	24.80
262	05b-Bisdisph-Fe1P1C1	-1964.8972611	24.81
263	02a-Antipr-FeC1P3	-1964.8972479	24.81
264	11a-DicapOh-Fe3C4P1	-1964.8971971	24.85
265	11a-DicapOh-Fe3C1P5	-1964.8971863	24.85
266	08a-Nido-Fe1C3P4	-1964.8961736	25.49
267	11a-DicapOh-Fe1C2P2	-1964.8937479	27.01
268	05b-Bisdisph-Fe2P3C2	-1964.8937407	27.02
269	08b-Nido-Fe2P3C3	-1964.8936718	27.06
270	11b-DicapOh-Fe3P1C5	-1964.8932853	27.30
271	09a-DicapTrPr-Fe1C1P5	-1964.8929009	27.54
272	10a-DicapTrPrism-Fe2C1P4	-1964.8928940	27.55
273	07b-Tdallcap-Fe2P1C1	-1964.8928565	27.57
274	10a-DicapTrPrism-Fe3C5P1	-1964.8928509	27.57
275	05b-Bisdisph-Fe1P5C1	-1964.8928470	27.58
276	08a-Nido-Fe1C1P1	-1964.8928354	27.58
277	02a-Antipr-FeC1P1	-1964.8928307	27.59
278	08a-Nido-Fe2C2P1	-1964.8928211	27.59
279	07a-Tdallcap-Fe2C1P1	-1964.8928173	27.60
280	05a-Bisdisph-Fe1C1P1	-1964.8928159	27.60
281	05b-Bisdisph-Fe2P1C2	-1964.8928092	27.60
282	02b-Antipr-FeP1C3	-1964.8928081	27.60
283	05a-Bisdisph-Fe1C5P1	-1964.8928070	27.60
284	05b-Bisdisph-Fe2P2C5	-1964.8927961	27.61
285	10b-DicapTrPrism-Fe3P5C1	-1964.8927898	27.61
286	11a-DicapOh-Fe3C4P2	-1964.8927770	27.62
287	07b-Tdallcap-Fe1P1C2	-1964.8921501	28.01
288	10b-DicapTrPrism-Fe2P2C3	-1964.8921391	28.02
289	07b-Tdallcap-Fe2P4C2	-1964.8921276	28.03
290	04b-AntiprTriP-FeP1C3	-1964.8916613	28.32
291	01a-Cube-FeC2P2	-1964.8916606	28.32

292	09b-DicapTrPr-Fe3P2C2	-1964.8916494	28.33
293	06a-Bipirhex-Fe1C1P4	-1964.8916424	28.33
294	09b-DicapTrPr-Fe2P2C4	-1964.8916370	28.34
295	01a-Cube-FeC1P4_r-91	-1964.8916359	28.34
296	07b-Tdallcap-Fe1P3C3	-1964.8916292	28.34
297	07b-Tdallcap-Fe1P2C2	-1964.8916236	28.34
298	04b-AntiprTriP-FeP2C3	-1964.8912388	28.59
299	11a-DicapOh-Fe3C5P1	-1964.8909134	28.79
300	09a-DicapTrPr-Fe3C2P5	-1964.8908867	28.81
301	02a-Antipr-FeC1P6	-1964.8908100	28.85
302	10a-DicapTrPrism-Fe2C3P4_r-12	-1964.8907866	28.87
303	09b-DicapTrPr-Fe3P3C3	-1964.8907849	28.87
304	10a-DicapTrPrism-Fe3C4P1	-1964.8907833	28.87
305	08a-Nido-Fe1C2P4	-1964.8907531	28.89
306	10b-DicapTrPrism-Fe2P1C6	-1964.8907459	28.90
307	05b-Bisdisph-Fe1P3C1	-1964.8907402	28.90
308	10a-DicapTrPrism-Fe2C3P4_i-12	-1964.8907360	28.90
309	08b-Nido-Fe1P1C2	-1964.8906733	28.94
310	11a-DicapOh-Fe3C6P1	-1964.8903988	29.11
311	06b-Bipirhex-Fe2P2C3	-1964.8900162	29.35
312	05b-Bisdisph-Fe2P4C1	-1964.8900126	29.36
313	10a-DicapTrPrism-Fe1C1P4	-1964.8900024	29.36
314	09a-DicapTrPr-Fe2C5P1	-1964.8900015	29.36
315	10a-DicapTrPrism-Fe1C2P5	-1964.8899966	29.37
316	02b-Antipr-FeP2C2	-1964.8899887	29.37
317	10a-DicapTrPrism-Fe1C1P3	-1964.8899837	29.37
318	05b-Bisdisph-Fe2P2C4	-1964.8899830	29.37
319	11a-DicapOh-Fe1C1P2	-1964.8899770	29.38
320	10a-DicapTrPrism-Fe1C3P3	-1964.8899519	29.39
321	10b-DicapTrPrism-Fe3P4C3	-1964.8899150	29.42
322	11b-DicapOh-Fe2P1C2	-1964.8888123	30.11
323	10a-DicapTrPrism-Fe3C1P2	-1964.8882543	30.46
324	10b-DicapTrPrism-Fe3P4C1_r-19	-1964.8882498	30.46
325	09b-DicapTrPr-Fe2P5C1_r-28	-1964.8882300	30.47
326	10b-DicapTrPrism-Fe1P2C3	-1964.8882297	30.47
327	08a-Nido-Fe2C3P1	-1964.8882205	30.48
328	05a-Bisdisph-Fe2C2P5	-1964.8882129	30.48
329	10b-DicapTrPrism-Fe1P2C5_r-18	-1964.8882103	30.49
330	02b-Antipr-FeP1C6	-1964.8881892	30.50
331	02b-Antipr-FeP1C1	-1964.8881872	30.50
332	10b-DicapTrPrism-Fe3P1C1_r-34	-1964.8881836	30.50
333	09a-DicapTrPr-Fe2C1P6	-1964.8881794	30.51

334	10b-DicapTrPrism-Fe1P2C5_i-18	-1964.8881579	30.52
335	09a-DicapTrPr-Fe2C3P4	-1964.8881424	30.53
336	08a-Nido-Fe2C1P6	-1964.8881318	30.54
337	09a-DicapTrPr-Fe3C1P6	-1964.8881268	30.54
338	10b-DicapTrPrism-Fe1P1C6	-1964.8881235	30.54
339	09a-DicapTrPr-Fe2C1P4	-1964.8881119	30.55
340	10a-DicapTrPrism-Fe1C1P6	-1964.8881038	30.55
341	01a-Cube-FeC1P4_i-91	-1964.8880783	30.57
342	07a-Tdallcap-Fe2C1P5	-1964.8880448	30.59
343	05a-Bisdisph-Fe1C4P3	-1964.8880377	30.59
344	09b-DicapTrPr-Fe3P1C6_r-31	-1964.8880126	30.61
345	10b-DicapTrPrism-Fe3P4C1_i-19	-1964.8877796	30.76
346	10b-DicapTrPrism-Fe3P1C1_i-34	-1964.8877742	30.76
347	09b-DicapTrPr-Fe2P5C1_i-28	-1964.8876955	30.81
348	09b-DicapTrPr-Fe3P1C6_i-31	-1964.8871654	31.14
349	07a-Tdallcap-Fe2C1P2	-1964.8870255	31.23
350	09a-DicapTrPr-Fe3C1P2	-1964.8869845	31.26
351	11b-DicapOh-Fe3P1C3	-1964.8869804	31.26
352	09b-DicapTrPr-Fe3P2C5	-1964.8865727	31.51
353	09b-DicapTrPr-Fe3P2C1	-1964.8865562	31.52
354	11b-DicapOh-Fe3P6C1	-1964.8865230	31.55
355	09b-DicapTrPr-Fe2P4C1	-1964.8865191	31.55
356	06a-Bipirhex-Fe1C1P1	-1964.8864991	31.56
357	09b-DicapTrPr-Fe2P1C4	-1964.8864294	31.60
358	11b-DicapOh-Fe2P1C4	-1964.8863672	31.64
359	08b-Nido-Fe2P4C1	-1964.8863375	31.66
360	04b-AntiprTriP-FeP1C4	-1964.8863211	31.67
361	08a-Nido-Fe2C1P2	-1964.8863184	31.67
362	08b-Nido-Fe2P3C4	-1964.8863056	31.68
363	11a-DicapOh-Fe2C2P1	-1964.8861946	31.75
364	11b-DicapOh-Fe2P2C1	-1964.8861938	31.75
365	09a-DicapTrPr-Fe1C1P4	-1964.8861675	31.77
366	09a-DicapTrPr-Fe3C3P2	-1964.8855654	32.15
367	10a-DicapTrPrism-Fe2C2P5	-1964.8850383	32.48
368	09b-DicapTrPr-Fe1P1C4	-1964.8850136	32.49
369	07a-Tdallcap-Fe1C4P1	-1964.8850044	32.50
370	08b-Nido-Fe1P2C4	-1964.8849981	32.50
371	05b-Bisdisph-Fe1P1C3_r-47	-1964.8849860	32.51
372	10b-DicapTrPrism-Fe3P2C4	-1964.8849293	32.55
373	10a-DicapTrPrism-Fe3C3P1	-1964.8849095	32.56
374	05b-Bisdisph-Fe2P2C3	-1964.8848547	32.59
375	05b-Bisdisph-Fe1P1C3_i-47	-1964.8846977	32.69

376	04b-AntiprTriP-FeP2C4	-1964.8833545	33.53
377	09a-DicapTrPr-Fe3C4P2	-1964.8831916	33.64
378	10b-DicapTrPrism-Fe3P3C1	-1964.8830952	33.70
379	05a-Bisdisph-Fe2C3P1	-1964.8830942	33.70
380	05a-Bisdisph-Fe2C2P3	-1964.8830681	33.71
381	10b-DicapTrPrism-Fe1P1C2	-1964.8830663	33.71
382	08b-Nido-Fe2P2C1	-1964.8830324	33.74
383	02b-Antipr-FeP3C2	-1964.8830288	33.74
384	09a-DicapTrPr-Fe2C4P1	-1964.8830243	33.74
385	06b-Bipirhex-Fe2P1C3	-1964.8830172	33.75
386	11a-DicapOh-Fe3C2P1	-1964.8826061	34.00
387	11a-DicapOh-Fe2C1P2	-1964.8825913	34.01
388	04a-AntiprTrig-FeC3P1	-1964.8825566	34.03
389	07a-Tdallcap-Fe1C3P3	-1964.8818747	34.46
390	03a-TrigPyr-FeC1P5	-1964.8818582	34.47
391	04a-AntiprTrig-FeC1P3	-1964.8812161	34.88
392	07a-Tdallcap-Fe1C1P5	-1964.8811635	34.91
393	09b-DicapTrPr-Fe3P6C1	-1964.8808382	35.11
394	11a-DicapOh-Fe3C3P4	-1964.8808030	35.13
395	08b-Nido-Fe2P4C3	-1964.8807782	35.15
396	08a-Nido-Fe2C3P2	-1964.8807457	35.17
397	11b-DicapOh-Fe3P2C1	-1964.8803416	35.42
398	04b-AntiprTriP-FeP3C1	-1964.8803076	35.45
399	09b-DicapTrPr-Fe2P2C1	-1964.8799933	35.64
400	09a-DicapTrPr-Fe3C5P2	-1964.8791945	36.14
401	07b-Tdallcap-Fe1P1C5	-1964.8789774	36.28
402	07b-Tdallcap-Fe1P3C2	-1964.8789487	36.30
403	01a-Cube-FeC1P2	-1964.8788972	36.33
404	03a-TrigPyr-FeC1P6	-1964.8788795	36.34
405	07b-Tdallcap-Fe1P1C3	-1964.8788463	36.36
406	11b-DicapOh-Fe1P2C2	-1964.8787109	36.45
407	06b-Bipirhex-Fe1P1C4	-1964.8771503	37.43
408	10b-DicapTrPrism-Fe2P3C3	-1964.8769191	37.57
409	11b-DicapOh-Fe3P3C1	-1964.8769172	37.57
410	08a-Nido-Fe1C3P1	-1964.8768742	37.60
411	07b-Tdallcap-Fe2P2C2	-1964.8768698	37.60
412	10b-DicapTrPrism-Fe3P2C5	-1964.8768587	37.61
413	05a-Bisdisph-Fe1C2P1	-1964.8768194	37.63
414	09a-DicapTrPr-Fe3C2P1	-1964.8760089	38.14
415	01b-Cube-FeP1C2	-1964.8754634	38.49
416	09b-DicapTrPr-Fe1P3C2	-1964.8744712	39.11
417	08a-Nido-Fe2C3P3	-1964.8744302	39.13

418	09b-DicapTrPr-Fe3P3C2_r-23	-1964.8739961	39.41
419	11b-DicapOh-Fe1P1C2	-1964.8737982	39.53
420	09a-DicapTrPr-Fe1C3P1	-1964.8735834	39.66
421	08b-Nido-Fe2P1C1	-1964.8735739	39.67
422	11a-DicapOh-Fe2C1P3	-1964.8735620	39.68
423	11b-DicapOh-Fe2P1C3	-1964.8735612	39.68
424	08a-Nido-Fe2C1P1	-1964.8735362	39.69
425	09b-DicapTrPr-Fe3P3C2_i-23	-1964.8735100	39.71
426	03a-TrigPyr-FeC2P2	-1964.8734802	39.73
427	11a-DicapOh-Fe3C3P3	-1964.8734533	39.75
428	09a-DicapTrPr-Fe1C3P2	-1964.8731865	39.91
429	10b-DicapTrPrism-Fe3P6C1	-1964.8730200	40.02
430	06b-Bipirhex-Fe2P3C2	-1964.8728962	40.10
431	04a-AntiprTrig-FeC1P4	-1964.8724475	40.38
432	07a-Tdallcap-Fe2C3P2	-1964.8723851	40.42
433	11b-DicapOh-Fe3P3C4	-1964.8718460	40.76
434	05b-Bisdisph-Fe1P2C1	-1964.8718298	40.77
435	06b-Bipirhex-Fe1P1C1	-1964.8717886	40.79
436	09b-DicapTrPr-Fe1P4C1	-1964.8717143	40.84
437	09a-DicapTrPr-Fe1C4P1	-1964.8717123	40.84
438	09a-DicapTrPr-Fe3C1P3_r-55	-1964.8717049	40.84
439	09b-DicapTrPr-Fe2P4C3	-1964.8711406	41.20
440	09b-DicapTrPr-Fe3P5C1	-1964.8709988	41.29
441	05b-Bisdisph-Fe1P2C3	-1964.8704769	41.61
442	07a-Tdallcap-Fe2C2P1	-1964.8704184	41.65
443	05a-Bisdisph-Fe2C1P4	-1964.8700421	41.89
444	11b-DicapOh-Fe2P2C3	-1964.8697068	42.10
445	09a-DicapTrPr-Fe3C3P4	-1964.8696696	42.12
446	09b-DicapTrPr-Fe2P3C1	-1964.8692536	42.38
447	10a-DicapTrPrism-Fe1C3P2	-1964.8692423	42.39
448	10b-DicapTrPrism-Fe3P3C4	-1964.8692422	42.39
449	05b-Bisdisph-Fe2P2C1	-1964.8692314	42.40
450	05a-Bisdisph-Fe2C3P2	-1964.8692224	42.40
451	10a-DicapTrPrism-Fe1C3P1	-1964.8692215	42.40
452	05a-Bisdisph-Fe2C2P6	-1964.8692098	42.41
453	10a-DicapTrPrism-Fe3C3P4	-1964.8692055	42.41
454	05b-Bisdisph-Fe2P2C6	-1964.8692007	42.42
455	08a-Nido-Fe2C2P2	-1964.8691912	42.42
456	02a-Antipr-FeC2P1	-1964.8691713	42.43
457	02a-Antipr-FeC3P1	-1964.8691705	42.43
458	02b-Antipr-FeP3C1	-1964.8691695	42.43
459	10a-DicapTrPrism-Fe3C2P1	-1964.8691690	42.44

460	06a-Bipirhex-Fe2C3P1	-1964.8691558	42.44
461	10b-DicapTrPrism-Fe1P3C2	-1964.8691536	42.44
462	07a-Tdallcap-Fe1C2P2	-1964.8690532	42.51
463	06a-Bipirhex-Fe2C2P3_r-42	-1964.8668719	43.88
464	09a-DicapTrPr-Fe3C1P3_i-55	-1964.8666492	44.02
465	03a-TrigPyr-FeC3P2_r-45	-1964.8666326	44.03
466	09b-DicapTrPr-Fe3P1C5	-1964.8666149	44.04
467	03b-TriPyr-FeP3C1	-1964.8663336	44.21
468	08a-Nido-Fe2C1P4	-1964.8662912	44.24
469	09a-DicapTrPr-Fe3C6P1	-1964.8662153	44.29
470	09a-DicapTrPr-Fe3C1P1	-1964.8661216	44.35
471	06a-Bipirhex-Fe2C2P3_i-42	-1964.8658073	44.54
472	08a-Nido-Fe2C4P2	-1964.8656499	44.64
473	10a-DicapTrPrism-Fe1C2P2	-1964.8655577	44.70
474	08b-Nido-Fe2P1C5	-1964.8655328	44.72
475	10b-DicapTrPrism-Fe1P3C1	-1964.8654450	44.77
476	09a-DicapTrPr-Fe2C1P1	-1964.8654180	44.79
477	03a-TrigPyr-FeC3P2_i-45	-1964.8652472	44.90
478	07a-Tdallcap-Fe1C1P3	-1964.8651995	44.93
479	11b-DicapOh-Fe3P4C1	-1964.8651380	44.96
480	09b-DicapTrPr-Fe3P3C1	-1964.8651284	44.97
481	11b-DicapOh-Fe3P2C4_i-14	-1964.8650480	45.02
482	10b-DicapTrPrism-Fe2P2C5	-1964.8636622	45.89
483	10a-DicapTrPrism-Fe3C1P1	-1964.8636493	45.90
484	05a-Bisdisph-Fe1C1P3	-1964.8636283	45.91
485	05a-Bisdisph-Fe2C2P1	-1964.8630642	46.27
486	09a-DicapTrPr-Fe2C3P1	-1964.8630559	46.27
487	02b-Antipr-FeP2C1	-1964.8630297	46.29
488	10b-DicapTrPrism-Fe3P2C1	-1964.8630280	46.29
489	03b-TriPyr-FeP2C3	-1964.8628995	46.37
490	11b-DicapOh-Fe3P5C1	-1964.8627791	46.44
491	11a-DicapOh-Fe2C1P4	-1964.8627068	46.49
492	03a-TrigPyr-FeC1P4	-1964.8626949	46.50
493	04a-AntiprTrig-FeC2P2	-1964.8626948	46.50
494	04a-AntiprTrig-FeC2P3	-1964.8625266	46.60
495	11a-DicapOh-Fe3C5P2	-1964.8624405	46.66
496	05a-Bisdisph-Fe2C2P2	-1964.8623544	46.71
497	11a-DicapOh-Fe3C1P1	-1964.8613843	47.32
498	06b-Bipirhex-Fe2P2C4	-1964.8609837	47.57
499	07a-Tdallcap-Fe1C3P2	-1964.8603475	47.97
500	09a-DicapTrPr-Fe1C2P2	-1964.8599160	48.24
501	09a-DicapTrPr-Fe2C4P3	-1964.8595870	48.45

502	06a-Bipirhex-Fe2C3P2	-1964.8593599	48.59
503	08a-Nido-Fe2C1P3	-1964.8587139	49.00
504	10a-DicapTrPrism-Fe3C2P5	-1964.8586647	49.03
505	10a-DicapTrPrism-Fe2C3P3	-1964.8586395	49.04
506	07a-Tdallcap-Fe2C2P2	-1964.8586345	49.05
507	07b-Tdallcap-Fe1P4C1	-1964.8585020	49.13
508	04a-AntiprTrig-FeC2P4	-1964.8577751	49.58
509	11a-DicapOh-Fe1C1P1	-1964.8571616	49.97
510	07b-Tdallcap-Fe2P1C2	-1964.8570222	50.06
511	03b-TriPyr-FeP1C4	-1964.8568615	50.16
512	11b-DicapOh-Fe3P2C2	-1964.8567203	50.25
513	09b-DicapTrPr-Fe3P4C1	-1964.8566683	50.28
514	09b-DicapTrPr-Fe3P4C3	-1964.8563154	50.50
515	09a-DicapTrPr-Fe3C1P5	-1964.8561876	50.58
516	06a-Bipirhex-Fe2C1P2	-1964.8557116	50.88
517	09a-DicapTrPr-Fe3C3P1	-1964.8551918	51.21
518	05b-Bisdisph-Fe2P1C1	-1964.8549634	51.35
519	08b-Nido-Fe2P1C6	-1964.8548521	51.42
520	08b-Nido-Fe2P1C4	-1964.8535924	52.21
521	04b-AntiprTriP-FeP4C1	-1964.8530944	52.52
522	07a-Tdallcap-Fe1C2P1	-1964.8528766	52.66
523	11a-DicapOh-Fe2C1P1	-1964.8519265	53.26
524	09b-DicapTrPr-Fe2P5C2	-1964.8514105	53.58
525	08a-Nido-Fe2C4P3	-1964.8512881	53.66
526	08b-Nido-Fe2P3C2	-1964.8512788	53.66
527	07b-Tdallcap-Fe1P1C6	-1964.8506360	54.06
528	07a-Tdallcap-Fe1C1P6	-1964.8506019	54.09
529	11b-DicapOh-Fe2P1C1	-1964.8504240	54.20
530	07b-Tdallcap-Fe1P3C1	-1964.8501264	54.38
531	01b-Cube-FeP2C2	-1964.8501219	54.39
532	09a-DicapTrPr-Fe3C5P1	-1964.8501121	54.39
533	04b-AntiprTriP-FeP3C3	-1964.8501114	54.39
534	04a-AntiprTrig-FeC4P1	-1964.8500353	54.44
535	09a-DicapTrPr-Fe1C1P1	-1964.8494114	54.83
536	11a-DicapOh-Fe1C1P4	-1964.8494106	54.83
537	06a-Bipirhex-Fe2C2P2	-1964.8487902	55.22
538	10a-DicapTrPrism-Fe1C2P4	-1964.8486554	55.31
539	04a-AntiprTrig-FeC2P5	-1964.8486449	55.31
540	10b-DicapTrPrism-Fe3P4C2	-1964.8481602	55.62
541	05b-Bisdisph-Fe2P3C1	-1964.8481600	55.62
542	02a-Antipr-FeC3P2	-1964.8481340	55.63
543	10a-DicapTrPrism-Fe1C1P2	-1964.8481227	55.64

544	11b-DicapOh-Fe1P1C4	-1964.8478912	55.79
545	09b-DicapTrPr-Fe3P1C1	-1964.8478649	55.80
546	11a-DicapOh-Fe1C1P5	-1964.8467198	56.52
547	09a-DicapTrPr-Fe2C1P3	-1964.8463342	56.76
548	03b-TriPyr-FeP2C2	-1964.8462280	56.83
549	04a-AntiprTrig-FeC1P2	-1964.8458204	57.09
550	04b-AntiprTriP-FeP2C2	-1964.8455209	57.27
551	09b-DicapTrPr-Fe1P3C1	-1964.8454859	57.30
552	06b-Bipirhex-Fe2P3C1	-1964.8454849	57.30
553	08b-Nido-Fe1P2C3	-1964.8453151	57.40
554	09b-DicapTrPr-Fe3P1C3	-1964.8451797	57.49
555	04a-AntiprTrig-FeC1P1_i-16	-1964.8446614	57.81
556	04a-AntiprTrig-FeC1P1_r-16	-1964.8445242	57.90
557	10a-DicapTrPrism-Fe3C4P2	-1964.8441148	58.16
558	11a-DicapOh-Fe3C2P2	-1964.8435585	58.51
559	11b-DicapOh-Fe3P1C2	-1964.8429475	58.89
560	03b-TriPyr-FeP2C1	-1964.8412938	59.93
561	09b-DicapTrPr-Fe2P1C1	-1964.8412450	59.96
562	11b-DicapOh-Fe3P3C2	-1964.8408719	60.19
563	03a-TrigPyr-FeC4P1	-1964.8391562	61.27
564	11b-DicapOh-Fe3P1C1	-1964.8391404	61.28
565	08b-Nido-Fe2P3C1	-1964.8390431	61.34
566	03a-TrigPyr-FeC1P1	-1964.8382116	61.86
567	11b-DicapOh-Fe1P2C1	-1964.8380416	61.97
568	11a-DicapOh-Fe3C1P2	-1964.8358349	63.35
569	11a-DicapOh-Fe3C1P6	-1964.8339576	64.53
570	03b-TriPyr-FeP3C2	-1964.8331372	65.05
571	04a-AntiprTrig-FeC3P3	-1964.8324415	65.48
572	11a-DicapOh-Fe1C2P1	-1964.8321500	65.67
573	03a-TrigPyr-FeC3P1	-1964.8312347	66.24
574	09a-DicapTrPr-Fe2C2P5	-1964.8305836	66.65
575	08b-Nido-Fe2P2C2	-1964.8291123	67.57
576	06a-Bipirhex-Fe2C1P3_r-139	-1964.8290938	67.58
577	03a-TrigPyr-FeC1P2	-1964.8267723	69.04
578	03b-TriPyr-FeP1C2	-1964.8249426	70.19
579	06a-Bipirhex-Fe2C1P4	-1964.8216563	72.25
580	06b-Bipirhex-Fe2P2C2	-1964.8216500	72.25
581	06b-Bipirhex-Fe2P1C4	-1964.8215993	72.29
582	07b-Tdallcap-Fe1P2C1	-1964.8196915	73.48
583	09b-DicapTrPr-Fe2P3C4	-1964.8193065	73.72
584	09b-DicapTrPr-Fe2P2C5	-1964.8183572	74.32
585	07a-Tdallcap-Fe1C3P1	-1964.8141160	76.98

586	09a-DicapTrPr-Fe1C2P3	-1964.8068823	81.52
587	06a-Bipirhex-Fe2C1P3_i-139	-1964.8051880	82.58
588	09b-DicapTrPr-Fe2P1C6	-1964.8039610	83.35
589	03b-TriPyr-FeP1C3	-1964.7980708	87.05
590	03a-TrigPyr-FeC1P3	-1964.7980675	87.05
591	03b-TriPyr-FeP4C1	-1964.7969920	87.73
592	11a-DicapOh-Fe1C2P3	-1964.7917901	90.99
593	11a-DicapOh-Fe1C1P3	-1964.7917332	91.03

Table S2A. Initial $CpFeCHPHHB_6H_6$ structures, 439 in all.

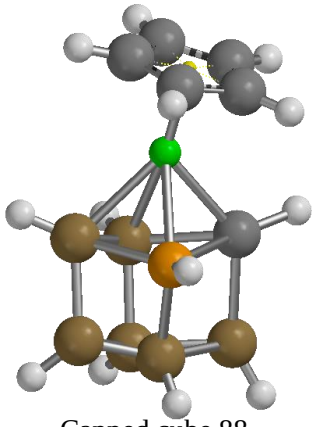
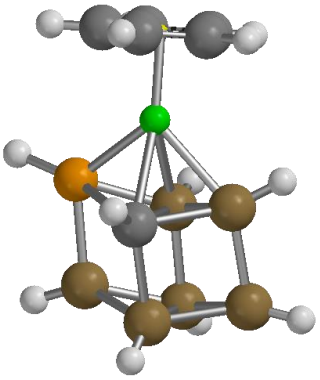
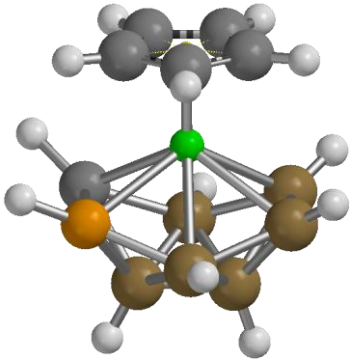
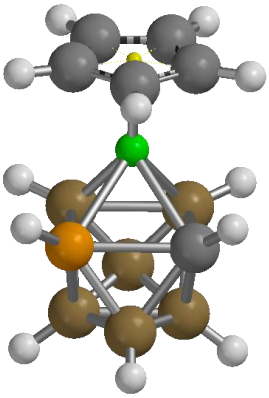
 Capped cube 88	 Compressed capped cube 136
 Isocloso structure 162	 Tricapped trigonal prism 53

Table S2B. Distance table for the lowest-lying $CpFeCHPCH_3B_6H_6$ 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.

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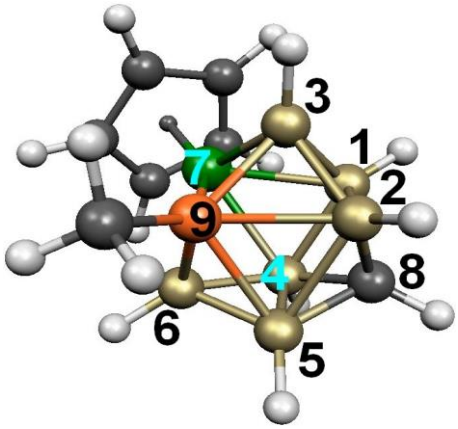
<td> 

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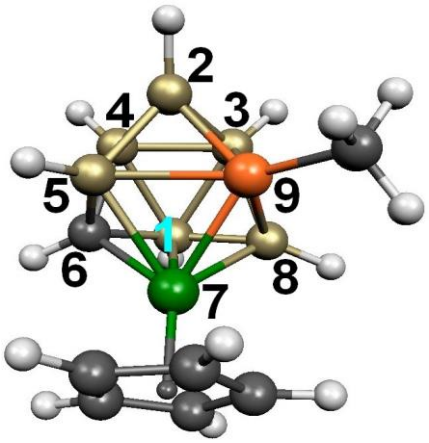
<td> 

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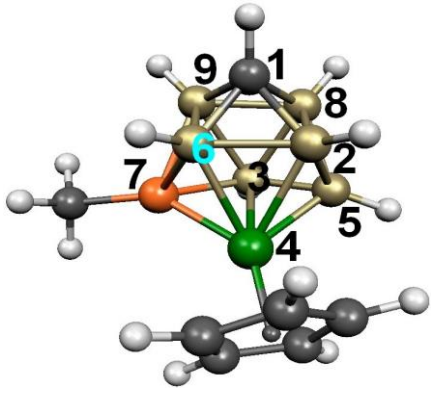
<td> 

3. -2029.6760146 +4.2
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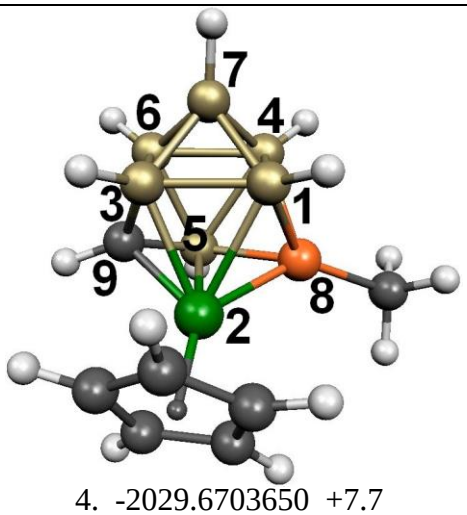
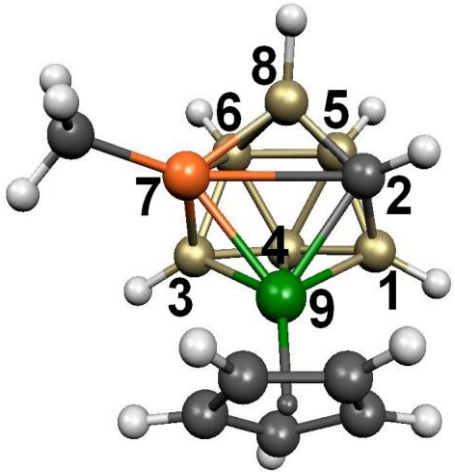


4. -2029.6703650 +7.7
C_1 H/L 1.91

		1	2	3	4	5
1	B	0.000000				
2	Fe	2.298913	0.000000			
3	B	1.898847	2.204324	0.000000		
4	B	1.878097	3.148064	2.630836	0.000000	
5	B	2.787045	2.221681	2.623600	2.034044	0.000000
6	B	2.645117	3.079367	1.793022	1.891904	1.897666
7	B	1.686287	3.327790	1.710718	1.687630	2.940681
8	P	1.933743	2.097426	3.056596	1.911840	1.931166
9	C	2.811579	1.939688	1.609287	2.785017	1.576098

		6	7	8	9
6	B	0.000000			
7	B	1.696180	0.000000		
8	P	3.068050	3.029829	0.000000	
9	C	1.615363	2.723576	2.895229	0.000000



5. -2029.6690718 +8.5
C_1 H/L 2.39

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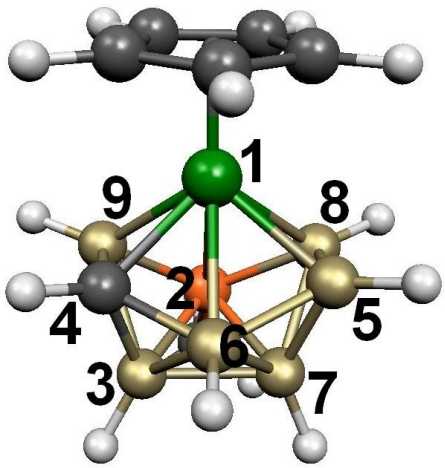
1	B	0.000000				
2	C	1.541217	0.000000			
3	B	2.964110	3.195700	0.000000		
4	B	1.727764	2.560629	1.680034	0.000000	
5	B	1.744493	1.675867	2.894392	1.816068	0.000000
6	B	2.887489	2.712521	1.786370	1.820126	1.768911
7	P	3.373490	2.674767	1.881484	2.869033	2.980294
8	B	2.761695	1.603847	2.950894	2.850500	1.766475
9	Fe	2.014789	2.142888	2.075807	2.212182	2.926388

		6	7	8	9
6	B	0.000000			
7	P	2.011092	0.000000		
8	B	1.882394	1.895147	0.000000	
9	Fe	2.954147	2.251434	2.849671	0.000000



6. -2029.6616382 +13.2
C_1 H/L 1.98

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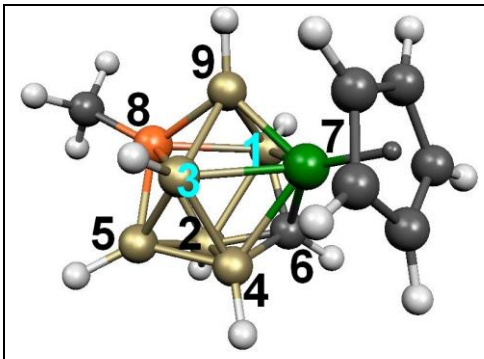
1	Fe	0.000000				
2	P	2.769661	0.000000			
3	B	2.865375	2.027203	0.000000		
4	C	1.937395	2.792823	1.608836	0.000000	
5	B	2.003177	2.938399	2.921652	2.861099	0.000000
6	B	2.151843	2.989286	1.808930	1.601307	1.729842
7	B	2.864021	2.031478	1.845908	2.760832	1.735885
8	B	2.237481	1.852442	2.981903	3.265039	1.656968
9	B	2.167234	1.879278	1.869317	1.551802	3.374504

		6	7	8	9
6	B	0.000000			
7	B	1.818718	0.000000		
8	B	2.770066	1.843393	0.000000	
9	B	2.727512	2.986085	2.957947	0.000000



7. -2029.6587869 +15.0
C_1 H/L 1.95

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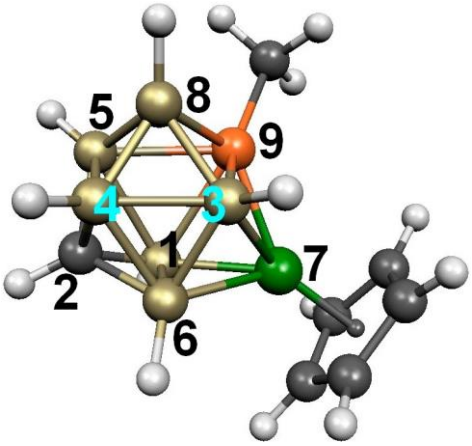
1	B	0.000000				
2	B	2.083666	0.000000			
3	B	2.755034	2.732728	0.000000		
4	B	2.634184	1.791540	1.854267	0.000000	
5	B	3.023311	1.724312	1.781485	1.717172	0.000000
6	C	1.578742	1.589355	2.792223	1.627533	2.728414
7	Fe	2.097874	3.044935	2.073429	2.087156	3.222705
8	P	2.110547	2.140354	2.039446	2.787817	1.885681
9	B	1.806983	3.116332	1.876233	2.966307	3.027840

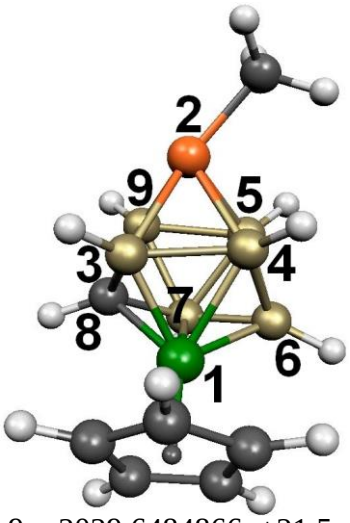
		6	7	8	9
6	C	0.000000			
7	Fe	1.949875	0.000000		
8	P	2.886719	3.107610	0.000000	
9	B	2.823857	1.937210	1.871728	0.000000



8. -2029.6541348 +17.9
C_1 H/L 1.34

		1	2	3	4	5
1	B	0.000000				
2	C	1.567105	0.000000			
3	B	2.765007	2.728755	0.000000		
4	B	2.680668	1.614730	1.847560	0.000000	
5	B	2.148737	1.589338	2.695004	1.783458	0.000000
6	B	1.787013	1.653021	1.825775	1.851965	2.670232
7	Fe	2.021733	3.114682	2.171310	3.357093	3.427636
8	B	3.096414	2.701759	1.753558	1.693527	1.721613
9	P	2.228332	2.907624	2.022051	2.826998	2.175228

		6	7	8	9
6	B	0.000000			
7	Fe	2.061468	0.000000		
8	B	2.867408	3.347773	0.000000	
9	P	2.776662	2.057701	1.913757	0.000000



9. -2029.6484866 +21.5
C_1 H/L 1.92

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1	Fe	0.000000				
2	P	3.452388	0.000000			
3	B	1.940145	2.100980	0.000000		
4	B	2.105649	1.956569	1.897802	0.000000	
5	B	2.951369	1.995406	2.818169	1.853397	0.000000
6	B	1.929702	3.165688	2.915702	1.737059	1.710938
7	B	2.103764	3.118727	2.671756	2.622323	1.854333
8	C	1.958134	2.799302	1.611166	2.720833	2.673077
9	B	3.091571	1.953774	2.285679	2.748350	1.858904

		6	7	8	9
6	B	0.000000			
7	B	1.756198	0.000000		
8	C	2.784679	1.606012	0.000000	
9	B	2.941904	1.826257	1.605764	0.000000

Table S2C. Energy ranking for all of the $CpFeCHPHB_6H_6$ optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	04a-TricTrPrism-Fe1C2P2	-1990.3967438	0.00
2	03b-Tl99-Fe2P3C3	-1990.3967382	0.00
3	03b-Tl99-Fe2P5C1	-1990.3967213	0.01
4	03a-Tl99-Fe4C4P1	-1990.3967089	0.02
5	03b-Tl99-Fe3P3C2	-1990.3967005	0.03
6	03a-Tl99-Fe3C2P3	-1990.3966953	0.03
7	02a-PressCapCube-Fe1C3P3	-1990.3966915	0.03
8	01a-CapCube-Fe3C5P3	-1990.3966755	0.04
9	04b-TricTrPrism-Fe2P3C1	-1990.3966715	0.05
10	01b-CapCube-Fe1P1C5	-1990.3966696	0.05
11	01b-CapCube-Fe2P4C2	-1990.3966212	0.08
12	03a-Tl99-Fe1C1P4	-1990.3957140	0.65
13	03b-Tl99-Fe4P2C1	-1990.3957069	0.65
14	02a-PressCapCube-Fe5C5P2	-1990.3957056	0.65
15	03b-Tl99-Fe4P1C1	-1990.3957051	0.65
16	02a-PressCapCube-Fe5C1P3	-1990.3957039	0.65
17	01b-CapCube-Fe3P4C2	-1990.3956950	0.66
18	01b-CapCube-Fe1P1C2	-1990.3956945	0.66
19	03a-Tl99-Fe2C4P2	-1990.3956925	0.66
20	03b-Tl99-Fe1P1C4	-1990.3956911	0.66
21	03b-Tl99-Fe2P1C1	-1990.3956836	0.67
22	04b-TricTrPrism-Fe2P1C2	-1990.3956836	0.67
23	02b-PressCapCube-Fe3P1C1	-1990.3956828	0.67
24	02a-PressCapCube-Fe3C1P1	-1990.3956659	0.68
25	01a-CapCube-Fe2C5P3	-1990.3956613	0.68
26	02b-PressCapCube-Fe2P2C3	-1990.3956594	0.68
27	03a-Tl99-Fe3C6P1	-1990.3956580	0.68
28	01b-CapCube-Fe3P1C1	-1990.3956534	0.68
29	03b-Tl99-Fe3P6C1	-1990.3956445	0.69
30	04b-TricTrPrism-Fe2P2C1	-1990.3956275	0.70
31	03b-Tl99-Fe3P1C3	-1990.3953476	0.88
32	01a-CapCube-Fe1C1P4	-1990.3906688	3.81
33	01b-CapCube-Fe2P2C4	-1990.3906632	3.82
34	02b-PressCapCube-Fe3P2C4	-1990.3906497	3.82
35	01a-CapCube-Fe2C3P2	-1990.3906463	3.83
36	01b-CapCube-Fe1P1C4	-1990.3906371	3.83
37	04b-TricTrPrism-Fe2P1C1_i-17	-1990.3906298	3.84
38	04a-TricTrPrism-Fe2C1P1	-1990.3906296	3.84
39	01a-CapCube-Fe2C2P4	-1990.3906289	3.84

40	04b-TricTrPrism-Fe2P1C1_r-17	-1990.3906192	3.84
41	03a-Tl99-Fe4C1P3	-1990.3906073	3.85
42	03a-Tl99-Fe1C1P3	-1990.3905968	3.86
43	03a-Tl99-Fe2C1P3	-1990.3905779	3.87
44	03b-Tl99-Fe1P1C3	-1990.3904618	3.94
45	04b-TricTrPrism-Fe2P2C2	-1990.3899013	4.29
46	04a-TricTrPrism-Fe2C2P2	-1990.3898282	4.34
47	02b-PressCapCube-Fe5P4C1	-1990.3898254	4.34
48	03b-Tl99-Fe2P3C2	-1990.3898196	4.35
49	03b-Tl99-Fe4P2C2	-1990.3898113	4.35
50	01b-CapCube-Fe3P1C5	-1990.3898012	4.36
51	03a-Tl99-Fe2C4P1	-1990.3897942	4.36
52	03a-Tl99-Fe2C3P2	-1990.3897909	4.36
53	01a-CapCube-Fe2C5P2	-1990.3897818	4.37
54	03b-Tl99-Fe2P4C1	-1990.3897708	4.38
55	01b-CapCube-Fe3P5C2	-1990.3897651	4.38
56	03a-Tl99-Fe4C2P2	-1990.3897475	4.39
57	02b-PressCapCube-Fe5P6C1	-1990.3897316	4.40
58	03a-Tl99-Fe3C1P4	-1990.3854161	7.11
59	03b-Tl99-Fe3P1C5	-1990.3854126	7.11
60	04a-TricTrPrism-Fe1C1P1	-1990.3853985	7.12
61	04b-TricTrPrism-Fe1P1C1	-1990.3853979	7.12
62	03b-Tl99-Fe3P6C2	-1990.3853762	7.13
63	01a-CapCube-Fe3C5P2	-1990.3853739	7.13
64	02b-PressCapCube-Fe1P1C2	-1990.3853719	7.14
65	03b-Tl99-Fe3P1C4	-1990.3853693	7.14
66	03a-Tl99-Fe3C1P5	-1990.3853429	7.15
67	02a-PressCapCube-Fe1C1P2	-1990.3853370	7.16
68	02a-PressCapCube-Fe5C6P1	-1990.3853366	7.16
69	02a-PressCapCube-Fe2C1P3	-1990.3842180	7.86
70	01b-CapCube-Fe3P1C2	-1990.3842114	7.86
71	01b-CapCube-Fe3P3C3	-1990.3842067	7.87
72	04b-TricTrPrism-Fe1P1C5	-1990.3842058	7.87
73	04a-TricTrPrism-Fe1C2P3	-1990.3841843	7.88
74	03b-Tl99-Fe3P3C4	-1990.3841811	7.88
75	04a-TricTrPrism-Fe2C2P3	-1990.3841709	7.89
76	02b-PressCapCube-Fe3P6C1	-1990.3841699	7.89
77	03a-Tl99-Fe3C1P2	-1990.3841641	7.89
78	03b-Tl99-Fe2P4C3	-1990.3838095	8.12
79	01b-CapCube-Fe3P6C1	-1990.3837756	8.14
80	03a-Tl99-Fe4C2P4	-1990.3837579	8.15
81	03b-Tl99-Fe2P5C2	-1990.3837533	8.15

82	02a-PressCapCube-Fe5C5P1	-1990.3837390	8.16
83	01a-CapCube-Fe3C6P1	-1990.3837355	8.16
84	04b-TricTrPrism-Fe2P1C7	-1990.3815742	9.52
85	01b-CapCube-Fe2P5C2	-1990.3804166	10.25
86	01a-CapCube-Fe2C6P1	-1990.3804106	10.25
87	03b-Tl99-Fe1P2C1	-1990.3804045	10.25
88	03b-Tl99-Fe1P1C5	-1990.3803957	10.26
89	04b-TricTrPrism-Fe2P2C3	-1990.3803409	10.29
90	02a-PressCapCube-Fe5C3P1	-1990.3777851	11.90
91	02a-PressCapCube-Fe2C1P2	-1990.3762983	12.83
92	02b-PressCapCube-Fe3P5C3	-1990.3762830	12.84
93	03b-Tl99-Fe3P1C7	-1990.3762696	12.85
94	03b-Tl99-Fe4P2C3	-1990.3762409	12.87
95	01a-CapCube-Fe3C1P2	-1990.3762381	12.87
96	03a-Tl99-Fe2C3P3	-1990.3762235	12.88
97	03a-Tl99-Fe2C2P2	-1990.3762103	12.89
98	03a-Tl99-Fe2C5P1	-1990.3762083	12.89
99	01b-CapCube-Fe3P2C4	-1990.3762060	12.89
100	02b-PressCapCube-Fe3P3C2	-1990.3761993	12.89
101	03a-Tl99-Fe3C2P2	-1990.3761968	12.89
102	04b-TricTrPrism-Fe2P2C4	-1990.3761931	12.90
103	01b-CapCube-Fe2P1C3	-1990.3761851	12.90
104	03a-Tl99-Fe4C3P2	-1990.3761816	12.90
105	01b-CapCube-Fe3P5C3	-1990.3761634	12.91
106	02a-PressCapCube-Fe2C2P3	-1990.3758374	13.12
107	04b-TricTrPrism-Fe1P1C6	-1990.3758275	13.13
108	03b-Tl99-Fe3P5C2	-1990.3758215	13.13
109	03a-Tl99-Fe3C2P5	-1990.3758145	13.13
110	03b-Tl99-Fe3P2C2	-1990.3758138	13.13
111	02b-PressCapCube-Fe5P1C4	-1990.3758120	13.14
112	03a-Tl99-Fe3C1P3	-1990.3758117	13.14
113	04b-TricTrPrism-Fe1P2C1	-1990.3757928	13.15
114	01b-CapCube-Fe2P6C1	-1990.3703144	16.58
115	02b-PressCapCube-Fe3P5C2	-1990.3702964	16.60
116	02a-PressCapCube-Fe3C5P2	-1990.3702645	16.62
117	02a-PressCapCube-Fe3C1P4	-1990.3702437	16.63
118	03a-Tl99-Fe4C1P6	-1990.3702429	16.63
119	01b-CapCube-Fe2P3C2	-1990.3692594	17.25
120	03b-Tl99-Fe3P2C5	-1990.3679823	18.05
121	03a-Tl99-Fe2C1P4	-1990.3679353	18.08
122	03a-Tl99-Fe2C5P2	-1990.3679340	18.08
123	04a-TricTrPrism-Fe2C1P7	-1990.3679163	18.09

124	01a-CapCube-Fe2C1P5	-1990.3678242	18.15
125	01a-CapCube-Fe2C4P1	-1990.3677821	18.17
126	02a-PressCapCube-Fe3C4P1	-1990.3677653	18.18
127	03b-Tl99-Fe4P2C4	-1990.3656137	19.53
128	01a-CapCube-Fe3C3P3	-1990.3656122	19.54
129	02a-PressCapCube-Fe2C5P2	-1990.3655571	19.57
130	03b-Tl99-Fe4P1C4_r-23	-1990.3655493	19.58
131	03a-Tl99-Fe3C7P1	-1990.3655255	19.59
132	02b-PressCapCube-Fe3P1C4	-1990.3655112	19.60
133	03a-Tl99-Fe1C1P5_r-200	-1990.3654792	19.62
134	03a-Tl99-Fe1C2P1	-1990.3654770	19.62
135	04b-TricTrPrism-Fe2P1C4	-1990.3654525	19.64
136	03b-Tl99-Fe4P1C4_i-23	-1990.3650338	19.90
137	02b-PressCapCube-Fe3P4C1	-1990.3644218	20.28
138	04a-TricTrPrism-Fe1C1P5	-1990.3626786	21.38
139	02b-PressCapCube-Fe5P1C2	-1990.3626570	21.39
140	02b-PressCapCube-Fe3P1C2	-1990.3626559	21.39
141	03b-Tl99-Fe1P3C2_r-21	-1990.3626384	21.40
142	03b-Tl99-Fe3P4C1	-1990.3626376	21.40
143	04a-TricTrPrism-Fe2C1P3	-1990.3626237	21.41
144	01a-CapCube-Fe2C4P2	-1990.3626221	21.41
145	03b-Tl99-Fe1P1C7	-1990.3626164	21.42
146	03a-Tl99-Fe2C1P2	-1990.3626159	21.42
147	03b-Tl99-Fe4P3C3	-1990.3625468	21.46
148	04b-TricTrPrism-Fe1P3C1	-1990.3625222	21.47
149	02a-PressCapCube-Fe2C3P3	-1990.3625148	21.48
150	01b-CapCube-Fe2P1C5	-1990.3625097	21.48
151	03a-Tl99-Fe4C3P3	-1990.3624691	21.51
152	04a-TricTrPrism-Fe1C3P1	-1990.3624639	21.51
153	01a-CapCube-Fe3C2P2	-1990.3624461	21.52
154	02b-PressCapCube-Fe2P3C3	-1990.3624455	21.52
155	03a-Tl99-Fe1C2P2	-1990.3623474	21.58
156	02b-PressCapCube-Fe1P3C3	-1990.3623158	21.60
157	04a-TricTrPrism-Fe1C1P3	-1990.3622940	21.62
158	03b-Tl99-Fe4P4C1	-1990.3622630	21.64
159	03b-Tl99-Fe1P2C2	-1990.3622624	21.64
160	03b-Tl99-Fe1P3C2_i-21	-1990.3622596	21.64
161	03b-Tl99-Fe2P4C2	-1990.3599954	23.06
162	03a-Tl99-Fe4C2P1	-1990.3599635	23.08
163	03a-Tl99-Fe4C1P1	-1990.3599290	23.10
164	04a-TricTrPrism-Fe2C1P2	-1990.3597282	23.23
165	04a-TricTrPrism-Fe2C2P1	-1990.3596847	23.26

166	03a-Tl99-Fe2C1P1	-1990.3596194	23.30
167	02b-PressCapCube-Fe3P1C5	-1990.3585504	23.97
168	03b-Tl99-Fe4P1C6	-1990.3585181	23.99
169	01b-CapCube-Fe2P2C3	-1990.3585167	23.99
170	03b-Tl99-Fe1P1C1	-1990.3585061	23.99
171	01b-CapCube-Fe3P5C1	-1990.3584796	24.01
172	02b-PressCapCube-Fe5P1C5_r-18	-1990.3584633	24.02
173	03b-Tl99-Fe3P1C6	-1990.3584570	24.03
174	01a-CapCube-Fe2C3P3	-1990.3584547	24.03
175	01a-CapCube-Fe2C2P3	-1990.3584514	24.03
176	01b-CapCube-Fe3P3C1	-1990.3581219	24.24
177	03a-Tl99-Fe3C3P1	-1990.3581200	24.24
178	03a-Tl99-Fe4C1P5	-1990.3580963	24.25
179	03a-Tl99-Fe1C1P2	-1990.3580937	24.25
180	01a-CapCube-Fe2C5P1	-1990.3580864	24.26
181	03a-Tl99-Fe3C3P5	-1990.3580855	24.26
182	04b-TricTrPrism-Fe2P1C5	-1990.3580824	24.26
183	02b-PressCapCube-Fe5P2C2	-1990.3580790	24.26
184	02b-PressCapCube-Fe5P1C1	-1990.3580768	24.26
185	02b-PressCapCube-Fe5P1C5_i-18	-1990.3580165	24.30
186	02b-PressCapCube-Fe5P1C3	-1990.3577418	24.47
187	02b-PressCapCube-Fe2P5C2	-1990.3577070	24.50
188	03b-Tl99-Fe3P7C1	-1990.3576902	24.51
189	01a-CapCube-Fe3C1P5	-1990.3576449	24.54
190	01b-CapCube-Fe2P5C3	-1990.3576260	24.55
191	04a-TricTrPrism-Fe2C1P4	-1990.3576245	24.55
192	03a-Tl99-Fe4C1P4	-1990.3576221	24.55
193	02a-PressCapCube-Fe1C2P1	-1990.3561698	25.46
194	04a-TricTrPrism-Fe2C2P6	-1990.3561013	25.50
195	03a-Tl99-Fe2C3P1	-1990.3559274	25.61
196	02b-PressCapCube-Fe2P1C4	-1990.3558937	25.63
197	03b-Tl99-Fe4P2C5	-1990.3558834	25.64
198	03a-Tl99-Fe2C3P5	-1990.3558582	25.66
199	02a-PressCapCube-Fe3C2P2	-1990.3558285	25.68
200	03b-Tl99-Fe2P3C1	-1990.3558227	25.68
201	04b-TricTrPrism-Fe2P2C5	-1990.3558112	25.69
202	02b-PressCapCube-Fe5P4C2	-1990.3557998	25.69
203	02b-PressCapCube-Fe2P2C1	-1990.3557658	25.71
204	04a-TricTrPrism-Fe2C2P4	-1990.3553372	25.98
205	03a-Tl99-Fe3C1P7	-1990.3553371	25.98
206	02a-PressCapCube-Fe3C3P2	-1990.3553288	25.99
207	02a-PressCapCube-Fe1C1P5	-1990.3553202	25.99

208	03b-Tl99-Fe2P2C2	-1990.3553114	26.00
209	04b-TricTrPrism-Fe2P1C6	-1990.3551464	26.10
210	02b-PressCapCube-Fe5P2C3	-1990.3551253	26.12
211	02a-PressCapCube-Fe3C2P3	-1990.3551112	26.13
212	01a-CapCube-Fe2C2P2	-1990.3550696	26.15
213	01a-CapCube-Fe2C1P3_r-84	-1990.3550630	26.16
214	03a-Tl99-Fe4C2P5	-1990.3546394	26.42
215	03a-Tl99-Fe4C2P3	-1990.3537082	27.01
216	02b-PressCapCube-Fe2P1C2	-1990.3536972	27.01
217	02b-PressCapCube-Fe1P2C3	-1990.3536962	27.01
218	03b-Tl99-Fe4P3C2	-1990.3536539	27.04
219	02b-PressCapCube-Fe2P3C2	-1990.3534700	27.16
220	02a-PressCapCube-Fe3C2P4	-1990.3534674	27.16
221	04b-TricTrPrism-Fe2P4C1	-1990.3534580	27.16
222	03b-Tl99-Fe4P3C4	-1990.3534574	27.16
223	03b-Tl99-Fe2P3C4	-1990.3534569	27.16
224	03a-Tl99-Fe3C2P1	-1990.3534404	27.17
225	03b-Tl99-Fe3P4C2	-1990.3534350	27.18
226	02a-PressCapCube-Fe1C1P4	-1990.3533606	27.22
227	02a-PressCapCube-Fe5C3P3	-1990.3533588	27.22
228	01b-CapCube-Fe1P1C3	-1990.3533428	27.23
229	02b-PressCapCube-Fe1P3C1	-1990.3533231	27.25
230	02a-PressCapCube-Fe1C2P3	-1990.3533140	27.25
231	02a-PressCapCube-Fe2C2P4	-1990.3533087	27.26
232	04a-TricTrPrism-Fe1C1P4_r-44	-1990.3532948	27.27
233	02b-PressCapCube-Fe5P2C4	-1990.3532764	27.28
234	01a-CapCube-Fe3C3P1	-1990.3531234	27.37
235	01b-CapCube-Fe2P2C2	-1990.3530706	27.41
236	03b-Tl99-Fe1P1C2	-1990.3529227	27.50
237	02b-PressCapCube-Fe3P2C3	-1990.3529083	27.51
238	04a-TricTrPrism-Fe1C1P4_i-44	-1990.3515486	28.36
239	01b-CapCube-Fe3P2C2	-1990.3513299	28.50
240	02a-PressCapCube-Fe3C1P2	-1990.3513032	28.51
241	02a-PressCapCube-Fe5C1P2	-1990.3512901	28.52
242	04b-TricTrPrism-Fe2P1C3	-1990.3512864	28.53
243	03b-Tl99-Fe2P1C2	-1990.3512633	28.54
244	03a-Tl99-Fe3C4P1	-1990.3512415	28.55
245	03b-Tl99-Fe4P1C2	-1990.3512392	28.56
246	01a-CapCube-Fe2C1P3_i-84	-1990.3512095	28.57
247	02b-PressCapCube-Fe5P5C1	-1990.3510123	28.70
248	02b-PressCapCube-Fe1P1C4	-1990.3496395	29.56
249	03b-Tl99-Fe3P1C2	-1990.3495700	29.60

250	02a-PressCapCube-Fe2C3P2	-1990.3492447	29.81
251	02b-PressCapCube-Fe5P3C1	-1990.3491018	29.90
252	03a-Tl99-Fe1C2P3	-1990.3489426	30.00
253	03a-Tl99-Fe1C1P5_i-200	-1990.3477603	30.74
254	03b-Tl99-Fe4P3C1	-1990.3473662	30.99
255	02b-PressCapCube-Fe2P5C3	-1990.3473551	30.99
256	02a-PressCapCube-Fe5C4P1	-1990.3465793	31.48
257	03b-Tl99-Fe3P2C1	-1990.3465493	31.50
258	03b-Tl99-Fe2P3C5	-1990.3460488	31.81
259	02a-PressCapCube-Fe5C4P2	-1990.3460143	31.83
260	02b-PressCapCube-Fe2P4C1	-1990.3460110	31.84
261	02b-PressCapCube-Fe1P2C2	-1990.3456236	32.08
262	02a-PressCapCube-Fe1C2P2	-1990.3456152	32.08
263	03b-Tl99-Fe3P2C3	-1990.3455954	32.10
264	04b-TricTrPrism-Fe1P2C2	-1990.3455651	32.12
265	04b-TricTrPrism-Fe1P1C4	-1990.3449044	32.53
266	02a-PressCapCube-Fe5C5P3	-1990.3448979	32.53
267	02a-PressCapCube-Fe5C2P4	-1990.3448872	32.54
268	01a-CapCube-Fe1C1P3	-1990.3448605	32.56
269	03a-Tl99-Fe3C4P2	-1990.3448210	32.58
270	01b-CapCube-Fe2P2C1	-1990.3447160	32.65
271	02a-PressCapCube-Fe2C1P1	-1990.3446643	32.68
272	02b-PressCapCube-Fe2P1C1	-1990.3446403	32.70
273	04a-TricTrPrism-Fe2C3P1	-1990.3445236	32.77
274	03a-Tl99-Fe3C3P2	-1990.3444938	32.79
275	03a-Tl99-Fe4C1P2	-1990.3444449	32.82
276	01a-CapCube-Fe2C2P1	-1990.3437236	33.27
277	03b-Tl99-Fe2P2C3	-1990.3425930	33.98
278	02b-PressCapCube-Fe5P2C1	-1990.3425791	33.99
279	01b-CapCube-Fe1P2C1	-1990.3425569	34.00
280	02a-PressCapCube-Fe2C3P1	-1990.3425513	34.01
281	01b-CapCube-Fe3P2C1	-1990.3425347	34.02
282	02b-PressCapCube-Fe3P3C3	-1990.3424883	34.05
283	03a-Tl99-Fe2C5P3	-1990.3424703	34.06
284	03a-Tl99-Fe1C3P2	-1990.3423167	34.15
285	03a-Tl99-Fe1C1P7	-1990.3422789	34.18
286	01b-CapCube-Fe2P1C1	-1990.3415588	34.63
287	03a-Tl99-Fe4C3P5	-1990.3412674	34.81
288	04b-TricTrPrism-Fe2P3C2	-1990.3412531	34.82
289	02b-PressCapCube-Fe5P5C2	-1990.3412270	34.84
290	03a-Tl99-Fe2C3P4	-1990.3412158	34.84
291	02b-PressCapCube-Fe5P3C3_r-94	-1990.3412061	34.85

292	01b-CapCube-Fe3P1C3	-1990.3411991	34.86
293	04a-TricTrPrism-Fe2C4P1	-1990.3411956	34.86
294	03a-Tl99-Fe2C2P1	-1990.3411747	34.87
295	02a-PressCapCube-Fe3C4P2	-1990.3411730	34.87
296	01a-CapCube-Fe3C1P1	-1990.3408985	35.04
297	03b-Tl99-Fe4P1C3	-1990.3405215	35.28
298	02b-PressCapCube-Fe2P5C1	-1990.3404944	35.30
299	01a-CapCube-Fe3C1P3	-1990.3404890	35.30
300	02b-PressCapCube-Fe1P1C5	-1990.3403541	35.39
301	01a-CapCube-Fe1C1P5	-1990.3402680	35.44
302	01b-CapCube-Fe1P1C1	-1990.3401473	35.52
303	02b-PressCapCube-Fe1P1C1	-1990.3401335	35.52
304	02a-PressCapCube-Fe5C1P4	-1990.3400351	35.59
305	02a-PressCapCube-Fe1C1P1	-1990.3396977	35.80
306	01b-CapCube-Fe2P5C1	-1990.3380959	36.80
307	02a-PressCapCube-Fe3C5P1_r-30	-1990.3380837	36.81
308	01a-CapCube-Fe3C5P1	-1990.3380826	36.81
309	02a-PressCapCube-Fe2C2P2	-1990.3380775	36.81
310	03b-Tl99-Fe4P2C6	-1990.3380663	36.82
311	03b-Tl99-Fe2P4C4	-1990.3380288	36.84
312	02a-PressCapCube-Fe5C2P3	-1990.3378779	36.94
313	03b-Tl99-Fe2P1C3	-1990.3377841	37.00
314	01a-CapCube-Fe3C4P2	-1990.3377699	37.01
315	02a-PressCapCube-Fe5C1P5	-1990.3377468	37.02
316	02b-PressCapCube-Fe3P4C2	-1990.3375429	37.15
317	02b-PressCapCube-Fe2P1C3	-1990.3375275	37.16
318	02a-PressCapCube-Fe3C5P1_i-30	-1990.3374806	37.19
319	04a-TricTrPrism-Fe2C1P6	-1990.3374446	37.21
320	03a-Tl99-Fe3C1P6	-1990.3372825	37.31
321	04b-TricTrPrism-Fe1P1C3	-1990.3372790	37.32
322	03a-Tl99-Fe3C1P1_r-29	-1990.3372473	37.34
323	02b-PressCapCube-Fe2P2C4	-1990.3370787	37.44
324	03a-Tl99-Fe3C1P1_i-29	-1990.3369474	37.52
325	03a-Tl99-Fe2C4P4	-1990.3356772	38.32
326	03b-Tl99-Fe3P1C1	-1990.3356315	38.35
327	04b-TricTrPrism-Fe2P2C6	-1990.3356176	38.36
328	02b-PressCapCube-Fe2P1C5	-1990.3356121	38.36
329	02b-PressCapCube-Fe3P5C1	-1990.3356110	38.36
330	03a-Tl99-Fe3C4P3	-1990.3355991	38.37
331	02b-PressCapCube-Fe2P2C2	-1990.3355873	38.38
332	01b-CapCube-Fe2P3C1	-1990.3354010	38.49
333	02a-PressCapCube-Fe1C3P2	-1990.3350129	38.74

334	02b-PressCapCube-Fe1P3C2	-1990.3349899	38.75
335	04b-TricTrPrism-Fe1P1C2	-1990.3349833	38.76
336	04a-TricTrPrism-Fe1C1P2	-1990.3349725	38.76
337	03a-Tl99-Fe3C5P1	-1990.3347168	38.92
338	03a-Tl99-Fe1C1P1	-1990.3347103	38.93
339	02a-PressCapCube-Fe1C1P3	-1990.3344254	39.11
340	03b-Tl99-Fe3P5C1	-1990.3344028	39.12
341	03a-Tl99-Fe4C3P1	-1990.3340585	39.34
342	01b-CapCube-Fe3P4C1	-1990.3326136	40.24
343	04a-TricTrPrism-Fe2C2P5	-1990.3326071	40.25
344	01b-CapCube-Fe2P1C4	-1990.3321330	40.54
345	01a-CapCube-Fe2C3P1	-1990.3320605	40.59
346	03b-Tl99-Fe2P1C4	-1990.3319701	40.65
347	02a-PressCapCube-Fe2C2P1	-1990.3319637	40.65
348	01a-CapCube-Fe1C1P2	-1990.3319438	40.66
349	02a-PressCapCube-Fe3C1P3	-1990.3319274	40.67
350	02a-PressCapCube-Fe3C2P1	-1990.3318928	40.70
351	03b-Tl99-Fe4P1C7	-1990.3318795	40.70
352	01a-CapCube-Fe1C1P1	-1990.3308619	41.34
353	02a-PressCapCube-Fe2C1P4	-1990.3308590	41.34
354	02b-PressCapCube-Fe3P2C2	-1990.3308392	41.36
355	03a-Tl99-Fe4C3P4	-1990.3293485	42.29
356	02b-PressCapCube-Fe5P3C2	-1990.3290475	42.48
357	03a-Tl99-Fe2C2P3	-1990.3289582	42.54
358	02a-PressCapCube-Fe3C5P3	-1990.3284765	42.84
359	03b-Tl99-Fe4P3C5	-1990.3284029	42.89
360	02b-PressCapCube-Fe3P1C3	-1990.3263328	44.18
361	03b-Tl99-Fe1P1C6	-1990.3263234	44.19
362	02b-PressCapCube-Fe3P2C1	-1990.3262568	44.23
363	03b-Tl99-Fe3P3C1	-1990.3262457	44.24
364	03a-Tl99-Fe3C2P4	-1990.3256940	44.59
365	03b-Tl99-Fe3P3C5	-1990.3256527	44.61
366	03a-Tl99-Fe3C2P6	-1990.3256369	44.62
367	04b-TricTrPrism-Fe1P2C3	-1990.3256183	44.63
368	03b-Tl99-Fe3P4C4	-1990.3256175	44.63
369	03b-Tl99-Fe3P5C3	-1990.3255760	44.66
370	02b-PressCapCube-Fe1P2C1_r-20	-1990.3255757	44.66
371	02b-PressCapCube-Fe1P2C1_i-20	-1990.3250436	44.99
372	01a-CapCube-Fe3C2P1	-1990.3249523	45.05
373	02a-PressCapCube-Fe3C3P3	-1990.3249064	45.08
374	03b-Tl99-Fe1P2C3	-1990.3248893	45.09
375	01b-CapCube-Fe2P4C1	-1990.3244527	45.36

376	01a-CapCube-Fe2C1P1	-1990.3243065	45.46
377	02a-PressCapCube-Fe2C5P3	-1990.3237851	45.78
378	01a-CapCube-Fe3C2P3	-1990.3235227	45.95
379	02a-PressCapCube-Fe5C1P1	-1990.3233568	46.05
380	01a-CapCube-Fe2C1P4	-1990.3224479	46.62
381	02a-PressCapCube-Fe3C1P5	-1990.3217113	47.08
382	01a-CapCube-Fe3C1P4	-1990.3214644	47.24
383	01b-CapCube-Fe2P3C3	-1990.3212153	47.40
384	03b-Tl99-Fe3P4C3	-1990.3211030	47.47
385	02a-PressCapCube-Fe5C3P2	-1990.3210621	47.49
386	01a-CapCube-Fe3C2P4	-1990.3210432	47.50
387	01b-CapCube-Fe3P3C2	-1990.3203669	47.93
388	02a-PressCapCube-Fe1C3P1	-1990.3185758	49.05
389	03a-Tl99-Fe1C1P6	-1990.3183652	49.18
390	03a-Tl99-Fe3C6P2	-1990.3178461	49.51
391	02b-PressCapCube-Fe2P4C2	-1990.3176239	49.65
392	03b-Tl99-Fe3P2C4	-1990.3175631	49.69
393	01a-CapCube-Fe3C3P2	-1990.3170888	49.99
394	03a-Tl99-Fe3C3P4	-1990.3169631	50.06
395	04a-TricTrPrism-Fe1C1P6	-1990.3165165	50.34
396	02a-PressCapCube-Fe2C4P2	-1990.3165149	50.35
397	04a-TricTrPrism-Fe1C2P1	-1990.3165142	50.35
398	02a-PressCapCube-Fe2C4P1	-1990.3162125	50.54
399	01b-CapCube-Fe3P1C4	-1990.3160601	50.63
400	01b-CapCube-Fe3P2C3	-1990.3159984	50.67
401	04a-TricTrPrism-Fe2C3P2	-1990.3158492	50.76
402	04a-TricTrPrism-Fe2C1P5	-1990.3151228	51.22
403	03b-Tl99-Fe1P3C1	-1990.3140803	51.87
404	03a-Tl99-Fe1C3P1	-1990.3140712	51.88
405	02a-PressCapCube-Fe5C2P1	-1990.3133649	52.32
406	02b-PressCapCube-Fe5P3C3_i-94	-1990.3105039	54.12
407	03b-Tl99-Fe2P5C3	-1990.3104672	54.14
408	02a-PressCapCube-Fe2C6P1	-1990.3101517	54.34
409	03a-Tl99-Fe4C1P7	-1990.3100595	54.40
410	03b-Tl99-Fe4P1C5	-1990.3071751	56.21
411	02a-PressCapCube-Fe5C2P2	-1990.3071342	56.23
412	03b-Tl99-Fe2P2C1	-1990.3058590	57.03
413	02a-PressCapCube-Fe3C6P1	-1990.3058055	57.07
414	01a-CapCube-Fe3C4P1	-1990.3053894	57.33
415	03a-Tl99-Fe2C4P3	-1990.3051424	57.48
416	03a-Tl99-Fe4C2P6	-1990.3026562	59.04
417	03a-Tl99-Fe3C3P3_i-14	-1990.3020776	59.40

418	03a-Tl99-Fe3C3P3_r-14	-1990.3019964	59.46
419	01b-CapCube-Fe2P1C2	-1990.3010538	60.05
420	01a-CapCube-Fe2C1P2	-1990.2999064	60.77
421	02b-PressCapCube-Fe3P3C1	-1990.2998710	60.79
422	02a-PressCapCube-Fe3C3P1_r-32	-1990.2998426	60.81
423	02a-PressCapCube-Fe3C3P1_i-32	-1990.2991510	61.24
424	02b-PressCapCube-Fe5P5C3	-1990.2983369	61.75
425	02a-PressCapCube-Fe2C1P5	-1990.2972500	62.43
426	02b-PressCapCube-Fe2P3C1	-1990.2964149	62.96
427	02b-PressCapCube-Fe2P6C1	-1990.2930267	65.08
428	01a-CapCube-Fe1C2P1	-1990.2880927	68.18
429	03b-Tl99-Fe3P2C6	-1990.2876739	68.44
430	02a-PressCapCube-Fe2C5P1	-1990.2874086	68.61
431	03a-Tl99-Fe3C5P2	-1990.2864189	69.23
432	01b-CapCube-Fe1P2C2	-1990.2863708	69.26
433	01a-CapCube-Fe1C2P2	-1990.2863390	69.28
434	03b-Tl99-Fe3P3C3	-1990.2850072	70.12
435	03a-Tl99-Fe3C5P3	-1990.2832796	71.20
436	03a-Tl99-Fe3C4P4	-1990.2832764	71.20
437	02a-PressCapCube-Fe1C4P1	-1990.2721090	78.21
438	02b-PressCapCube-Fe1P4C1	-1990.2720738	78.23
439	02b-PressCapCube-Fe1P1C3	-1990.2635528	83.58

Table S3A. Initial $CpFeCHPHB_7H_7$ structures, 648 in all.

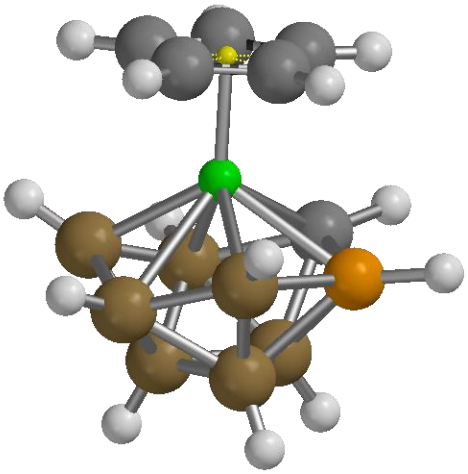
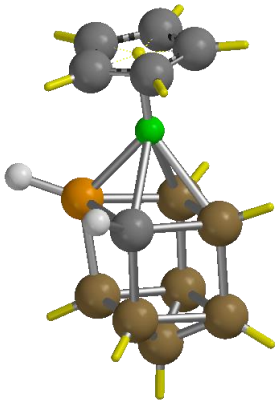
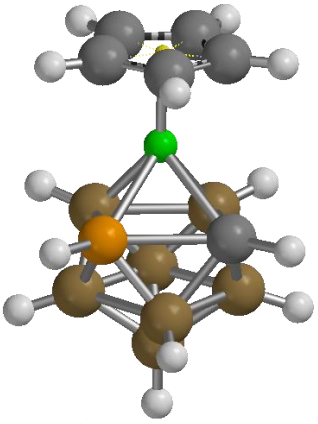
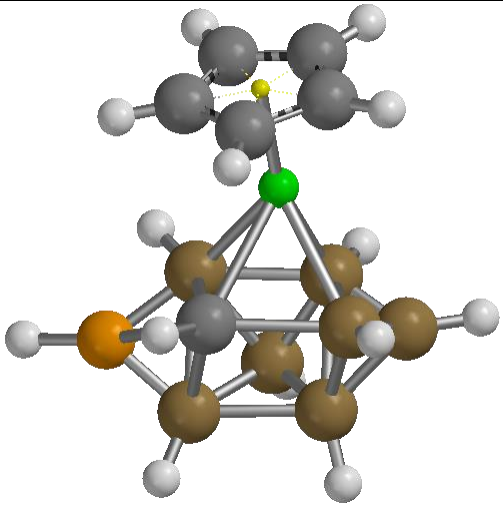
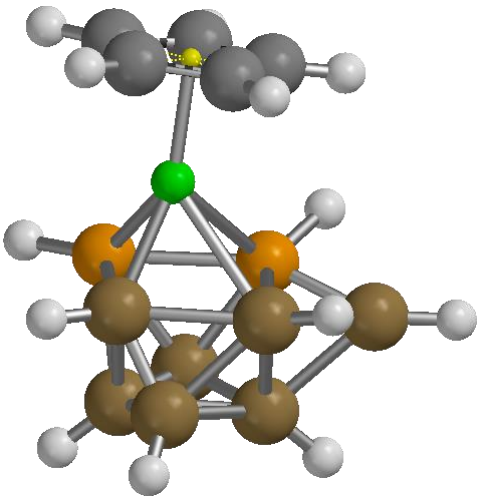
Initial structures	 Isocloso 146
 Bicapped cube 62	 Bicapped square antiprism 68
 Tetracapped trigonal prism C_{2v} 200	 Tetracapped trigonal prism C_{3v} 172

Table S3B. Distance table for the lowest-lying $CpFeCHPCH_3B_7H_7$ 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.

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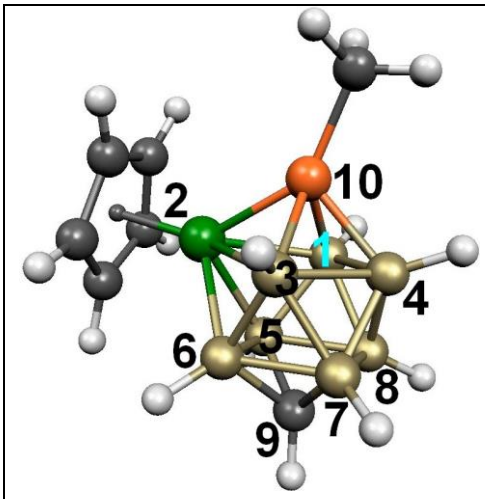
<td> 

1. -2055.17509380 0.0
C_S H/L 2.59</td>
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<tr><td>2</td><td>Fe</td><td>2.246414</td><td>0.000000</td><td></td><td></td><td></td></tr>
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<tr><td>9</td><td>C</td><td>1.598466</td><td>1.589485</td><td>1.589722</td><td>0.000000</td><td></td></tr>
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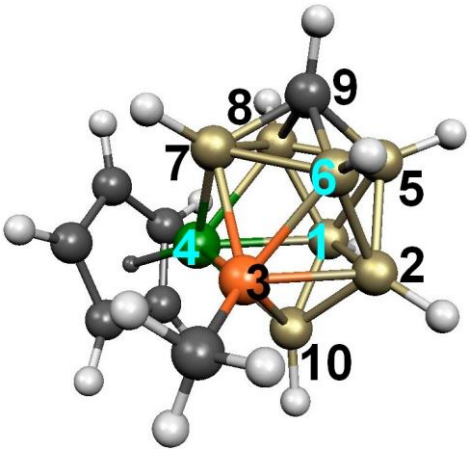
<td> 

2. -2055.17152180 +2.2
C_1 H/L 2.55</td>
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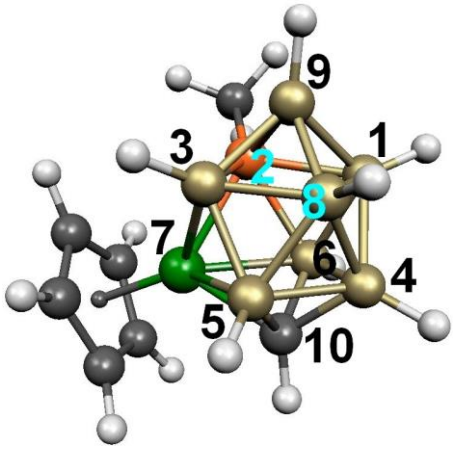
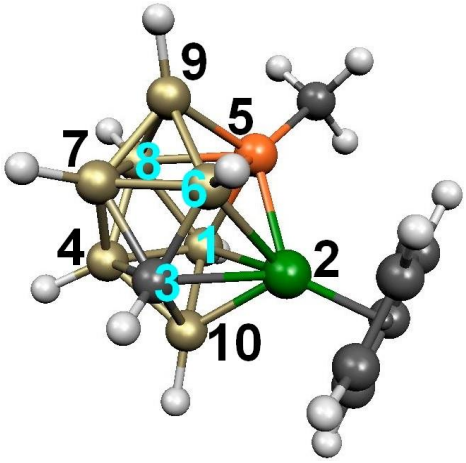


3. -2055.17131630 +2.4
C_1 H/L 2.60

	1	2	3	4	5
1 B	0.000000				
2 P	2.018078	0.000000			
3 B	2.685607	2.058168	0.000000		
4 B	1.772200	2.990854	2.852465	0.000000	
5 B	2.829666	2.969878	1.778180	1.833461	0.000000
6 B	1.883340	2.006653	2.991583	1.811090	2.587074
7 Fe	3.281702	2.122049	2.162606	3.009126	2.138487
8 B	1.798002	2.727053	1.795889	1.782708	1.806435
9 B	1.760046	1.876025	1.786112	2.936104	2.950188
10 C	2.799442	2.952557	2.857080	1.599327	1.599785

	6	7	8	9	10
6 B	0.000000				
7 Fe	2.175051	0.000000			
8 B	2.846152	3.233747	0.000000		
9 B	3.069191	3.348235	1.678270	0.000000	
10 C	1.585797	1.918744	2.769145	3.646416	0.000000



4. -2055.15165010 +14.7
C_1 H/L 2.84

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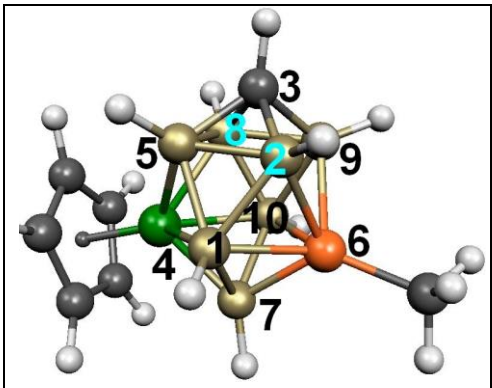
1 B	0.000000				
2 Fe	2.210142	0.000000			
3 C	2.500007	2.080395	0.000000		
4 B	1.784065	2.977187	1.732810	0.000000	
5 P	1.977853	2.120269	2.883381	2.956244	0.000000
6 B	3.001090	2.097059	1.658823	2.807891	2.150704
7 B	2.839058	3.199358	1.710072	1.766611	2.746790
8 B	1.889637	3.279226	2.698578	1.751047	2.019247
9 B	3.050998	3.258708	2.807761	2.918415	1.866734
10 B	1.711494	1.950637	1.637512	1.712845	3.062166

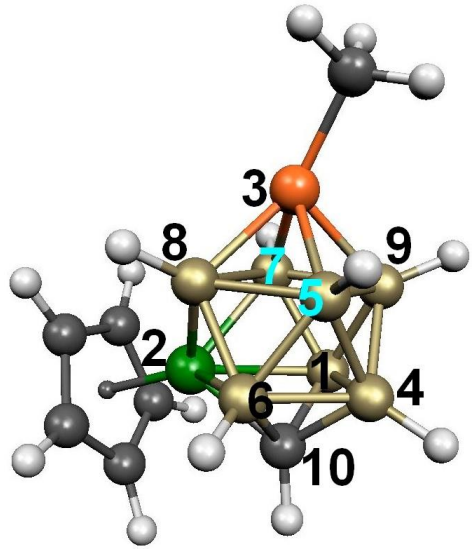
	6	7	8	9	10
6 B	0.000000				
7 B	1.790295	0.000000			
8 B	2.704398	1.774031	0.000000		
9 B	1.782141	1.683541	1.776377	0.000000	
10 B	2.911120	2.892233	2.956784	3.756612	0.000000



5. -2055.14589270 +18.3
C_S H/L 2.64

	1	2	3	4	5
1 B	0.000000				
2 B	1.857306	0.000000			
3 C	2.802593	1.577864	0.000000		
4 Fe	2.089465	3.207995	3.106176	0.000000	
5 B	1.789635	1.806238	1.623435	2.042451	0.000000
6 P	2.023474	1.995030	2.902587	3.067956	2.989389
7 B	1.845510	3.112520	3.692740	1.900545	3.022195
8 B	2.864325	2.620129	1.623692	2.042451	1.835100
9 B	2.966592	1.963100	1.577804	3.208022	2.619964
10 B	2.726000	2.966773	2.802963	2.089981	2.864744

	6	7	8	9	10
6 P	0.000000				
7 B	1.886672	0.000000			
8 B	2.989287	3.021986	0.000000		
9 B	1.995194	3.112553	1.806051	0.000000	
10 B	2.023416	1.845440	1.789792	1.857418	0.000000



6. -2055.14560420 +18.5
C_S H/L 2.64

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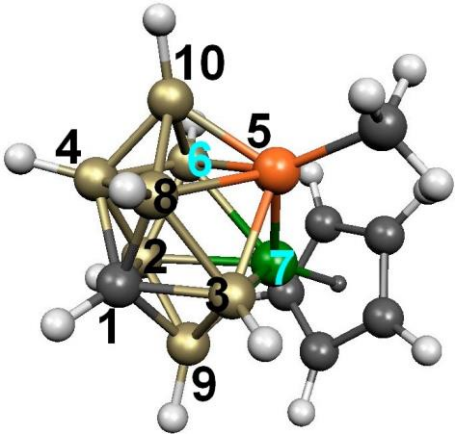
2 Fe	2.134269	0.000000			
3 P	3.090674	3.251280	0.000000		
4 B	1.829314	2.963923	3.113442	0.000000	
5 B	2.832681	3.159444	1.928834	1.761749	0.000000
6 B	2.617400	2.134179	3.090542	1.829326	1.775077
7 B	1.770240	2.004689	1.952551	2.911036	2.805325
8 B	3.000991	2.004636	1.952425	2.911125	1.921815
9 B	1.775159	3.159503	1.928922	1.761681	1.861700
10 C	1.604042	1.884483	3.726151	1.601091	2.736481

	6	7	8	9	10
6 B	0.000000				
7 B	3.000909	0.000000			
8 B	1.770282	2.243400	0.000000		
9 B	2.832603	1.921813	2.805346	0.000000	
10 C	1.604111	2.808291	2.808387	2.736449	0.000000



7. -2055.14540260 +18.6
C1 H/L 2.82

		1	2	3	4	5
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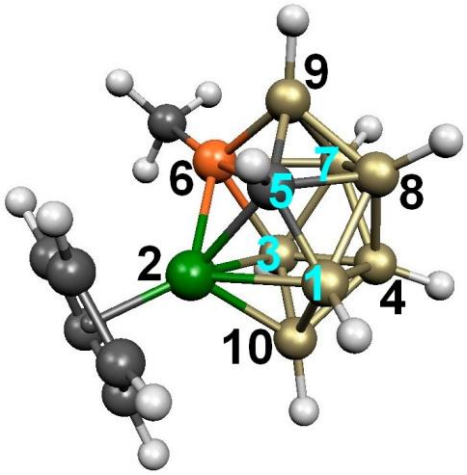
2	B	1.733592	0.000000			
3	B	1.699419	2.600469	0.000000		
4	B	1.707828	1.775097	2.831367	0.000000	
5	P	2.840904	2.975924	1.980124	2.747192	0.000000
6	B	2.697415	1.736650	2.997260	1.774778	2.112208
7	Fe	2.846195	2.141667	2.179205	3.216527	2.108920
8	B	1.680812	2.809483	1.852332	1.794531	2.034294
9	B	1.647085	1.714302	1.705230	2.908283	3.077668
10	B	2.806026	2.921840	3.020696	1.686925	1.870218

		6	7	8	9	10
6	B	0.000000				
7	Fe	2.166956	0.000000			
8	B	2.693524	3.267162	0.000000		
9	B	2.977406	1.959589	2.937249	0.000000	
10	B	1.795290	3.314006	1.749125	3.781866	0.000000



8. -2055.14245680 +20.5
C_1 H/L 2.19

		1	2	3	4	5
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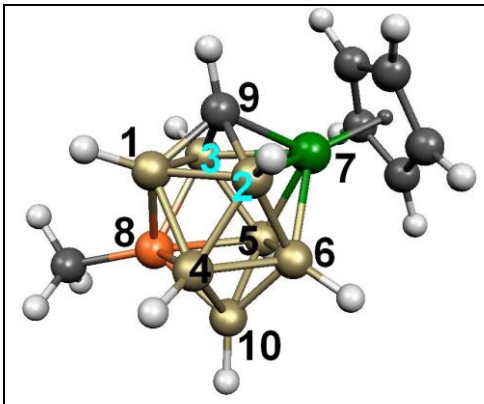
2	Fe	2.131479	0.000000			
3	B	2.638015	2.203141	0.000000		
4	B	1.833253	2.954838	1.779923	0.000000	
5	C	1.592457	2.051993	2.957223	2.710614	0.000000
6	P	3.174343	2.144192	1.932271	3.045348	2.410986
7	B	2.812508	3.192787	1.850822	1.767777	2.624466
8	B	1.794101	3.138325	2.811791	1.780541	1.679171
9	B	2.835505	2.997396	2.965804	2.954941	1.650487
10	B	1.739367	1.970806	1.719359	1.727104	2.860395

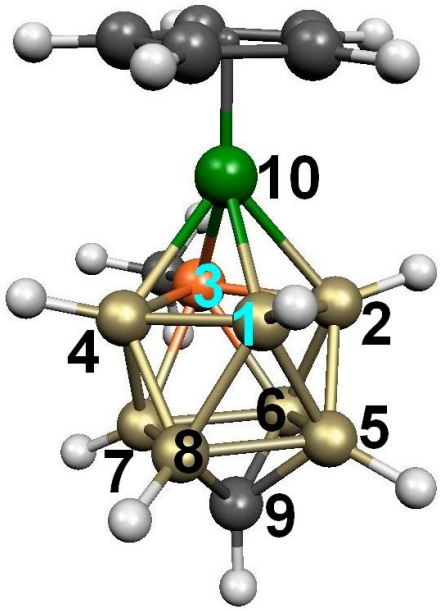
		6	7	8	9	10
6	P	0.000000				
7	B	2.031900	0.000000			
8	B	2.888876	1.739213	0.000000		
9	B	1.876912	1.824438	1.727459	0.000000	
10	B	3.124551	2.956413	2.926582	3.692384	0.000000



9. -2055.14038670 +21.8
C_1 H/L 2.43

		1	2	3	4	5
1	B	0.000000				
2	B	1.799446	0.000000			
3	B	1.962774	2.600259	0.000000		
4	B	1.842073	1.803028	2.951976	0.000000	
5	B	3.025717	2.863232	1.947554	2.723896	0.000000
6	B	2.842327	1.805798	2.853611	1.823766	1.791947
7	Fe	2.990817	2.110784	2.063926	3.236608	2.002281
8	P	1.993516	2.984651	1.986024	2.012620	2.080966
9	C	1.580812	1.612587	1.606759	2.812793	2.897846
10	B	3.050559	2.966533	3.081559	1.774268	1.816268

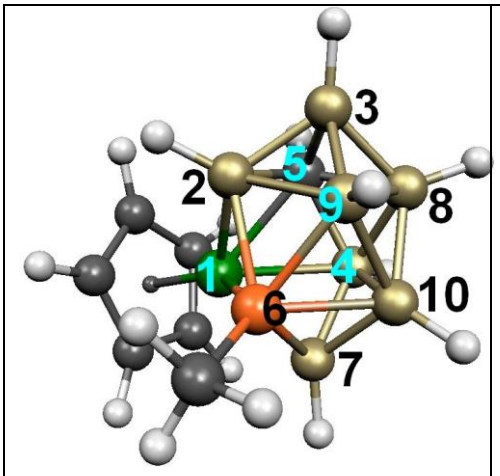
		6	7	8	9	10
6	B	0.000000				
7	Fe	2.064923	0.000000			
8	P	2.716830	3.347679	0.000000		
9	C	2.823045	1.899653	2.924061	0.000000	
10	B	1.697795	3.298303	1.859668	3.675948	0.000000



10. -2055.14015130 +21.9
C_S H/L 1.96

		1	2	3	4	5
1	B	0.000000				
2	B	1.799514	0.000000			
3	P	2.719301	2.039009	0.000000		
4	B	1.799522	2.693081	2.038042	0.000000	
5	B	1.811662	1.768940	3.018432	2.834895	0.000000
6	B	2.825184	1.850396	2.028468	2.933820	1.787845
7	B	2.825815	2.933548	2.025987	1.850302	2.590280
8	B	1.813011	2.836374	3.017914	1.767994	1.824434
9	C	2.778269	2.792649	2.972920	2.791728	1.599322
10	Fe	2.042304	2.112902	2.061828	2.109187	3.378535

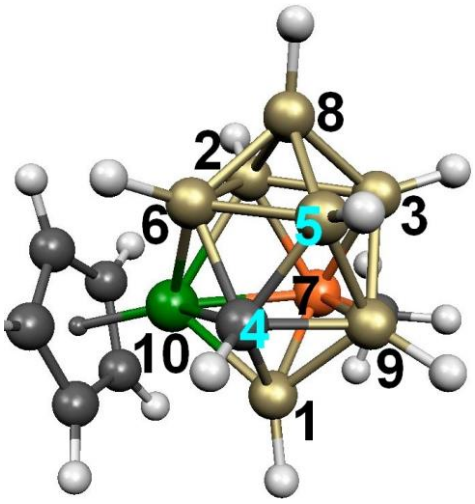
		6	7	8	9	10
6	B	0.000000				
7	B	1.924455	0.000000			
8	B	2.590040	1.788683	0.000000		
9	C	1.586042	1.586582	1.598878	0.000000	
10	Fe	3.420646	3.418174	3.377343	4.068785	0.000000



11. -2055.13893840 +22.7
C_1 H/L 2.33

	1	2	3	4	5
1	Fe	0.000000			
2	B	2.090359	0.000000		
3	B	3.293782	1.688222	0.000000	
4	B	2.122540	2.802995	2.873545	0.000000
5	C	2.069978	1.700890	1.625988	1.694772	0.000000
6	P	2.191078	2.016016	3.064566	2.678975	2.841989
7	B	2.040898	3.143975	3.833093	1.690842	2.905863
8	B	3.253058	2.591671	1.680111	1.791910	1.726733
9	B	3.308065	1.939285	1.676016	2.836861	2.466448
10	B	3.056615	2.969782	2.931454	1.814607	2.706715

	6	7	8	9	10
6	P	0.000000			
7	B	1.900335	0.000000		
8	B	2.952334	2.951964	0.000000	
9	B	1.992449	3.102431	1.795351	0.000000	
10	B	2.019454	1.774148	1.754760	1.893069	0.000000



12. -2055.13824110 +23.1
C_1 H/L 2.44

	1	2	3	4	5
1	B	0.000000			
2	B	3.154664	0.000000		
3	B	3.081050	1.940935	0.000000	
4	C	1.600680	2.756221	2.716713	0.000000	
5	B	2.921276	2.611244	1.799742	1.719121	0.000000
6	B	2.931727	1.809141	2.600409	1.712829	1.822028
7	P	1.924338	2.005419	1.986044	2.581251	2.960826
8	B	3.804144	1.689331	1.692176	2.795405	1.677770
9	B	1.769871	2.960736	1.848033	1.720824	1.753793
10	Fe	1.992149	2.147702	3.312756	2.094178	3.258031

	6	7	8	9	10
6	B	0.000000			
7	P	2.936836	0.000000		
8	B	1.707005	3.058742	0.000000	
9	B	2.807581	2.010808	2.909771	0.000000	
10	Fe	2.096234	2.171978	3.312216	3.035180	0.000000

Table S3C. Energy ranking for all of the $CpFeCHPHB_7H_7$ optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	04a-BicapSqAntipr-Fe2C4P2	-2015.87275530	0.00
2	02b-TetrcTriPri2-Fe1P2C7	-2015.87273300	0.01
3	02b-TetrcTriPri2-Fe1P1C3	-2015.87270590	0.03
4	01a-TetrcTriPri1-Fe1C2P4	-2015.87270340	0.03
5	02a-TetrcTriPri2-Fe2C3P1	-2015.87267860	0.05
6	02a-TetrcTriPri2-Fe3C3P4	-2015.87267780	0.05
7	05b-Isocloso-Fe3P4C2	-2015.87267580	0.05
8	02b-TetrcTriPri2-Fe1P4C4	-2015.87267270	0.05
9	05b-Isocloso-Fe3P2C7	-2015.87267240	0.05
10	02b-TetrcTriPri2-Fe2P2C6	-2015.87267190	0.05
11	05a-Isocloso-Fe3C3P6	-2015.87266910	0.05
12	02a-TetrcTriPri2-Fe3C2P5	-2015.87266270	0.06
13	02a-TetrcTriPri2-Fe2C1P5	-2015.87264040	0.07
14	03a-BicapCub-Fe2C1P5	-2015.87263780	0.07
15	02b-TetrcTriPri2-Fe1P3C4	-2015.87263140	0.08
16	02b-TetrcTriPri2-Fe2P4C2	-2015.87089920	1.16
17	01b-TetrcTriPri1-Fe1P1C4	-2015.86889960	2.42
18	05a-Isocloso-Fe2C1P4_r-22	-2015.86888880	2.43
19	04b-BicapSqAntipr-Fe1P1C1	-2015.86887880	2.43
20	01b-TetrcTriPri1-Fe3P3C4_i-14	-2015.86885550	2.45
21	05a-Isocloso-Fe3C1P3	-2015.86885380	2.45
22	01b-TetrcTriPri1-Fe1P2C7	-2015.86885320	2.45
23	01b-TetrcTriPri1-Fe2P1C5	-2015.86884380	2.45
24	01b-TetrcTriPri1-Fe3P2C6	-2015.86884360	2.45
25	05b-Isocloso-Fe3P3C4	-2015.86884170	2.46
26	02a-TetrcTriPri2-Fe2C1P4	-2015.86883320	2.46
27	01b-TetrcTriPri1-Fe2P3C4	-2015.86883020	2.46
28	02a-TetrcTriPri2-Fe2C2P5	-2015.86882450	2.47
29	02a-TetrcTriPri2-Fe1C1P6	-2015.86881640	2.47
30	03a-BicapCub-Fe1C1P1	-2015.86881560	2.47
31	04a-BicapSqAntipr-Fe1C1P1	-2015.86881540	2.47
32	02b-TetrcTriPri2-Fe1P1C6	-2015.86880210	2.48
33	05a-Isocloso-Fe2C1P6	-2015.86879200	2.49
34	02b-TetrcTriPri2-Fe2P2C1	-2015.86877230	2.50
35	02a-TetrcTriPri2-Fe1C2P3	-2015.86876840	2.50
36	02b-TetrcTriPri2-Fe1P3C3	-2015.86876450	2.50
37	01b-TetrcTriPri1-Fe3P3C4_r-14	-2015.86875490	2.51
38	03b-BicapCub-Fe2P1C6	-2015.86874960	2.51
39	01b-TetrcTriPri1-Fe2P1C6	-2015.86874700	2.52

40	05b-Isocloso-Fe2P1C6	-2015.86873780	2.52
41	03b-BicapCub-Fe1P1C2_i-18	-2015.86873230	2.52
42	03b-BicapCub-Fe1P1C1	-2015.86871970	2.53
43	05a-Isocloso-Fe2C1P4_i-22	-2015.86871440	2.54
44	03b-BicapCub-Fe1P1C2_r-18	-2015.86869360	2.55
45	01a-TetrcTriPri1-Fe1C1P6	-2015.86862680	2.59
46	03b-BicapCub-Fe2P4C1	-2015.86755580	3.26
47	01a-TetrcTriPri1-Fe3C4P4	-2015.86754540	3.27
48	04b-BicapSqAntipr-Fe2P1C5	-2015.86753730	3.27
49	02b-TetrcTriPri2-Fe3P2C6	-2015.86753610	3.28
50	02a-TetrcTriPri2-Fe3C4P4	-2015.86753330	3.28
51	02b-TetrcTriPri2-Fe1P1C8	-2015.86753150	3.28
52	02a-TetrcTriPri2-Fe2C3P2	-2015.86751940	3.29
53	05b-Isocloso-Fe3P2C2	-2015.86751460	3.29
54	01b-TetrcTriPri1-Fe2P4C5	-2015.86751080	3.29
55	01b-TetrcTriPri1-Fe3P4C5	-2015.86751040	3.29
56	01b-TetrcTriPri1-Fe2P3C6	-2015.86750850	3.29
57	02a-TetrcTriPri2-Fe3C2P6	-2015.86750210	3.30
58	01a-TetrcTriPri1-Fe2C7P2	-2015.86749670	3.30
59	02b-TetrcTriPri2-Fe1P3C2	-2015.86748350	3.31
60	04b-BicapSqAntipr-Fe2P1C7	-2015.86746770	3.32
61	02a-TetrcTriPri2-Fe3C3P6	-2015.86746300	3.32
62	01b-TetrcTriPri1-Fe3P7C1	-2015.86745680	3.32
63	02b-TetrcTriPri2-Fe1P8C1	-2015.86745420	3.33
64	01b-TetrcTriPri1-Fe1P4C4	-2015.86744780	3.33
65	05a-Isocloso-Fe3C1P8	-2015.86744090	3.33
66	02b-TetrcTriPri2-Fe3P1C1	-2015.86743920	3.34
67	02a-TetrcTriPri2-Fe2C2P4	-2015.86742420	3.35
68	05b-Isocloso-Fe2P2C2	-2015.86741620	3.35
69	02b-TetrcTriPri2-Fe3P2C5_r-30	-2015.85037030	14.05
70	05b-Isocloso-Fe3P3C6	-2015.85034110	14.07
71	02a-TetrcTriPri2-Fe1C4P4	-2015.85033460	14.07
72	02b-TetrcTriPri2-Fe2P1C5	-2015.85033260	14.07
73	05a-Isocloso-Fe3C4P2	-2015.85032590	14.07
74	03b-BicapCub-Fe2P1C5	-2015.85031870	14.08
75	02a-TetrcTriPri2-Fe1C2P7	-2015.85030380	14.09
76	05a-Isocloso-Fe3C2P7	-2015.85030340	14.09
77	02b-TetrcTriPri2-Fe2P3C1	-2015.85030070	14.09
78	05b-Isocloso-Fe1P2C6	-2015.85029970	14.09
79	02a-TetrcTriPri2-Fe2C4P2	-2015.85029520	14.09
80	02a-TetrcTriPri2-Fe1C3P4	-2015.85029050	14.10
81	05a-Isocloso-Fe1C1P8	-2015.85028020	14.10

82	01b-TetrcTriPri1-Fe3P2C7	-2015.85027330	14.11
83	04b-BicapSqAntipr-Fe2P4C2	-2015.85026480	14.11
84	05a-Isocloso-Fe1C4P1	-2015.85025950	14.12
85	02b-TetrcTriPri2-Fe3P3C4	-2015.85024720	14.12
86	02a-TetrcTriPri2-Fe3C1P4	-2015.84974280	14.44
87	03a-BicapCub-Fe2C5P2	-2015.84973580	14.45
88	05a-Isocloso-Fe2C4P1	-2015.84973260	14.45
89	05b-Isocloso-Fe1P4C1	-2015.84972620	14.45
90	01b-TetrcTriPri1-Fe3P1C6	-2015.84971900	14.46
91	02b-TetrcTriPri2-Fe2P2C3	-2015.84970050	14.47
92	05b-Isocloso-Fe1P1C8	-2015.84969790	14.47
93	01a-TetrcTriPri1-Fe2C3P1	-2015.84968740	14.48
94	01a-TetrcTriPri1-Fe3C3P1	-2015.84967310	14.48
95	05a-Isocloso-Fe1C2P6	-2015.84964350	14.50
96	01b-TetrcTriPri1-Fe2P2C6	-2015.84964120	14.50
97	02b-TetrcTriPri2-Fe3P2C5_i-30	-2015.84938440	14.67
98	04a-BicapSqAntipr-Fe2C2P7	-2015.84918460	14.79
99	04b-BicapSqAntipr-Fe2P2C5	-2015.84916870	14.80
100	04a-BicapSqAntipr-Fe2C1P4	-2015.84909620	14.85
101	01a-TetrcTriPri1-Fe3C3P3	-2015.84892630	14.95
102	04a-BicapSqAntipr-Fe2C2P3	-2015.84605610	16.75
103	01a-TetrcTriPri1-Fe1C1P4	-2015.84597630	16.80
104	05b-Isocloso-Fe3P1C1	-2015.84596540	16.81
105	05a-Isocloso-Fe1C1P4	-2015.84595780	16.82
106	04b-BicapSqAntipr-Fe2P2C3	-2015.84595070	16.82
107	02a-TetrcTriPri2-Fe3C1P2	-2015.84594730	16.82
108	05b-Isocloso-Fe1P1C6	-2015.84594570	16.82
109	02b-TetrcTriPri2-Fe3P3C5	-2015.84593210	16.83
110	05a-Isocloso-Fe1C1P6	-2015.84591940	16.84
111	02b-TetrcTriPri2-Fe3P1C2	-2015.84591490	16.84
112	01b-TetrcTriPri1-Fe3P4C3	-2015.84591170	16.84
113	02a-TetrcTriPri2-Fe3C3P5	-2015.84590390	16.85
114	05b-Isocloso-Fe1P1C4	-2015.84588040	16.86
115	05a-Isocloso-Fe2C2P7	-2015.84089300	19.99
116	02a-TetrcTriPri2-Fe3C2P7	-2015.84088020	20.00
117	04b-BicapSqAntipr-Fe2P5C1	-2015.84087550	20.01
118	04a-BicapSqAntipr-Fe2C3P3	-2015.84086630	20.01
119	02b-TetrcTriPri2-Fe2P5C1	-2015.84084710	20.02
120	02a-TetrcTriPri2-Fe3C4P3	-2015.84084470	20.02
121	04b-BicapSqAntipr-Fe2P3C3	-2015.84084450	20.02
122	02a-TetrcTriPri2-Fe2C1P1	-2015.84083920	20.03
123	03b-BicapCub-Fe2P2C4	-2015.84083650	20.03

124	05a-Isocloso-Fe2C2P3	-2015.84083610	20.03
125	05b-Isocloso-Fe2P3C6	-2015.84082440	20.04
126	03b-BicapCub-Fe2P4C3	-2015.84081740	20.04
127	01b-TetrcTriPri1-Fe3P5C4	-2015.84081180	20.05
128	05b-Isocloso-Fe3P5C1	-2015.84080480	20.05
129	02b-TetrcTriPri2-Fe1P1C2	-2015.84079530	20.06
130	01b-TetrcTriPri1-Fe1P1C1	-2015.84079050	20.06
131	01b-TetrcTriPri1-Fe2P5C4	-2015.84077860	20.07
132	05b-Isocloso-Fe1P2C3	-2015.84076000	20.08
133	05b-Isocloso-Fe1P1C1	-2015.84075890	20.08
134	04b-BicapSqAntipr-Fe2P2C2	-2015.84074760	20.09
135	05b-Isocloso-Fe3P1C5	-2015.84074130	20.09
136	01b-TetrcTriPri1-Fe1P2C6	-2015.84019310	20.43
137	01b-TetrcTriPri1-Fe1P1C2	-2015.84019100	20.43
138	01b-TetrcTriPri1-Fe1P3C5	-2015.84019070	20.43
139	02a-TetrcTriPri2-Fe1C6P1	-2015.84018940	20.44
140	02a-TetrcTriPri2-Fe1C2P4	-2015.84018800	20.44
141	04b-BicapSqAntipr-Fe2P3C4	-2015.84014880	20.46
142	01b-TetrcTriPri1-Fe1P2C3	-2015.84012250	20.48
143	02a-TetrcTriPri2-Fe1C5P1	-2015.84010920	20.49
144	01b-TetrcTriPri1-Fe3P2C4	-2015.84010850	20.49
145	03b-BicapCub-Fe2P1C2	-2015.84010290	20.49
146	05a-Isocloso-Fe3C3P2	-2015.84010250	20.49
147	03b-BicapCub-Fe2P1C4	-2015.84009720	20.49
148	02a-TetrcTriPri2-Fe1C2P6	-2015.84007690	20.51
149	02a-TetrcTriPri2-Fe1C8P1	-2015.84005400	20.52
150	01a-TetrcTriPri1-Fe1C3P4	-2015.83862830	21.42
151	02a-TetrcTriPri2-Fe3C2P1_r-17	-2015.83860140	21.43
152	05a-Isocloso-Fe2C3P4	-2015.83858660	21.44
153	05b-Isocloso-Fe3P2C5	-2015.83858030	21.45
154	05a-Isocloso-Fe1C1P5	-2015.83857640	21.45
155	05a-Isocloso-Fe2C3P3	-2015.83857240	21.45
156	05b-Isocloso-Fe1P1C7	-2015.83855790	21.46
157	05b-Isocloso-Fe3P1C4	-2015.83854610	21.47
158	05a-Isocloso-Fe1C3P5	-2015.83852900	21.48
159	04a-BicapSqAntipr-Fe2C2P6_r-33	-2015.83852400	21.48
160	03a-BicapCub-Fe2C2P5	-2015.83847860	21.51
161	04a-BicapSqAntipr-Fe2C2P6_i-33	-2015.83836080	21.58
162	04b-BicapSqAntipr-Fe1P1C5_r-36	-2015.83738030	22.20
163	03b-BicapCub-Fe1P1C6	-2015.83734330	22.22
164	05b-Isocloso-Fe2P5C1	-2015.83734300	22.22
165	02a-TetrcTriPri2-Fe1C1P7	-2015.83731570	22.24

166	05b-Isocloso-Fe2P1C5_r-22	-2015.83731290	22.24
167	05b-Isocloso-Fe2P4C2	-2015.83729230	22.25
168	02a-TetrcTriPri2-Fe1C4P3	-2015.83727640	22.26
169	04b-BicapSqAntipr-Fe1P1C5_i-36	-2015.83653630	22.73
170	03b-BicapCub-Fe2P3C3	-2015.83651510	22.74
171	05b-Isocloso-Fe2P1C5_i-22	-2015.83646570	22.77
172	01b-TetrcTriPri1-Fe3P3C6	-2015.83641500	22.80
173	03a-BicapCub-Fe2C1P6	-2015.83608640	23.01
174	02b-TetrcTriPri2-Fe1P2C5	-2015.83607120	23.02
175	02b-TetrcTriPri2-Fe2P1C4	-2015.83606340	23.02
176	05b-Isocloso-Fe3P1C3	-2015.83605270	23.03
177	02a-TetrcTriPri2-Fe1C4P2	-2015.83604520	23.04
178	02b-TetrcTriPri2-Fe1P2C3	-2015.83603810	23.04
179	05b-Isocloso-Fe2P1C4	-2015.83603710	23.04
180	01b-TetrcTriPri1-Fe1P4C3	-2015.83602820	23.05
181	02b-TetrcTriPri2-Fe2P1C3	-2015.83601660	23.05
182	02a-TetrcTriPri2-Fe1C1P1	-2015.83601190	23.06
183	05a-Isocloso-Fe3C3P4	-2015.83600960	23.06
184	05a-Isocloso-Fe3C3P5	-2015.83599180	23.07
185	04a-BicapSqAntipr-Fe2C2P5	-2015.83598720	23.07
186	02a-TetrcTriPri2-Fe2C1P3	-2015.83598670	23.07
187	02a-TetrcTriPri2-Fe2C2P3	-2015.83597920	23.08
188	05b-Isocloso-Fe3P1C7	-2015.83597290	23.08
189	01a-TetrcTriPri1-Fe2C1P5	-2015.83597130	23.08
190	02a-TetrcTriPri2-Fe1C2P5	-2015.83596770	23.08
191	05b-Isocloso-Fe3P3C5	-2015.83594840	23.10
192	02b-TetrcTriPri2-Fe2P2C5	-2015.83593060	23.11
193	05a-Isocloso-Fe3C1P7	-2015.83519160	23.57
194	04b-BicapSqAntipr-Fe2P1C4	-2015.83516370	23.59
195	04b-BicapSqAntipr-Fe2P2C7	-2015.83516060	23.59
196	01a-TetrcTriPri1-Fe1C4P3_r-35	-2015.83513610	23.61
197	01a-TetrcTriPri1-Fe2C2P6	-2015.83511780	23.62
198	05b-Isocloso-Fe2P4C1	-2015.83511390	23.62
199	02b-TetrcTriPri2-Fe3P1C4	-2015.83506570	23.65
200	03b-BicapCub-Fe2P5C2	-2015.83503960	23.67
201	01a-TetrcTriPri1-Fe3C2P5	-2015.83475580	23.85
202	01a-TetrcTriPri1-Fe1C4P3_i-35	-2015.83412200	24.24
203	02a-TetrcTriPri2-Fe1C1P3	-2015.83340320	24.69
204	04a-BicapSqAntipr-Fe2C1P8	-2015.83337990	24.71
205	03a-BicapCub-Fe2C5P1	-2015.83336770	24.72
206	04b-BicapSqAntipr-Fe2P1C8	-2015.83332690	24.74
207	04b-BicapSqAntipr-Fe2P3C6	-2015.83123820	26.05

208	04b-BicapSqAntipr-Fe2P1C3	-2015.83123640	26.05
209	05b-Isocloso-Fe2P2C7	-2015.83121080	26.07
210	05b-Isocloso-Fe3P3C3	-2015.83105510	26.17
211	02b-TetrcTriPri2-Fe1P2C6	-2015.83104490	26.17
212	03a-BicapCub-Fe2C1P4	-2015.83104450	26.17
213	05b-Isocloso-Fe3P3C2	-2015.83104040	26.18
214	01a-TetrcTriPri1-Fe3C2P3	-2015.83103490	26.18
215	02b-TetrcTriPri2-Fe2P3C4	-2015.83103100	26.18
216	03a-BicapCub-Fe2C1P2	-2015.83102980	26.18
217	04a-BicapSqAntipr-Fe2C3P4	-2015.83100190	26.20
218	02b-TetrcTriPri2-Fe1P2C4	-2015.83099790	26.20
219	02b-TetrcTriPri2-Fe1P5C1	-2015.83099030	26.21
220	01b-TetrcTriPri1-Fe2P2C3	-2015.83097280	26.22
221	01a-TetrcTriPri1-Fe1C2P6	-2015.83096750	26.22
222	02b-TetrcTriPri2-Fe1P6C1	-2015.83094660	26.24
223	01b-TetrcTriPri1-Fe3P1C8	-2015.83057600	26.47
224	05b-Isocloso-Fe2P1C7	-2015.83055410	26.48
225	01b-TetrcTriPri1-Fe1P4C5	-2015.83054230	26.49
226	01a-TetrcTriPri1-Fe1C2P3	-2015.83034630	26.61
227	01b-TetrcTriPri1-Fe2P2C7	-2015.83034220	26.62
228	02b-TetrcTriPri2-Fe3P3C6	-2015.82914180	27.37
229	02b-TetrcTriPri2-Fe3P2C3	-2015.82914000	27.37
230	02a-TetrcTriPri2-Fe2C2P6	-2015.82912730	27.38
231	02a-TetrcTriPri2-Fe1C3P2	-2015.82912360	27.38
232	05b-Isocloso-Fe3P1C8	-2015.82911120	27.39
233	02a-TetrcTriPri2-Fe2C3P4	-2015.82910000	27.39
234	05a-Isocloso-Fe3C2P5	-2015.82909960	27.39
235	02b-TetrcTriPri2-Fe2P2C4	-2015.82909350	27.40
236	02a-TetrcTriPri2-Fe1C1P8	-2015.82908790	27.40
237	02b-TetrcTriPri2-Fe2P3C2	-2015.82908780	27.40
238	05a-Isocloso-Fe3C3P3	-2015.82908320	27.41
239	05a-Isocloso-Fe1C2P7	-2015.82907520	27.41
240	02b-TetrcTriPri2-Fe3P4C4	-2015.82906690	27.42
241	05a-Isocloso-Fe2C1P5_r-77	-2015.82905270	27.42
242	04a-BicapSqAntipr-Fe2C1P5	-2015.82903840	27.43
243	05b-Isocloso-Fe1P2C7	-2015.82903260	27.44
244	03b-BicapCub-Fe2P2C1	-2015.82903250	27.44
245	03a-BicapCub-Fe2C6P1	-2015.82902050	27.44
246	02a-TetrcTriPri2-Fe2C1P8_r-24	-2015.82900510	27.45
247	03b-BicapCub-Fe2P6C1	-2015.82899920	27.46
248	01b-TetrcTriPri1-Fe1P1C7	-2015.82898170	27.47
249	03a-BicapCub-Fe2C3P4	-2015.82894400	27.49

250	02a-TetrcTriPri2-Fe2C1P8_i-24	-2015.82893090	27.50
251	04b-BicapSqAntipr-Fe2P2C4	-2015.82892280	27.51
252	01b-TetrcTriPri1-Fe2P1C3	-2015.82890530	27.52
253	01b-TetrcTriPri1-Fe3P2C2	-2015.82889790	27.52
254	01b-TetrcTriPri1-Fe3P2C1	-2015.82889420	27.52
255	01a-TetrcTriPri1-Fe1C3P1	-2015.82889230	27.52
256	04b-BicapSqAntipr-Fe2P1C6	-2015.82889150	27.53
257	03b-BicapCub-Fe2P1C1	-2015.82886930	27.54
258	04b-BicapSqAntipr-Fe2P3C2	-2015.82886660	27.54
259	01a-TetrcTriPri1-Fe2C2P2	-2015.82886640	27.54
260	02a-TetrcTriPri2-Fe1C2P2	-2015.82885860	27.55
261	01a-TetrcTriPri1-Fe3C1P4	-2015.82885490	27.55
262	05b-Isocloso-Fe3P3C1	-2015.82875190	27.61
263	02a-TetrcTriPri2-Fe2C1P6	-2015.82870390	27.64
264	01a-TetrcTriPri1-Fe1C2P7	-2015.82827110	27.91
265	05b-Isocloso-Fe2P1C2	-2015.82820090	27.96
266	03b-BicapCub-Fe2P5C1	-2015.82818010	27.97
267	01b-TetrcTriPri1-Fe1P2C5	-2015.82814600	27.99
268	05a-Isocloso-Fe1C2P4	-2015.82724930	28.56
269	05a-Isocloso-Fe1C3P1	-2015.82721030	28.58
270	01a-TetrcTriPri1-Fe1C3P3	-2015.82716070	28.61
271	02b-TetrcTriPri2-Fe3P2C2	-2015.82715450	28.62
272	05a-Isocloso-Fe1C2P1	-2015.82709740	28.65
273	05b-Isocloso-Fe2P1C3	-2015.82090800	32.54
274	05b-Isocloso-Fe3P1C6	-2015.82089400	32.54
275	03a-BicapCub-Fe1C1P4	-2015.82088400	32.55
276	02b-TetrcTriPri2-Fe1P1C4	-2015.82087330	32.56
277	02a-TetrcTriPri2-Fe1C1P4	-2015.82084640	32.57
278	05a-Isocloso-Fe3C1P6	-2015.82081580	32.59
279	05a-Isocloso-Fe2C1P3	-2015.82038740	32.86
280	05a-Isocloso-Fe2C1P5_i-77	-2015.82022850	32.96
281	05a-Isocloso-Fe1C3P6	-2015.82014350	33.01
282	02b-TetrcTriPri2-Fe3P2C7	-2015.82013770	33.02
283	02b-TetrcTriPri2-Fe2P3C3	-2015.82013230	33.02
284	02a-TetrcTriPri2-Fe1C3P6	-2015.82012110	33.03
285	02b-TetrcTriPri2-Fe3P4C3	-2015.82012030	33.03
286	04a-BicapSqAntipr-Fe2C5P1	-2015.82011090	33.04
287	01a-TetrcTriPri1-Fe3C5P4	-2015.82010680	33.04
288	05a-Isocloso-Fe3C5P1	-2015.82010100	33.04
289	01a-TetrcTriPri1-Fe2C5P4	-2015.82009580	33.04
290	02b-TetrcTriPri2-Fe1P3C6	-2015.82008650	33.05
291	05a-Isocloso-Fe2C3P6	-2015.82008280	33.05

292	05a-Isocloso-Fe1C5P1	-2015.82008120	33.05
293	05b-Isocloso-Fe1P2C5	-2015.82008030	33.05
294	02a-TetrcTriPri2-Fe2C3P3	-2015.82007970	33.05
295	02b-TetrcTriPri2-Fe3P5C1	-2015.82007240	33.06
296	04b-BicapSqAntipr-Fe1P2C2	-2015.82005620	33.07
297	04b-BicapSqAntipr-Fe2P1C1	-2015.82001560	33.10
298	01a-TetrcTriPri1-Fe3C4P3	-2015.81995040	33.14
299	03b-BicapCub-Fe2P5C3	-2015.81994430	33.14
300	01b-TetrcTriPri1-Fe2P4C3	-2015.81973290	33.27
301	04a-BicapSqAntipr-Fe2C1P1_i-17	-2015.81973130	33.27
302	01b-TetrcTriPri1-Fe1P4C2	-2015.81971380	33.28
303	01a-TetrcTriPri1-Fe1C4P2	-2015.81962790	33.34
304	04a-BicapSqAntipr-Fe2C1P1_r-17	-2015.81962570	33.34
305	01a-TetrcTriPri1-Fe1C4P5	-2015.81849970	34.05
306	05b-Isocloso-Fe1P2C4	-2015.81734020	34.77
307	05b-Isocloso-Fe1P3C1	-2015.81733710	34.78
308	05b-Isocloso-Fe1P2C1	-2015.81733260	34.78
309	02b-TetrcTriPri2-Fe3P4C1	-2015.81731090	34.79
310	01a-TetrcTriPri1-Fe3C6P2	-2015.81661450	35.23
311	02a-TetrcTriPri2-Fe1C4P1	-2015.81653780	35.28
312	01a-TetrcTriPri1-Fe2C7P1	-2015.81652230	35.29
313	01a-TetrcTriPri1-Fe2C6P1	-2015.81649730	35.30
314	05b-Isocloso-Fe3P1C2	-2015.81614660	35.52
315	01b-TetrcTriPri1-Fe1P1C3	-2015.81613810	35.53
316	04b-BicapSqAntipr-Fe2P2C1	-2015.81609530	35.56
317	02a-TetrcTriPri2-Fe2C1P7	-2015.81606760	35.57
318	01b-TetrcTriPri1-Fe2P3C1	-2015.81536380	36.01
319	01b-TetrcTriPri1-Fe3P3C1	-2015.81533070	36.04
320	01a-TetrcTriPri1-Fe1C1P2	-2015.81450410	36.55
321	05a-Isocloso-Fe1C2P3	-2015.81416060	36.77
322	02b-TetrcTriPri2-Fe3P2C1	-2015.81409290	36.81
323	02a-TetrcTriPri2-Fe1C1P2	-2015.81408420	36.82
324	03b-BicapCub-Fe2P2C5	-2015.81407570	36.82
325	04a-BicapSqAntipr-Fe2C2P2	-2015.81405080	36.84
326	01b-TetrcTriPri1-Fe3P3C3	-2015.81401760	36.86
327	05a-Isocloso-Fe1C1P1	-2015.81397840	36.88
328	04b-BicapSqAntipr-Fe1P1C2	-2015.81365740	37.09
329	03a-BicapCub-Fe1C1P2	-2015.81363410	37.10
330	04a-BicapSqAntipr-Fe1C1P2	-2015.81360680	37.12
331	02a-TetrcTriPri2-Fe1C3P1	-2015.81357270	37.14
332	05a-Isocloso-Fe2C2P6	-2015.81355920	37.15
333	04a-BicapSqAntipr-Fe1C2P1	-2015.81350320	37.18

334	05b-Isocloso-Fe2P2C6	-2015.81350280	37.18
335	04a-BicapSqAntipr-Fe2C3P6	-2015.81171580	38.30
336	05a-Isocloso-Fe3C1P4	-2015.81170490	38.31
337	02b-TetrcTriPri2-Fe1P5C3	-2015.81169130	38.32
338	01b-TetrcTriPri1-Fe2P3C3	-2015.81167870	38.33
339	05a-Isocloso-Fe2C4P2	-2015.81167820	38.33
340	04a-BicapSqAntipr-Fe2C1P3	-2015.81166900	38.33
341	05a-Isocloso-Fe2C2P5	-2015.81120710	38.62
342	05b-Isocloso-Fe2P1C8	-2015.81115600	38.65
343	04b-BicapSqAntipr-Fe1P1C4_r-34	-2015.81108450	38.70
344	01a-TetrcTriPri1-Fe2C4P4	-2015.81102040	38.74
345	04b-BicapSqAntipr-Fe1P1C4_i-34	-2015.81035370	39.16
346	04b-BicapSqAntipr-Fe2P1C2	-2015.80964840	39.60
347	01a-TetrcTriPri1-Fe3C4P2	-2015.80963430	39.61
348	05b-Isocloso-Fe2P3C1	-2015.80963420	39.61
349	02b-TetrcTriPri2-Fe2P4C1	-2015.80962990	39.61
350	01b-TetrcTriPri1-Fe1P4C1	-2015.80960740	39.63
351	03b-BicapCub-Fe2P3C1	-2015.80959770	39.63
352	01a-TetrcTriPri1-Fe2C4P2	-2015.80958750	39.64
353	05b-Isocloso-Fe3P4C1	-2015.80956700	39.65
354	01a-TetrcTriPri1-Fe1C2P5	-2015.80831960	40.43
355	02a-TetrcTriPri2-Fe3C1P3	-2015.80817360	40.53
356	01a-TetrcTriPri1-Fe3C2P7	-2015.80816490	40.53
357	05a-Isocloso-Fe2C2P2	-2015.80782280	40.75
358	01b-TetrcTriPri1-Fe3P2C5	-2015.80762040	40.87
359	01a-TetrcTriPri1-Fe1C1P8	-2015.80758040	40.90
360	01a-TetrcTriPri1-Fe3C3P2	-2015.80745690	40.98
361	03b-BicapCub-Fe2P3C4	-2015.80726420	41.10
362	01b-TetrcTriPri1-Fe2P1C8	-2015.80720090	41.14
363	01a-TetrcTriPri1-Fe1C1P3	-2015.80685220	41.36
364	02a-TetrcTriPri2-Fe3C2P2	-2015.80680770	41.38
365	05b-Isocloso-Fe1P3C5	-2015.80673770	41.43
366	01b-TetrcTriPri1-Fe1P3C4	-2015.80668610	41.46
367	01b-TetrcTriPri1-Fe1P3C1	-2015.80663050	41.49
368	01a-TetrcTriPri1-Fe2C5P2	-2015.80636670	41.66
369	04b-BicapSqAntipr-Fe2P2C6	-2015.80633160	41.68
370	01a-TetrcTriPri1-Fe2C4P1	-2015.80627910	41.72
371	05a-Isocloso-Fe2C1P7	-2015.80627450	41.72
372	05b-Isocloso-Fe2P3C4	-2015.80626390	41.72
373	05b-Isocloso-Fe2P3C3	-2015.80622610	41.75
374	01a-TetrcTriPri1-Fe3C3P4	-2015.80587520	41.97
375	03a-BicapCub-Fe2C4P1	-2015.80565040	42.11

376	01a-TetrcTriPri1-Fe2C3P4	-2015.80555370	42.17
377	01b-TetrcTriPri1-Fe1P3C3	-2015.80444200	42.87
378	01a-TetrcTriPri1-Fe1C3P6	-2015.80384480	43.24
379	05a-Isocloso-Fe1C1P7	-2015.80376330	43.29
380	05b-Isocloso-Fe1P1C5	-2015.80375820	43.30
381	01b-TetrcTriPri1-Fe2P1C7	-2015.80374100	43.31
382	02b-TetrcTriPri2-Fe3P1C3	-2015.80367370	43.35
383	02b-TetrcTriPri2-Fe3P1C5	-2015.80320310	43.65
384	01a-TetrcTriPri1-Fe2C1P7	-2015.80290210	43.83
385	02b-TetrcTriPri2-Fe2P1C6	-2015.80284430	43.87
386	02b-TetrcTriPri2-Fe1P2C2	-2015.80283000	43.88
387	02b-TetrcTriPri2-Fe1P1C1	-2015.80280470	43.90
388	05a-Isocloso-Fe3C1P1	-2015.80280060	43.90
389	02b-TetrcTriPri2-Fe2P1C2	-2015.80279660	43.90
390	05a-Isocloso-Fe2C1P1	-2015.80279550	43.90
391	04a-BicapSqAntipr-Fe2C1P6	-2015.80277310	43.92
392	02b-TetrcTriPri2-Fe1P4C2	-2015.80273500	43.94
393	04b-BicapSqAntipr-Fe2P3C1	-2015.80259710	44.03
394	02a-TetrcTriPri2-Fe2C3P5	-2015.80258690	44.03
395	02a-TetrcTriPri2-Fe2C3P6	-2015.80258680	44.03
396	01b-TetrcTriPri1-Fe2P7C2	-2015.80256180	44.05
397	05a-Isocloso-Fe2C2P4	-2015.80255830	44.05
398	05b-Isocloso-Fe3P2C3	-2015.80252950	44.07
399	05a-Isocloso-Fe3C2P4	-2015.80250930	44.08
400	05a-Isocloso-Fe1C3P2	-2015.80239360	44.15
401	05a-Isocloso-Fe3C3P1	-2015.80229420	44.22
402	02a-TetrcTriPri2-Fe1C5P4	-2015.80222650	44.26
403	01a-TetrcTriPri1-Fe3C5P2	-2015.80219740	44.28
404	01b-TetrcTriPri1-Fe1P3C2	-2015.80219250	44.28
405	03b-BicapCub-Fe2P2C3	-2015.80216260	44.30
406	01b-TetrcTriPri1-Fe1P2C4	-2015.80213170	44.32
407	02a-TetrcTriPri2-Fe1C3P3	-2015.80211530	44.33
408	03b-BicapCub-Fe2P2C2	-2015.80210870	44.33
409	01b-TetrcTriPri1-Fe1P3C6	-2015.80208990	44.34
410	01a-TetrcTriPri1-Fe2C5P3	-2015.80207910	44.35
411	01b-TetrcTriPri1-Fe1P1C8	-2015.80202030	44.39
412	04b-BicapSqAntipr-Fe1P2C1	-2015.80104190	45.00
413	03a-BicapCub-Fe2C2P1	-2015.80103480	45.01
414	02b-TetrcTriPri2-Fe1P4C5	-2015.80102950	45.01
415	01b-TetrcTriPri1-Fe3P3C2	-2015.80101360	45.02
416	03b-BicapCub-Fe1P2C1	-2015.80098030	45.04
417	02a-TetrcTriPri2-Fe3C1P1	-2015.80097800	45.04

418	01b-TetrcTriPri1-Fe2P3C2	-2015.80089470	45.09
419	01a-TetrcTriPri1-Fe3C4P5	-2015.79972730	45.83
420	01a-TetrcTriPri1-Fe2C4P5	-2015.79970500	45.84
421	01b-TetrcTriPri1-Fe2P5C2	-2015.79954820	45.94
422	02b-TetrcTriPri2-Fe1P2C1	-2015.79932440	46.08
423	05b-Isocloso-Fe3P2C1	-2015.79932370	46.08
424	03a-BicapCub-Fe2C1P3	-2015.79930460	46.09
425	02b-TetrcTriPri2-Fe2P2C7	-2015.79929710	46.10
426	04a-BicapSqAntipr-Fe2C4P1	-2015.79922950	46.14
427	02b-TetrcTriPri2-Fe1P6C3	-2015.79920680	46.15
428	03a-BicapCub-Fe2C2P4	-2015.79906070	46.24
429	03a-BicapCub-Fe2C3P1	-2015.79853330	46.58
430	02a-TetrcTriPri2-Fe2C4P1	-2015.79850580	46.59
431	05a-Isocloso-Fe3C1P2	-2015.79847860	46.61
432	02a-TetrcTriPri2-Fe1C1P5	-2015.79843800	46.64
433	04a-BicapSqAntipr-Fe2C2P1	-2015.79842950	46.64
434	02b-TetrcTriPri2-Fe1P4C1	-2015.79841570	46.65
435	01a-TetrcTriPri1-Fe2C1P4	-2015.79817300	46.80
436	05b-Isocloso-Fe1P3C2	-2015.79778790	47.04
437	01a-TetrcTriPri1-Fe3C8P1	-2015.79758140	47.17
438	01b-TetrcTriPri1-Fe3P3C5	-2015.79727970	47.36
439	05a-Isocloso-Fe1C3P3	-2015.79707700	47.49
440	05b-Isocloso-Fe1P3C3	-2015.79700750	47.53
441	05a-Isocloso-Fe3C2P2	-2015.79694270	47.57
442	04a-BicapSqAntipr-Fe2C1P7	-2015.79693350	47.58
443	04b-BicapSqAntipr-Fe2P4C1	-2015.79618240	48.05
444	02a-TetrcTriPri2-Fe1C2P1	-2015.79612960	48.08
445	05a-Isocloso-Fe3C2P1	-2015.79606150	48.13
446	02a-TetrcTriPri2-Fe1C6P3	-2015.79604250	48.14
447	01b-TetrcTriPri1-Fe1P2C2	-2015.79603240	48.15
448	03b-BicapCub-Fe2P1C3	-2015.79602620	48.15
449	02a-TetrcTriPri2-Fe3C2P4	-2015.79601770	48.15
450	01a-TetrcTriPri1-Fe3C7P2_r-36	-2015.79542580	48.53
451	04a-BicapSqAntipr-Fe2C3P1	-2015.79539960	48.54
452	02b-TetrcTriPri2-Fe3P2C4	-2015.79539440	48.55
453	05b-Isocloso-Fe2P2C4	-2015.79537040	48.56
454	05a-Isocloso-Fe2C2P1	-2015.79536810	48.56
455	03a-BicapCub-Fe2C3P3	-2015.79536050	48.57
456	01a-TetrcTriPri1-Fe2C1P3	-2015.79513740	48.71
457	01a-TetrcTriPri1-Fe3C2P2	-2015.79508300	48.74
458	01a-TetrcTriPri1-Fe1C1P7	-2015.79493610	48.83
459	02b-TetrcTriPri2-Fe2P1C8	-2015.79489320	48.86

460	04a-BicapSqAntipr-Fe2C3P2	-2015.79488380	48.87
461	04a-BicapSqAntipr-Fe2C2P4	-2015.79477310	48.94
462	01a-TetrcTriPri1-Fe3C7P2_i-36	-2015.79455380	49.07
463	05b-Isocloso-Fe1P1C3	-2015.79427910	49.25
464	02a-TetrcTriPri2-Fe3C2P3	-2015.79404570	49.39
465	05a-Isocloso-Fe1C2P2	-2015.79399540	49.42
466	05b-Isocloso-Fe1P2C2	-2015.79388130	49.50
467	05b-Isocloso-Fe1P1C2	-2015.79303070	50.03
468	05b-Isocloso-Fe1P4C2	-2015.79302630	50.03
469	02b-TetrcTriPri2-Fe3P3C1	-2015.79301460	50.04
470	02a-TetrcTriPri2-Fe2C2P7	-2015.79299100	50.05
471	02b-TetrcTriPri2-Fe2P3C5	-2015.79291990	50.10
472	02b-TetrcTriPri2-Fe1P6C2	-2015.79258570	50.31
473	05a-Isocloso-Fe3C4P1	-2015.79257670	50.31
474	05a-Isocloso-Fe2C3P1	-2015.79254170	50.34
475	04a-BicapSqAntipr-Fe2C1P2	-2015.79253410	50.34
476	01a-TetrcTriPri1-Fe1C2P1	-2015.79244860	50.39
477	03a-BicapCub-Fe2C5P3	-2015.79244290	50.40
478	01a-TetrcTriPri1-Fe1C3P5	-2015.79151050	50.98
479	01a-TetrcTriPri1-Fe2C3P5	-2015.79112470	51.22
480	05b-Isocloso-Fe3P2C6	-2015.79103550	51.28
481	05a-Isocloso-Fe3C2P6	-2015.79103280	51.28
482	01a-TetrcTriPri1-Fe3C7P1	-2015.79102920	51.28
483	01b-TetrcTriPri1-Fe1P1C6	-2015.79074780	51.46
484	03b-BicapCub-Fe1P1C4	-2015.79061740	51.54
485	04b-BicapSqAntipr-Fe1P1C3	-2015.79060060	51.55
486	03b-BicapCub-Fe1P1C3	-2015.79051190	51.61
487	02a-TetrcTriPri2-Fe3C4P2	-2015.79019490	51.81
488	05b-Isocloso-Fe2P1C1	-2015.78995290	51.96
489	02b-TetrcTriPri2-Fe2P1C1	-2015.78989830	51.99
490	02b-TetrcTriPri2-Fe1P1C5	-2015.78962300	52.17
491	05a-Isocloso-Fe2C1P2	-2015.78960260	52.18
492	01b-TetrcTriPri1-Fe2P1C4	-2015.78921480	52.42
493	01b-TetrcTriPri1-Fe3P2C3	-2015.78914750	52.47
494	02a-TetrcTriPri2-Fe3C1P5	-2015.78914710	52.47
495	02a-TetrcTriPri2-Fe3C2P1_i-17	-2015.78908950	52.50
496	02a-TetrcTriPri2-Fe1C6P2	-2015.78744020	53.54
497	05b-Isocloso-Fe2P2C3	-2015.78734220	53.60
498	01a-TetrcTriPri1-Fe3C4P1	-2015.78710910	53.74
499	05a-Isocloso-Fe3C2P3	-2015.78708570	53.76
500	03a-BicapCub-Fe1C1P3	-2015.78708170	53.76
501	02b-TetrcTriPri2-Fe1P4C3	-2015.78706040	53.78

502	02b-TetrcTriPri2-Fe1P1C7	-2015.78700230	53.81
503	05a-Isocloso-Fe1C2P5	-2015.78678040	53.95
504	05b-Isocloso-Fe1P3C6	-2015.78676390	53.96
505	01a-TetrcTriPri1-Fe3C5P3	-2015.78614920	54.35
506	05a-Isocloso-Fe3C1P5	-2015.78544910	54.79
507	01a-TetrcTriPri1-Fe3C6P1	-2015.78512690	54.99
508	02a-TetrcTriPri2-Fe2C5P1	-2015.78496830	55.09
509	02b-TetrcTriPri2-Fe2P1C7	-2015.78486450	55.15
510	05a-Isocloso-Fe1C4P2	-2015.78475850	55.22
511	05a-Isocloso-Fe1C1P2	-2015.78475770	55.22
512	01b-TetrcTriPri1-Fe2P2C1	-2015.78460490	55.32
513	01b-TetrcTriPri1-Fe3P1C2	-2015.78460030	55.32
514	01b-TetrcTriPri1-Fe1P1C5	-2015.78455240	55.35
515	01a-TetrcTriPri1-Fe1C1P5	-2015.78446080	55.41
516	01b-TetrcTriPri1-Fe1P2C1	-2015.78426030	55.53
517	05a-Isocloso-Fe2C3P2	-2015.78357640	55.96
518	05b-Isocloso-Fe3P2C4	-2015.78348810	56.02
519	02b-TetrcTriPri2-Fe2P3C6	-2015.78344230	56.05
520	02b-TetrcTriPri2-Fe1P3C1	-2015.78341250	56.06
521	01a-TetrcTriPri1-Fe3C1P8	-2015.78326420	56.16
522	01a-TetrcTriPri1-Fe1C4P4	-2015.78318130	56.21
523	01a-TetrcTriPri1-Fe2C2P7	-2015.78315730	56.22
524	03a-BicapCub-Fe1C1P6	-2015.78263530	56.55
525	05b-Isocloso-Fe2P3C5	-2015.78188190	57.02
526	02b-TetrcTriPri2-Fe1P5C4	-2015.78185150	57.04
527	05a-Isocloso-Fe2C3P5	-2015.78184860	57.05
528	01b-TetrcTriPri1-Fe2P5C1	-2015.78184400	57.05
529	01b-TetrcTriPri1-Fe3P5C1	-2015.78184170	57.05
530	03a-BicapCub-Fe2C2P3	-2015.78181960	57.06
531	04a-BicapSqAntipr-Fe2C3P5	-2015.78180760	57.07
532	03a-BicapCub-Fe2C2P2	-2015.78179080	57.08
533	01b-TetrcTriPri1-Fe2P1C1	-2015.78172760	57.12
534	01b-TetrcTriPri1-Fe3P1C1	-2015.78170230	57.14
535	01b-TetrcTriPri1-Fe2P1C2	-2015.78166390	57.16
536	03a-BicapCub-Fe2C4P3	-2015.78122090	57.44
537	05b-Isocloso-Fe2P3C2	-2015.78115790	57.48
538	03a-BicapCub-Fe2C1P1	-2015.78048250	57.90
539	01b-TetrcTriPri1-Fe2P2C2	-2015.78047910	57.91
540	01b-TetrcTriPri1-Fe3P1C4	-2015.78045710	57.92
541	02b-TetrcTriPri2-Fe1P5C2	-2015.78041330	57.95
542	05b-Isocloso-Fe1P3C4	-2015.78003660	58.18
543	05a-Isocloso-Fe1C3P4	-2015.78002910	58.19

544	02a-TetrcTriPri2-Fe1C4P5	-2015.77992380	58.25
545	01a-TetrcTriPri1-Fe1C1P1	-2015.77990390	58.27
546	05b-Isocloso-Fe1P5C1	-2015.77861400	59.08
547	05a-Isocloso-Fe1C1P3	-2015.77852980	59.13
548	01a-TetrcTriPri1-Fe2C1P6	-2015.77845370	59.18
549	01b-TetrcTriPri1-Fe2P2C4	-2015.77829450	59.28
550	02b-TetrcTriPri2-Fe3P3C3	-2015.77828910	59.28
551	01b-TetrcTriPri1-Fe3P1C7	-2015.77826490	59.29
552	01b-TetrcTriPri1-Fe3P1C5	-2015.77825890	59.30
553	01a-TetrcTriPri1-Fe1C4P1	-2015.77825190	59.30
554	01a-TetrcTriPri1-Fe2C3P2	-2015.77824250	59.31
555	02a-TetrcTriPri2-Fe3C4P1	-2015.77822140	59.32
556	01b-TetrcTriPri1-Fe2P2C5	-2015.77805740	59.42
557	01a-TetrcTriPri1-Fe2C2P5	-2015.77782960	59.57
558	03a-BicapCub-Fe1C2P3	-2015.77760080	59.71
559	04b-BicapSqAntipr-Fe2P3C5	-2015.77741870	59.83
560	01a-TetrcTriPri1-Fe1C3P2	-2015.77736570	59.86
561	02a-TetrcTriPri2-Fe3C3P1	-2015.77575820	60.87
562	02b-TetrcTriPri2-Fe3P4C2	-2015.77490700	61.40
563	02a-TetrcTriPri2-Fe3C3P3	-2015.77484660	61.44
564	04a-BicapSqAntipr-Fe1C1P4	-2015.77447690	61.67
565	03a-BicapCub-Fe1C1P5	-2015.77444590	61.69
566	05b-Isocloso-Fe2P2C5	-2015.77442010	61.71
567	05a-Isocloso-Fe2C1P8	-2015.77438660	61.73
568	02a-TetrcTriPri2-Fe3C3P2	-2015.77431960	61.77
569	01b-TetrcTriPri1-Fe2P7C1	-2015.77363710	62.20
570	01b-TetrcTriPri1-Fe2P6C1	-2015.77363210	62.20
571	01b-TetrcTriPri1-Fe3P6C2	-2015.77360670	62.22
572	01b-TetrcTriPri1-Fe3P7C2	-2015.77236120	63.00
573	02b-TetrcTriPri2-Fe3P4C5	-2015.77084610	63.95
574	02a-TetrcTriPri2-Fe3C4P5	-2015.77083430	63.96
575	01b-TetrcTriPri1-Fe3P6C1	-2015.77062820	64.09
576	01b-TetrcTriPri1-Fe2P6C2	-2015.77061680	64.09
577	01b-TetrcTriPri1-Fe3P8C1	-2015.77053440	64.15
578	02a-TetrcTriPri2-Fe1C7P2	-2015.77038690	64.24
579	04b-BicapSqAntipr-Fe1P2C3	-2015.77035920	64.26
580	02a-TetrcTriPri2-Fe1C3P5	-2015.77032060	64.28
581	02a-TetrcTriPri2-Fe1C5P2	-2015.77031970	64.28
582	03a-BicapCub-Fe2C3P2	-2015.77022020	64.34
583	03b-BicapCub-Fe2P3C2	-2015.76989060	64.55
584	01a-TetrcTriPri1-Fe2C1P1	-2015.76920010	64.98
585	01a-TetrcTriPri1-Fe3C3P5	-2015.76909200	65.05

586	02b-TetrcTriPri2-Fe1P3C5	-2015.76895730	65.14
587	02b-TetrcTriPri2-Fe1P7C1	-2015.76890950	65.17
588	02b-TetrcTriPri2-Fe1P7C2	-2015.76887460	65.19
589	01b-TetrcTriPri1-Fe3P6C3	-2015.76794890	65.77
590	01b-TetrcTriPri1-Fe2P6C3	-2015.76792240	65.78
591	01a-TetrcTriPri1-Fe3C1P5	-2015.76657630	66.63
592	01a-TetrcTriPri1-Fe3C1P7	-2015.76656360	66.64
593	01a-TetrcTriPri1-Fe2C2P4	-2015.76654600	66.65
594	01a-TetrcTriPri1-Fe3C1P1	-2015.76591490	67.04
595	03a-BicapCub-Fe2C4P2	-2015.76464600	67.84
596	01a-TetrcTriPri1-Fe2C6P3	-2015.76364000	68.47
597	01a-TetrcTriPri1-Fe2C8P1	-2015.76360710	68.49
598	01a-TetrcTriPri1-Fe3C6P3	-2015.76358040	68.51
599	02a-TetrcTriPri2-Fe1C5P3	-2015.76353430	68.54
600	03b-BicapCub-Fe1P1C5	-2015.76340400	68.62
601	01b-TetrcTriPri1-Fe2P3C5	-2015.76170950	69.68
602	01a-TetrcTriPri1-Fe2C5P1	-2015.76137630	69.89
603	01a-TetrcTriPri1-Fe3C5P1	-2015.76137570	69.89
604	01b-TetrcTriPri1-Fe2P8C1	-2015.75969510	70.95
605	05b-Isocloso-Fe2P2C1	-2015.75913070	71.30
606	05a-Isocloso-Fe2C5P1	-2015.75782340	72.12
607	04a-BicapSqAntipr-Fe1C1P5	-2015.75729860	72.45
608	03b-BicapCub-Fe1P2C3	-2015.75681470	72.76
609	01a-TetrcTriPri1-Fe3C2P6	-2015.75575940	73.42
610	01a-TetrcTriPri1-Fe3C1P6	-2015.75567090	73.47
611	01a-TetrcTriPri1-Fe3C1P2	-2015.75553790	73.56
612	01a-TetrcTriPri1-Fe2C2P1	-2015.75551580	73.57
613	04a-BicapSqAntipr-Fe1C2P2	-2015.75519980	73.77
614	03a-BicapCub-Fe1C2P2	-2015.75516400	73.79
615	03b-BicapCub-Fe1P2C2	-2015.75503880	73.87
616	01a-TetrcTriPri1-Fe2C4P3	-2015.75416960	74.41
617	01b-TetrcTriPri1-Fe2P4C2	-2015.75394990	74.55
618	01b-TetrcTriPri1-Fe3P4C2	-2015.75387160	74.60
619	04a-BicapSqAntipr-Fe1C1P3	-2015.75273230	75.32
620	01a-TetrcTriPri1-Fe2C2P3	-2015.75249870	75.46
621	01a-TetrcTriPri1-Fe2C3P6	-2015.75239180	75.53
622	01a-TetrcTriPri1-Fe3C3P6	-2015.75237540	75.54
623	01a-TetrcTriPri1-Fe3C1P3	-2015.75237060	75.54
624	02a-TetrcTriPri2-Fe1C7P1	-2015.75195270	75.81
625	02a-TetrcTriPri2-Fe3C5P1	-2015.74916260	77.56
626	03b-BicapCub-Fe2P4C2	-2015.74763090	78.52
627	01b-TetrcTriPri1-Fe3P1C3	-2015.74606780	79.50

628	01b-TetrcTriPri1-Fe3P5C2	-2015.74597800	79.56
629	01b-TetrcTriPri1-Fe2P5C3	-2015.74590470	79.60
630	01a-TetrcTriPri1-Fe2C6P2	-2015.74495280	80.20
631	04a-BicapSqAntipr-Fe1C2P3	-2015.74300440	81.42
632	02a-TetrcTriPri2-Fe2C2P2	-2015.74176040	82.20
633	02b-TetrcTriPri2-Fe2P2C2	-2015.74141640	82.42
634	01a-TetrcTriPri1-Fe2C3P3	-2015.74096180	82.70
635	02a-TetrcTriPri2-Fe2C1P2	-2015.73910230	83.87
636	03a-BicapCub-Fe1C2P1	-2015.73730720	85.00
637	02b-TetrcTriPri2-Fe3P3C2	-2015.73688540	85.26
638	01b-TetrcTriPri1-Fe3P5C3	-2015.73246960	88.03
639	01b-TetrcTriPri1-Fe2P4C1	-2015.73210610	88.26
640	01b-TetrcTriPri1-Fe3P4C1	-2015.73204170	88.30
641	02a-TetrcTriPri2-Fe2C2P1	-2015.73008150	89.53
642	01a-TetrcTriPri1-Fe2C1P8	-2015.72774710	91.00
643	01a-TetrcTriPri1-Fe3C2P4	-2015.72773860	91.00
644	01b-TetrcTriPri1-Fe2P4C4	-2015.72005390	95.82
645	01b-TetrcTriPri1-Fe3P4C4	-2015.72004550	95.83
646	01a-TetrcTriPri1-Fe2C1P2	-2015.71881160	96.60
647	01a-TetrcTriPri1-Fe3C2P1	-2015.71306340	100.21
648	01a-TetrcTriPri1-Fe1C2P2	-2015.69214870	113.33

Table S4A. Initial $CpFeCHPHB_8H_8$ structures, 938 in all.

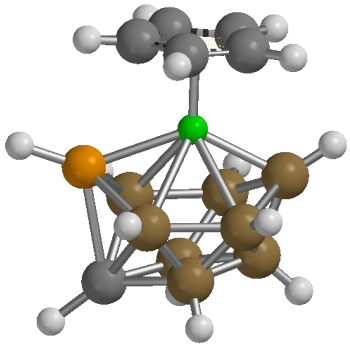
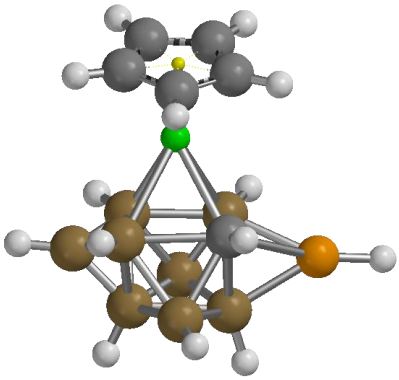
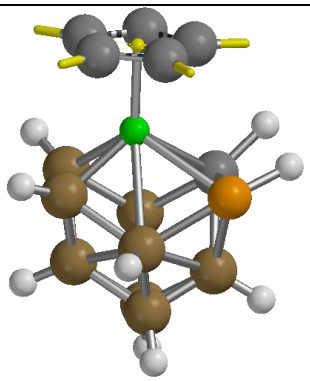
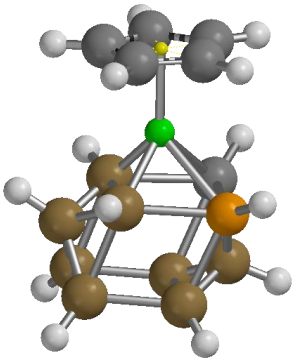
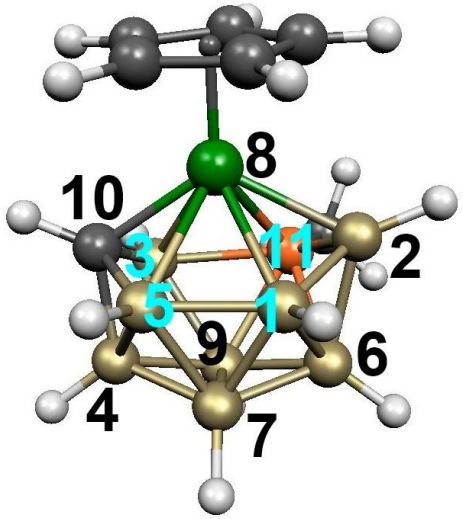
 Edge-coalesced icosahedron 316	 Pentacapped trigonal prism 100
 Tricapped cube C_{3v} 243	 Tricapped cube C_{2v} 279

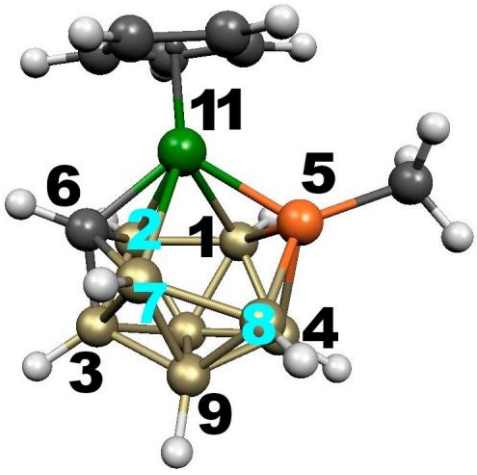
Table S4B. Distance table for the lowest-lying $CpFeCHPCH_3B_8H_8$ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol), HOMO/LUMO gaps (eV) and symmetry.



1. -2080.6268794 0.0
C_1 H/L 2.14

		1	2	3	4	5
1	B	0.000000				
2	B	1.681038	0.000000			
3	B	3.235196	3.290628	0.000000		
4	B	2.915699	3.788570	1.792698	0.000000	
5	B	1.796982	3.099490	2.611129	1.805835	0.000000
6	B	1.774566	1.831012	3.095267	2.959331	2.922489
7	B	1.780116	2.945712	2.843816	1.748376	1.791609
8	Fe	2.222742	2.130111	2.331539	3.091425	2.210017
9	B	2.817334	3.038648	1.854360	1.748851	2.809758
10	C	2.905284	3.548932	1.550259	1.640698	1.575496
11	P	2.728331	1.848625	2.010499	3.098352	3.316141

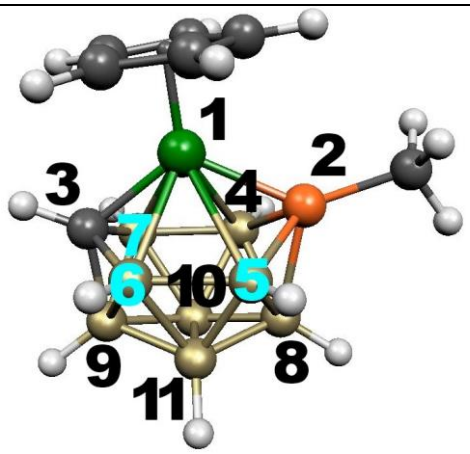
		6	7	8	9	10
6	B	0.000000				
7	B	1.725459	0.000000			
8	Fe	3.137490	3.198112	0.000000		
9	B	1.840661	1.788244	3.251996	0.000000	
10	C	3.560025	2.736352	1.980145	2.747563	0.000000
11	P	2.032656	2.978325	2.327326	1.976128	3.035042



2. -2080.6218910 +3.1
C_1 H/L 2.25

		1	2	3	4	5
1	B	0.000000				
2	B	1.771993	0.000000			
3	B	2.857240	1.798658	0.000000		
4	B	1.849645	2.966073	2.915721	0.000000	
5	P	1.948627	3.175709	3.636565	1.994888	0.000000
6	C	2.822564	1.617539	1.600069	3.507429	3.294299
7	B	3.025440	2.635304	1.868788	2.872995	2.688524
8	B	2.928676	3.566691	3.041385	1.865141	1.843419
9	B	2.800562	2.855903	1.764979	1.752065	2.892006
10	B	1.772417	1.787203	1.753088	1.732335	3.056057
11	Fe	2.182267	2.145409	3.091902	3.327763	2.146467

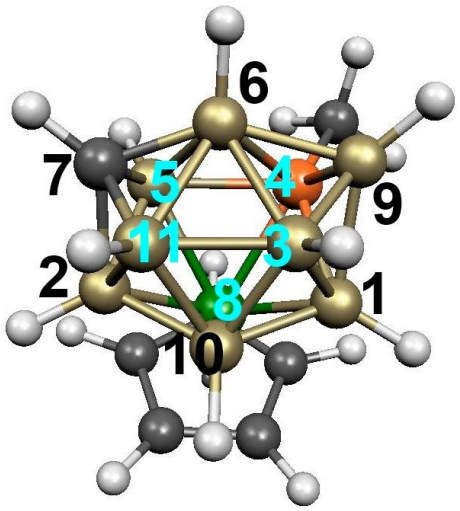
		6	7	8	9	10
6	C	0.000000				
7	B	1.578552	0.000000			
8	B	3.215571	1.886393	0.000000		
9	B	2.746338	1.838351	1.698565	0.000000	
10	B	2.719399	2.792663	2.926703	1.787229	0.000000
11	Fe	1.911854	2.355588	3.094610	3.464131	3.244934



3. -2080.6212890 +3.5
C_S H/L 2.25

		1	2	3	4	5
1	Fe	0.000000				
2	P	2.158164	0.000000			
3	C	1.960771	3.517236	0.000000		
4	B	2.410438	1.875746	2.941886	0.000000	
5	B	2.409938	1.875897	2.941910	2.812553	0.000000
6	B	2.267476	3.156136	1.569048	3.259948	1.807387
7	B	2.268159	3.156226	1.569018	1.807520	3.260051
8	B	3.235109	1.952820	3.519933	1.900840	1.900784
9	B	3.103818	3.786236	1.623054	2.926223	2.926100
10	B	3.272034	3.020467	2.721855	1.756281	2.864545
11	B	3.271667	3.020393	2.721776	2.864357	1.756239

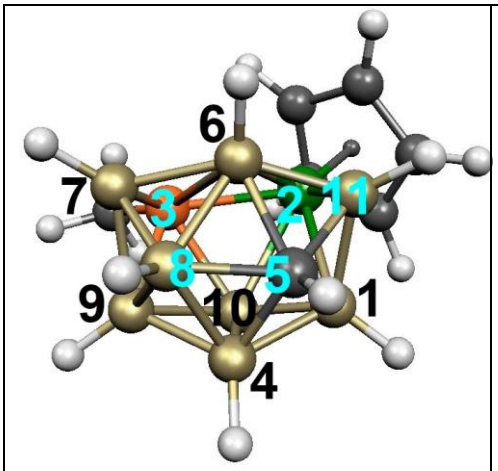
		6	7	8	9	10
6	B	0.000000				
7	B	2.617092	0.000000			
8	B	2.962551	2.962648	0.000000		
9	B	1.811160	1.811229	2.894016	0.000000	
10	B	2.829078	1.799544	1.733934	1.745486	0.000000
11	B	1.799579	2.828903	1.733762	1.745278	1.820634



4. -2080.6089567 +11.3
C_1 H/L 2.18

		1	2	3	4	5
1	B	0.000000				
2	B	3.004718	0.000000			
3	B	1.762760	2.903654	0.000000		
4	P	2.049345	3.140868	2.811905	0.000000	
5	B	3.107186	1.795992	3.214663	2.029593	0.000000
6	B	2.794037	2.677061	1.887692	2.295541	2.089397
7	C	3.502155	1.664022	2.782532	3.052353	1.570397
8	Fe	2.118779	2.066518	3.218295	2.111403	2.081872
9	B	1.876450	3.676080	1.669249	1.841416	3.108584
10	B	1.746440	1.768543	1.784841	3.019227	2.849092
11	B	2.934893	1.787118	1.793329	3.459289	2.670746

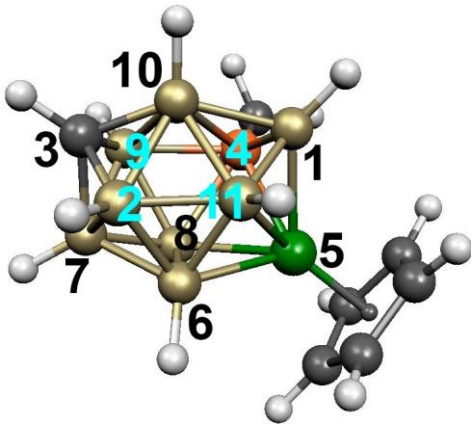
		6	7	8	9	10
6	B	0.000000				
7	C	1.600094	0.000000			
8	Fe	3.279996	3.109723	0.000000		
9	B	1.824443	3.251278	3.305141	0.000000	
10	B	2.767538	2.710645	2.130808	2.932038	0.000000
11	B	1.917346	1.579748	3.245909	3.032082	1.764894



5. -2080.6073424 +12.3
C_1 H/L 2.73

		1	2	3	4	5
1	B	0.000000				
2	Fe	2.116144	0.000000			
3	P	3.150008	2.129706	0.000000		
4	B	1.765357	3.224731	3.054736	0.000000	
5	C	1.698622	2.908928	3.404789	1.672869	0.000000
6	B	2.631401	2.292298	2.465556	2.766902	1.797569
7	B	3.607278	3.196298	1.840170	2.935811	2.922096
8	B	2.845598	3.475862	2.861149	1.778316	1.679170
9	B	2.950563	3.330187	2.011133	1.736787	2.777253
10	B	1.745062	2.149008	1.972283	1.773440	2.691477
11	B	1.750304	1.944675	3.348895	2.871084	1.621699

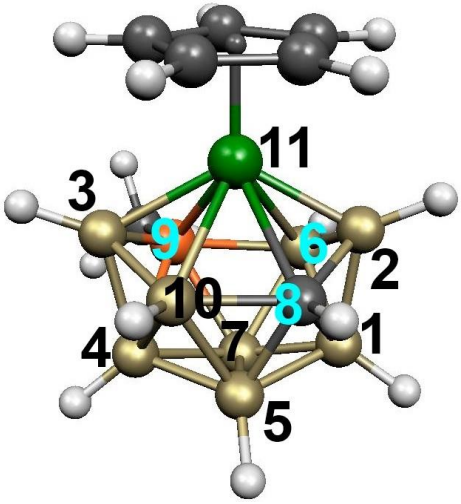
		6	7	8	9	10
6	B	0.000000				
7	B	1.833607	0.000000			
8	B	1.836856	1.697435	0.000000		
9	B	2.775032	1.843738	1.745317	0.000000	
10	B	2.924731	2.961383	2.796553	1.858198	0.000000
11	B	1.706643	3.392678	2.886967	3.661285	2.949479



6. -2080.6068605 +12.6
C_1 H/L 1.98

		1	2	3	4	5
1	B	0.000000				
2	B	3.072145	0.000000			
3	C	3.262374	1.592838	0.000000		
4	P	1.856215	3.489902	3.077901	0.000000	
5	Fe	2.090534	3.346911	3.895726	2.159111	0.000000
6	B	2.970173	1.775859	2.723131	3.013703	2.070110
7	B	3.690040	1.782570	1.634897	3.134005	3.364591
8	B	3.046455	2.842598	2.765665	1.979168	2.110900
9	B	3.056296	2.665132	1.570779	1.994584	3.366093
10	B	1.871326	1.888934	1.594929	2.424855	3.202357
11	B	1.692771	1.785735	2.757202	2.798560	2.097378

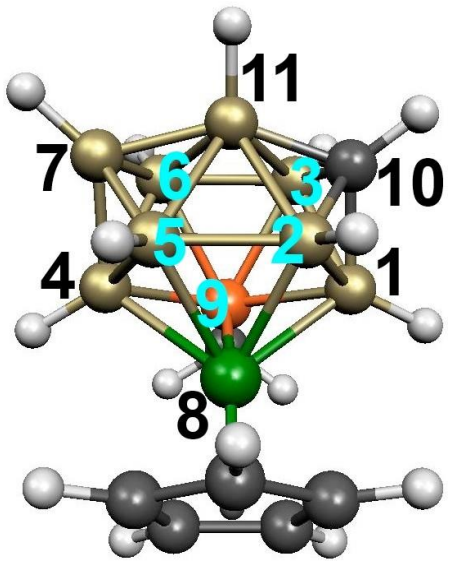
		6	7	8	9	10
6	B	0.000000				
7	B	1.794926	0.000000			
8	B	1.780645	1.774386	0.000000		
9	B	2.829364	1.780425	1.859957	0.000000	
10	B	2.787192	2.674912	2.981158	2.117766	0.000000
11	B	1.779102	2.879789	2.815154	3.138947	1.845792



7. -2080.6065968 +12.7
C_1 H/L 2.00

		1	2	3	4	5
1	B	0.000000				
2	B	1.732515	0.000000			
3	B	3.749663	3.622999	0.000000		
4	B	2.933711	3.676253	1.825049	0.000000	
5	B	1.752280	2.853882	2.943365	1.714661	0.000000
6	B	1.769841	1.679851	3.272549	3.091069	2.856229
7	B	1.731332	2.901031	3.035697	1.841972	1.788948
8	C	1.707072	1.600154	3.008188	2.787275	1.686580
9	P	3.052479	3.140456	1.840826	2.037557	2.976215
10	B	2.884316	2.957737	1.692370	1.776154	1.778764
11	Fe	3.072432	2.012236	2.119507	3.136077	3.210226

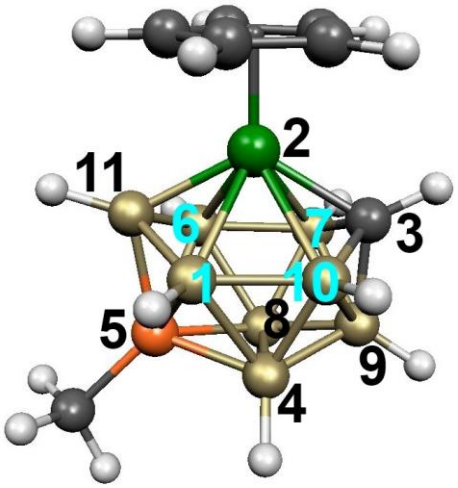
		6	7	8	9	10
6	B	0.000000				
7	B	1.865370	0.000000			
8	C	2.525006	2.679313	0.000000		
9	P	1.987392	1.978410	3.188704	0.000000	
10	B	3.226213	2.820624	1.710712	2.728437	0.000000
11	Fe	2.349724	3.277261	2.180664	2.334691	2.205265



8. -2080.6053738 +13.5
C_1 H/L 2.56

		1	2	3	4	5
1	B	0.000000				
2	B	1.785183	0.000000			
3	B	1.899179	2.665150	0.000000		
4	B	3.210433	2.979629	3.108815	0.000000	
5	B	3.032555	1.838962	3.269260	1.755003	0.000000
6	B	3.102189	3.238011	1.868854	1.918960	2.682644
7	B	3.716750	2.981596	3.010261	1.726797	1.676724
8	Fe	2.086526	2.051902	3.268102	2.113969	2.091694
9	P	1.992475	2.944385	1.968735	1.996821	2.962261
10	C	1.631380	1.585650	1.563567	3.540845	2.880394
11	B	2.688176	1.968882	1.925971	2.695087	2.007329

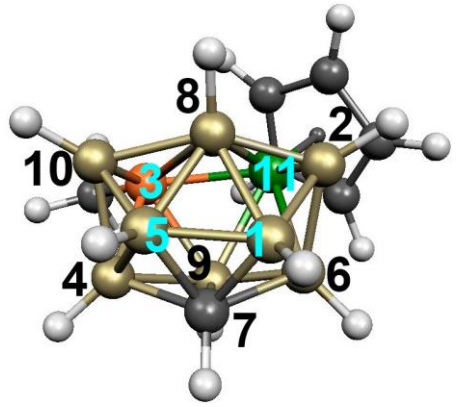
		6	7	8	9	10
6	B	0.000000				
7	B	1.665975	0.000000			
8	Fe	3.286963	3.269134	0.000000		
9	P	1.965183	3.017756	2.121210	0.000000	
10	C	2.865889	3.226645	3.094019	2.867810	0.000000
11	B	1.936706	1.748035	3.196727	2.902219	1.621706



9. -2080.6038284 +14.5
C_S H/L 2.17

		1	2	3	4	5
1	B	0.000000				
2	Fe	2.194999	0.000000			
3	C	2.908034	1.970656	0.000000		
4	B	1.916193	3.215848	2.703892	0.000000	
5	P	1.989691	3.155980	3.606985	1.926529	0.000000
6	B	2.739800	2.194739	2.908099	2.993381	1.989537
7	B	3.237167	2.229300	1.564507	2.860432	3.049135
8	B	2.993486	3.215752	2.703971	1.930400	1.926497
9	B	3.005126	3.078248	1.621666	1.741913	3.038898
10	B	1.819416	2.229627	1.564458	1.769467	3.049174
11	B	1.750092	2.009086	3.459530	3.048111	1.885986

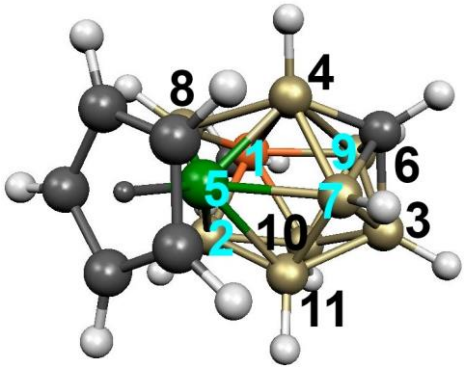
		6	7	8	9	10
6	B	0.000000				
7	B	1.819439	0.000000			
8	B	1.916161	1.769529	0.000000		
9	B	3.005073	1.827347	1.741908	0.000000	
10	B	3.237175	2.616600	2.860479	1.827383	0.000000
11	B	1.750167	3.103901	3.048185	3.760619	3.103871



10. -2080.6002569 +16.7
C_1 H/L 2.79

		1	2	3	4	5
1	B	0.000000				
2	B	1.694491	0.000000			
3	P	3.565449	3.354191	0.000000		
4	B	2.897813	3.663880	2.011880	0.000000	
5	B	1.756851	2.900551	2.860733	1.750524	0.000000
6	B	1.770844	1.741570	3.172768	2.950374	2.846186
7	C	1.682772	2.769924	2.932732	1.658752	1.690867
8	B	1.892056	1.717160	2.472737	2.770225	1.820946
9	B	2.815927	2.939751	1.982370	1.839852	2.786043
10	B	3.055190	3.425062	1.838860	1.829668	1.690555
11	Fe	3.050031	1.965425	2.117938	3.299609	3.477349

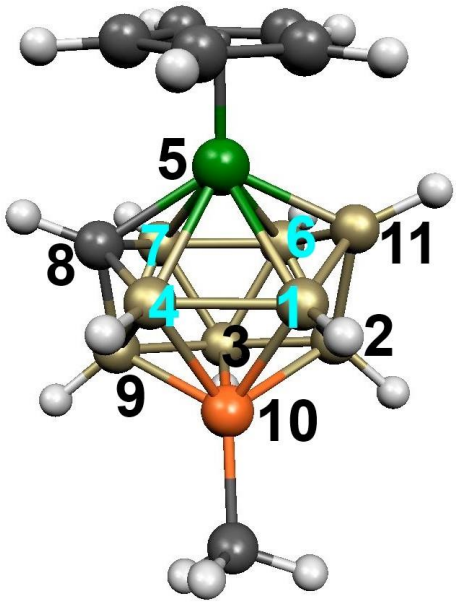
		6	7	8	9	10
6	B	0.000000				
7	C	1.708091	0.000000			
8	B	2.626912	2.615238	0.000000		
9	B	1.754057	1.686855	2.914131	0.000000	
10	B	3.622260	2.803677	1.860899	2.951680	0.000000
11	Fe	2.109004	3.076786	2.331512	2.102573	3.221608



11. -2080.5997639 +17.0
C_1 H/L 1.97

		1	2	3	4	5
1	P	0.000000				
2	B	2.035755	0.000000			
3	B	3.118626	2.946642	0.000000		
4	B	2.771612	2.943832	2.754734	0.000000	
5	Fe	3.221000	2.059904	3.253738	1.968689	0.000000
6	C	3.006791	3.407610	1.648320	1.604880	3.050186
7	B	3.569128	2.948994	1.768755	1.810040	2.052547
8	B	1.897003	1.872357	3.722790	2.109600	1.899566
9	B	1.971765	3.006346	1.766593	2.473679	3.607134
10	B	1.988873	1.819771	1.752130	3.187032	3.218078
11	B	3.077676	1.746715	1.788376	2.819520	2.103845

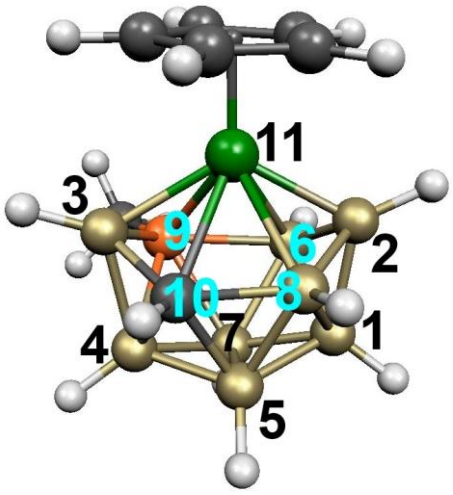
		6	7	8	9	10
6	C	0.000000				
7	B	1.642766	0.000000			
8	B	3.273893	3.207600	0.000000		
9	B	1.583258	2.748372	3.145329	0.000000	
10	B	2.727915	2.839901	3.038223	1.836860	0.000000
11	B	2.719908	1.762269	3.017005	2.858601	1.777491



12. -2080.5941628 +20.5
C_1 H/L 2.25

		1	2	3	4	5
1	B	0.000000				
2	B	1.919515	0.000000			
3	B	2.974688	1.864943	0.000000		
4	B	1.925824	3.128100	2.988530	0.000000	
5	Fe	2.204600	3.042263	3.181529	2.148225	0.000000
6	B	2.664478	1.762658	1.771647	3.244784	2.229096
7	B	3.246118	2.971536	1.791946	2.639571	2.189767
8	C	3.000977	3.596508	2.761586	1.554860	1.989372
9	B	3.134342	3.099146	1.803747	2.001033	3.080936
10	P	1.950829	1.966660	2.003981	1.999940	3.278693
11	B	1.686507	1.699191	2.936046	3.110593	2.032503

		6	7	8	9	10
6	B	0.000000				
7	B	1.817446	0.000000			
8	C	2.949964	1.581627	0.000000		
9	B	2.957555	1.793427	1.617461	0.000000	
10	P	2.956041	2.968589	2.848413	1.951104	0.000000
11	B	1.692973	3.056053	3.493222	3.770262	3.020387



13. -2080.5936576 +20.9
C_1 H/L 2.06

		1	2	3	4	5
1	B	0.000000				
2	B	1.730800	0.000000			
3	B	3.696445	3.602379	0.000000		
4	B	2.931241	3.713997	1.831868	0.000000	
5	B	1.754725	2.893766	2.886372	1.714949	0.000000
6	B	1.774324	1.686836	3.245489	3.070452	2.853229
7	B	1.761114	2.931789	3.012122	1.803858	1.786118
8	B	1.803317	1.692597	2.973793	2.886152	1.777004
9	P	3.053946	3.143389	1.855634	2.032625	2.974343
10	C	2.790148	2.967367	1.585584	1.690038	1.682431
11	Fe	3.057534	2.022766	2.101565	3.168821	3.241929

		6	7	8	9	10
6	B	0.000000				
7	B	1.866719	0.000000			
8	B	2.639780	2.814052	0.000000		
9	P	1.970269	1.983285	3.274894	0.000000	
10	C	3.136461	2.690625	1.713399	2.624271	0.000000
11	Fe	2.303817	3.266681	2.242756	2.276683	2.265365

Table S4C. Energy ranking for all of the $CpFeCHPHB_8H_8$ optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	02b-TricapCubeA-Fe2P3C1	-2041.3248836	0.00
2	03b-TricapCubeB-Fe4P1C8	-2041.3248444	0.02
3	04a-Icos-1vx-Fe1C1P6	-2041.3248174	0.04
4	01b-PentaCapTriPri-Fe1P1C6	-2041.3248046	0.05
5	03a-TricapCubeB-Fe3C2P2	-2041.3248036	0.05
6	03b-TricapCubeB-Fe3P4C2	-2041.3247964	0.05
7	03b-TricapCubeB-Fe1P1C8	-2041.3247857	0.06
8	02b-TricapCubeA-Fe3P3C2	-2041.3247800	0.07
9	01a-PentaCapTriPri-Fe1C1P6_r-11	-2041.3247708	0.07
10	02b-TricapCubeA-Fe2P1C6	-2041.3247674	0.07
11	01a-PentaCapTriPri-Fe1C1P6_i-11	-2041.3247601	0.08
12	04a-Icos-1vx-Fe2C1P4	-2041.3247493	0.08
13	03a-TricapCubeB-Fe4C4P2	-2041.3247353	0.09
14	03a-TricapCubeB-Fe3C1P8	-2041.3247349	0.09
15	02a-TricapCubeA-Fe1C1P5	-2041.3247336	0.09
16	04b-Icos-1vx-Fe5P2C5	-2041.3247288	0.10
17	01a-PentaCapTriPri-Fe1C2P5	-2041.3247219	0.10
18	02a-TricapCubeA-Fe2C3P1	-2041.3247178	0.10
19	03a-TricapCubeB-Fe1C1P8	-2041.3247060	0.11
20	04b-Icos-1vx-Fe1P1C6	-2041.3246925	0.12
21	02a-TricapCubeA-Fe3C3P7	-2041.3246784	0.13
22	04b-Icos-1vx-Fe3P1C5_r-10	-2041.3246759	0.13
23	02a-TricapCubeA-Fe2C1P4	-2041.3246731	0.13
24	04b-Icos-1vx-Fe5P1C7	-2041.3246670	0.14
25	04b-Icos-1vx-Fe2P1C3	-2041.3246658	0.14
26	04b-Icos-1vx-Fe3P1C5_i-10	-2041.3246572	0.14
27	02b-TricapCubeA-Fe4P3C1	-2041.3246397	0.15
28	03a-TricapCubeB-Fe4C1P8	-2041.3246357	0.16
29	02a-TricapCubeA-Fe4C3P1	-2041.3246346	0.16
30	04a-Icos-1vx-Fe3C1P5	-2041.3246332	0.16
31	03a-TricapCubeB-Fe4C2P6	-2041.3246318	0.16
32	02b-TricapCubeA-Fe1P1C5_r-24	-2041.3246195	0.17
33	02b-TricapCubeA-Fe1P1C5_i-24	-2041.3246002	0.18
34	03b-TricapCubeB-Fe4P4C2	-2041.3244615	0.26
35	04a-Icos-1vx-Fe3C1P4	-2041.3233174	0.98
36	04b-Icos-1vx-Fe5P1C5	-2041.3232897	1.00
37	02a-TricapCubeA-Fe1C1P9	-2041.3232868	1.00
38	02b-TricapCubeA-Fe3P8C1	-2041.3232817	1.01
39	01b-PentaCapTriPri-Fe1P1C8	-2041.3232682	1.01

40	04a-Icos-1vx-Fe3C2P4	-2041.3232625	1.02
41	02b-TricapCubeA-Fe1P1C1	-2041.3232609	1.02
42	02b-TricapCubeA-Fe4P1C1	-2041.3232571	1.02
43	04a-Icos-1vx-Fe3C6P1	-2041.3232533	1.02
44	01b-PentaCapTriPri-Fe1P2C5_r-11	-2041.3232494	1.03
45	01b-PentaCapTriPri-Fe1P2C4	-2041.3232437	1.03
46	03b-TricapCubeB-Fe1P3C6	-2041.3232406	1.03
47	04a-Icos-1vx-Fe5C2P4	-2041.3232363	1.03
48	02b-TricapCubeA-Fe3P1C9	-2041.3232351	1.03
49	03a-TricapCubeB-Fe3C4P2	-2041.3232260	1.04
50	04a-Icos-1vx-Fe1C3P7	-2041.3232216	1.04
51	04b-Icos-1vx-Fe2P4C1	-2041.3232197	1.04
52	02b-TricapCubeA-Fe4P4C3	-2041.3232160	1.05
53	04a-Icos-1vx-Fe5C1P1	-2041.3232105	1.05
54	02b-TricapCubeA-Fe3P1C7_r-43	-2041.3232030	1.05
55	04b-Icos-1vx-Fe3P1C6	-2041.3231961	1.06
56	03a-TricapCubeB-Fe1C1P7	-2041.3231946	1.06
57	03b-TricapCubeB-Fe1P3C1	-2041.3231898	1.06
58	04b-Icos-1vx-Fe4P1C2	-2041.3231890	1.06
59	03a-TricapCubeB-Fe3C2P4	-2041.3231865	1.06
60	02a-TricapCubeA-Fe1C2P2	-2041.3231827	1.07
61	02b-TricapCubeA-Fe4P2C2	-2041.3231766	1.07
62	01a-PentaCapTriPri-Fe2C5P4	-2041.3231665	1.08
63	04a-Icos-1vx-Fe1C1P5	-2041.3231514	1.09
64	04b-Icos-1vx-Fe2P2C3	-2041.3231442	1.09
65	03a-TricapCubeB-Fe3C1P5	-2041.3230463	1.15
66	01b-PentaCapTriPri-Fe1P2C5_i-11	-2041.3229776	1.20
67	02a-TricapCubeA-Fe4C8P1	-2041.3082073	10.46
68	02b-TricapCubeA-Fe2P3C7	-2041.3081981	10.47
69	02a-TricapCubeA-Fe2C5P1	-2041.3081733	10.49
70	03a-TricapCubeB-Fe4C4P3	-2041.3081659	10.49
71	01a-PentaCapTriPri-Fe1C2P3	-2041.3081599	10.49
72	02b-TricapCubeA-Fe3P4C5	-2041.3081517	10.50
73	04b-Icos-1vx-Fe3P7C2	-2041.3081322	10.51
74	03a-TricapCubeB-Fe3C2P3	-2041.3081283	10.51
75	04a-Icos-1vx-Fe3C5P4	-2041.3081267	10.52
76	04a-Icos-1vx-Fe4C1P6	-2041.3081207	10.52
77	04b-Icos-1vx-Fe5P1C4	-2041.3081190	10.52
78	02a-TricapCubeA-Fe4C4P6	-2041.3081179	10.52
79	03b-TricapCubeB-Fe2P4C3	-2041.3081125	10.52
80	02b-TricapCubeA-Fe3P1C3	-2041.3081118	10.52
81	02b-TricapCubeA-Fe4P6C2	-2041.3081017	10.53

82	03a-TricapCubeB-Fe3C5P1	-2041.3080998	10.53
83	02a-TricapCubeA-Fe3C6P2	-2041.3080987	10.53
84	03a-TricapCubeB-Fe2C5P2	-2041.3080961	10.53
85	04b-Icos-1vx-Fe4P4C3	-2041.3080959	10.53
86	04b-Icos-1vx-Fe3P6C3	-2041.3080936	10.54
87	03b-TricapCubeB-Fe1P5C2	-2041.3080916	10.54
88	01a-PentaCapTriPri-Fe2C4P3	-2041.3080892	10.54
89	03b-TricapCubeB-Fe3P2C5	-2041.3071968	11.10
90	02b-TricapCubeA-Fe1P3C7	-2041.3071966	11.10
91	02a-TricapCubeA-Fe4C4P3	-2041.3071835	11.11
92	03a-TricapCubeB-Fe4C2P7	-2041.3071783	11.11
93	04b-Icos-1vx-Fe3P4C2	-2041.3071756	11.11
94	04b-Icos-1vx-Fe5P4C4	-2041.3071694	11.12
95	03b-TricapCubeB-Fe3P1C5	-2041.3071651	11.12
96	03b-TricapCubeB-Fe4P3C3	-2041.3071624	11.12
97	04a-Icos-1vx-Fe5C3P4	-2041.3071617	11.12
98	02a-TricapCubeA-Fe4C2P2	-2041.3071606	11.12
99	02b-TricapCubeA-Fe4P6C3	-2041.3071605	11.12
100	04a-Icos-1vx-Fe5C1P9	-2041.3071440	11.13
101	03a-TricapCubeB-Fe4C2P2	-2041.3071399	11.13
102	04b-Icos-1vx-Fe4P1C4	-2041.3071382	11.14
103	04b-Icos-1vx-Fe5P2C3	-2041.3071065	11.16
104	03a-TricapCubeB-Fe1C3P1	-2041.3071063	11.16
105	02b-TricapCubeA-Fe1P1C8	-2041.3071057	11.16
106	03a-TricapCubeB-Fe4C1P4	-2041.3070902	11.17
107	04b-Icos-1vx-Fe5P2C7	-2041.3070774	11.17
108	04a-Icos-1vx-Fe3C5P5	-2041.3070747	11.18
109	02a-TricapCubeA-Fe3C7P2	-2041.3070711	11.18
110	03b-TricapCubeB-Fe3P3C1	-2041.3070414	11.20
111	03b-TricapCubeB-Fe4P2C3	-2041.3056179	12.09
112	04a-Icos-1vx-Fe3C3P5	-2041.3056088	12.10
113	02a-TricapCubeA-Fe4C2P7	-2041.3056032	12.10
114	02b-TricapCubeA-Fe4P2C7	-2041.3055931	12.11
115	02a-TricapCubeA-Fe2C4P1	-2041.3055887	12.11
116	03a-TricapCubeB-Fe3C1P7	-2041.3055845	12.11
117	03a-TricapCubeB-Fe3C3P5	-2041.3055663	12.12
118	02b-TricapCubeA-Fe3P5C5	-2041.3055655	12.12
119	04a-Icos-1vx-Fe5C3P6	-2041.3055628	12.12
120	03a-TricapCubeB-Fe2C2P8	-2041.3055623	12.12
121	02b-TricapCubeA-Fe2P2C5	-2041.3055556	12.13
122	03a-TricapCubeB-Fe2C2P4	-2041.3055532	12.13
123	04b-Icos-1vx-Fe3P4C6	-2041.3055531	12.13

124	04a-Icos-1vx-Fe4C2P3	-2041.3055516	12.13
125	03b-TricapCubeB-Fe2P2C8	-2041.3055453	12.14
126	02a-TricapCubeA-Fe1C2P3	-2041.3055439	12.14
127	03b-TricapCubeB-Fe3P1C6	-2041.3055365	12.14
128	02b-TricapCubeA-Fe1P2C3	-2041.3055343	12.14
129	04a-Icos-1vx-Fe2C1P5	-2041.3055303	12.14
130	02b-TricapCubeA-Fe4P7C1	-2041.3055279	12.15
131	02a-TricapCubeA-Fe2C2P5	-2041.3055212	12.15
132	04b-Icos-1vx-Fe1P2C3	-2041.3055200	12.15
133	01b-PentaCapTriPri-Fe2P5C4	-2041.3055181	12.15
134	02a-TricapCubeA-Fe2C2P2	-2041.3055154	12.15
135	02a-TricapCubeA-Fe4C5P5	-2041.3055074	12.16
136	02b-TricapCubeA-Fe2P2C2	-2041.3055060	12.16
137	03a-TricapCubeB-Fe3C1P6	-2041.3055051	12.16
138	04b-Icos-1vx-Fe3P3C2	-2041.3055015	12.16
139	04b-Icos-1vx-Fe4P2C3	-2041.3055009	12.16
140	04b-Icos-1vx-Fe5P3C6	-2041.3054991	12.16
141	02a-TricapCubeA-Fe1C3P4	-2041.3054916	12.17
142	04a-Icos-1vx-Fe3C4P6	-2041.3054873	12.17
143	02b-TricapCubeA-Fe1P3C4	-2041.3054720	12.18
144	02b-TricapCubeA-Fe2P1C7	-2041.3054653	12.19
145	03a-TricapCubeB-Fe4C1P5	-2041.3054615	12.19
146	03b-TricapCubeB-Fe4P1C5	-2041.3054537	12.19
147	02a-TricapCubeA-Fe1C1P1	-2041.3054508	12.19
148	04b-Icos-1vx-Fe5P2C4	-2041.3054420	12.20
149	04b-Icos-1vx-Fe2P2C2	-2041.3054268	12.21
150	04b-Icos-1vx-Fe5P1C1	-2041.3054256	12.21
151	04b-Icos-1vx-Fe3P1C4	-2041.3054253	12.21
152	02b-TricapCubeA-Fe2P1C5	-2041.3054090	12.22
153	03b-TricapCubeB-Fe1P1C7	-2041.3054086	12.22
154	01a-PentaCapTriPri-Fe1C1P8	-2041.3054025	12.22
155	02a-TricapCubeA-Fe3C1P7	-2041.3053941	12.23
156	04b-Icos-1vx-Fe3P6C1	-2041.3053929	12.23
157	01a-PentaCapTriPri-Fe1C2P4	-2041.3053923	12.23
158	04a-Icos-1vx-Fe2C2P3	-2041.3052896	12.30
159	02b-TricapCubeA-Fe3P3C4	-2041.3014044	14.73
160	01b-PentaCapTriPri-Fe2P2C1	-2041.3013389	14.77
161	03b-TricapCubeB-Fe3P1C9	-2041.3013377	14.78
162	03a-TricapCubeB-Fe4C5P1	-2041.3013374	14.78
163	03b-TricapCubeB-Fe4P2C8	-2041.3013225	14.79
164	01b-PentaCapTriPri-Fe1P1C4	-2041.3013129	14.79
165	03b-TricapCubeB-Fe4P3C5	-2041.3012975	14.80

166	04b-Icos-1vx-Fe1P2C5	-2041.3012951	14.80
167	04b-Icos-1vx-Fe4P3C2	-2041.3012940	14.80
168	04a-Icos-1vx-Fe2C4P1	-2041.3012812	14.81
169	02a-TricapCubeA-Fe3C4P1	-2041.3012736	14.82
170	04a-Icos-1vx-Fe1C1P3	-2041.3012610	14.82
171	04a-Icos-1vx-Fe3C1P9	-2041.3012564	14.83
172	04b-Icos-1vx-Fe5P2C6	-2041.3012280	14.84
173	02a-TricapCubeA-Fe4C1P1	-2041.3012236	14.85
174	03b-TricapCubeB-Fe4P1C7	-2041.3012233	14.85
175	04a-Icos-1vx-Fe3C1P6	-2041.3012232	14.85
176	03a-TricapCubeB-Fe2C1P8	-2041.3012140	14.85
177	03a-TricapCubeB-Fe4C1P7	-2041.3012130	14.85
178	04a-Icos-1vx-Fe5C2P6	-2041.3012068	14.86
179	04b-Icos-1vx-Fe1P1C5	-2041.3011944	14.87
180	02b-TricapCubeA-Fe1P1C9	-2041.3011919	14.87
181	04b-Icos-1vx-Fe1P3C7	-2041.3011754	14.88
182	04a-Icos-1vx-Fe1C3P2	-2041.3007289	15.16
183	03a-TricapCubeB-Fe1C4P1	-2041.3007184	15.16
184	03a-TricapCubeB-Fe1C3P5	-2041.3006879	15.18
185	04b-Icos-1vx-Fe3P2C3	-2041.3006712	15.19
186	04a-Icos-1vx-Fe3C4P3	-2041.3006692	15.20
187	02b-TricapCubeA-Fe4P1C6	-2041.3006661	15.20
188	04a-Icos-1vx-Fe3C2P3	-2041.3006566	15.20
189	04b-Icos-1vx-Fe1P3C2	-2041.3006274	15.22
190	03a-TricapCubeB-Fe1C3P7	-2041.2988639	16.33
191	03b-TricapCubeB-Fe2P3C7	-2041.2988328	16.35
192	03b-TricapCubeB-Fe1P4C1	-2041.2988003	16.37
193	02b-TricapCubeA-Fe3P1C8	-2041.2987878	16.38
194	03b-TricapCubeB-Fe2P2C7	-2041.2987701	16.39
195	04b-Icos-1vx-Fe3P4C3	-2041.2987670	16.39
196	02a-TricapCubeA-Fe4C4P1	-2041.2986894	16.44
197	03b-TricapCubeB-Fe2P4C2	-2041.2986708	16.45
198	04b-Icos-1vx-Fe4P3C5	-2041.2984225	16.60
199	04b-Icos-1vx-Fe4P1C8	-2041.2983895	16.63
200	01a-PentaCapTriPri-Fe2C1P4	-2041.2983708	16.64
201	03a-TricapCubeB-Fe2C4P1	-2041.2983704	16.64
202	02a-TricapCubeA-Fe4C4P4	-2041.2983642	16.64
203	02b-TricapCubeA-Fe2P1C1	-2041.2983631	16.64
204	04a-Icos-1vx-Fe4C3P1	-2041.2983566	16.65
205	03a-TricapCubeB-Fe2C3P5	-2041.2983539	16.65
206	03b-TricapCubeB-Fe1P3C5	-2041.2983425	16.66
207	03b-TricapCubeB-Fe4P1C9	-2041.2983395	16.66

208	02a-TricapCubeA-Fe4C1P6	-2041.2983388	16.66
209	04a-Icos-1vx-Fe5C4P3	-2041.2983352	16.66
210	02b-TricapCubeA-Fe1P1C6	-2041.2983235	16.67
211	03b-TricapCubeB-Fe3P3C6	-2041.2983165	16.67
212	04b-Icos-1vx-Fe5P2C8	-2041.2982996	16.68
213	03b-TricapCubeB-Fe3P2C8	-2041.2982793	16.69
214	04a-Icos-1vx-Fe5C3P5	-2041.2982790	16.69
215	02a-TricapCubeA-Fe4C3P5	-2041.2982630	16.70
216	02b-TricapCubeA-Fe1P3C6	-2041.2982420	16.72
217	02a-TricapCubeA-Fe3C3P4	-2041.2954866	18.45
218	03b-TricapCubeB-Fe3P5C1	-2041.2954304	18.48
219	04b-Icos-1vx-Fe1P1C3	-2041.2954219	18.49
220	04a-Icos-1vx-Fe3C3P3	-2041.2954094	18.50
221	02b-TricapCubeA-Fe4P4C1	-2041.2954009	18.50
222	02b-TricapCubeA-Fe4P3C5	-2041.2954004	18.50
223	03b-TricapCubeB-Fe4P5C1	-2041.2953725	18.52
224	04a-Icos-1vx-Fe1C2P5	-2041.2952742	18.58
225	03b-TricapCubeB-Fe4P4C3	-2041.2952046	18.62
226	03a-TricapCubeB-Fe2C2P3	-2041.2949631	18.78
227	03b-TricapCubeB-Fe4P2C7	-2041.2949370	18.79
228	03a-TricapCubeB-Fe2C2P6	-2041.2949165	18.80
229	03a-TricapCubeB-Fe2C1P5	-2041.2949057	18.81
230	04b-Icos-1vx-Fe4P3C7	-2041.2948667	18.84
231	02b-TricapCubeA-Fe4P2C5	-2041.2948404	18.85
232	04b-Icos-1vx-Fe4P2C7	-2041.2948144	18.87
233	02a-TricapCubeA-Fe4C1P5	-2041.2948098	18.87
234	04a-Icos-1vx-Fe3C2P2	-2041.2947987	18.88
235	02a-TricapCubeA-Fe3C7P1	-2041.2947939	18.88
236	03b-TricapCubeB-Fe2P1C9	-2041.2947775	18.89
237	02a-TricapCubeA-Fe4C6P3	-2041.2941725	19.27
238	02b-TricapCubeA-Fe4P1C8	-2041.2941487	19.29
239	04a-Icos-1vx-Fe2C3P1	-2041.2941480	19.29
240	04a-Icos-1vx-Fe3C4P2	-2041.2941480	19.29
241	04a-Icos-1vx-Fe4C2P2	-2041.2941480	19.29
242	04b-Icos-1vx-Fe5P1C9	-2041.2941361	19.29
243	02a-TricapCubeA-Fe2C3P2	-2041.2941275	19.30
244	02a-TricapCubeA-Fe2C1P3	-2041.2941247	19.30
245	04a-Icos-1vx-Fe4C1P4	-2041.2941239	19.30
246	04b-Icos-1vx-Fe3P5C5	-2041.2941132	19.31
247	02a-TricapCubeA-Fe4C1P9	-2041.2940852	19.33
248	04b-Icos-1vx-Fe2P2C1	-2041.2940816	19.33
249	04b-Icos-1vx-Fe4P1C5	-2041.2940494	19.35

250	04b-Icos-1vx-Fe1P1C2	-2041.2926432	20.23
251	01a-PentaCapTriPri-Fe2C4P5	-2041.2926005	20.26
252	04a-Icos-1vx-Fe2C3P2	-2041.2925917	20.26
253	03b-TricapCubeB-Fe4P3C1	-2041.2925854	20.27
254	04a-Icos-1vx-Fe3C1P7	-2041.2925662	20.28
255	03b-TricapCubeB-Fe3P1C7	-2041.2913157	21.06
256	04a-Icos-1vx-Fe5C3P3	-2041.2912962	21.08
257	04b-Icos-1vx-Fe3P2C8	-2041.2911923	21.14
258	02a-TricapCubeA-Fe4C3P7	-2041.2883419	22.93
259	04b-Icos-1vx-Fe3P1C8	-2041.2883225	22.94
260	02b-TricapCubeA-Fe4P4C6	-2041.2883014	22.96
261	03a-TricapCubeB-Fe4C3P3	-2041.2882999	22.96
262	04a-Icos-1vx-Fe1C1P2	-2041.2882981	22.96
263	04b-Icos-1vx-Fe2P5C1	-2041.2882864	22.97
264	03b-TricapCubeB-Fe1P1C4	-2041.2882823	22.97
265	04b-Icos-1vx-Fe2P3C2_r-34	-2041.2882557	22.98
266	04b-Icos-1vx-Fe3P1C7	-2041.2882279	23.00
267	04a-Icos-1vx-Fe3C6P2	-2041.2882181	23.01
268	04b-Icos-1vx-Fe2P3C5_r-13	-2041.2882001	23.02
269	04b-Icos-1vx-Fe2P3C2_i-34	-2041.2875608	23.42
270	02a-TricapCubeA-Fe2C3P7	-2041.2873151	23.57
271	04b-Icos-1vx-Fe3P5C4	-2041.2873003	23.58
272	03a-TricapCubeB-Fe3C3P3	-2041.2872754	23.60
273	01a-PentaCapTriPri-Fe1C3P2	-2041.2872722	23.60
274	04a-Icos-1vx-Fe3C6P3	-2041.2872494	23.62
275	04b-Icos-1vx-Fe2P1C6	-2041.2872430	23.62
276	02b-TricapCubeA-Fe4P4C4	-2041.2872429	23.62
277	04a-Icos-1vx-Fe5C1P4	-2041.2872360	23.62
278	01b-PentaCapTriPri-Fe1P1C9	-2041.2872276	23.63
279	02b-TricapCubeA-Fe3P6C2	-2041.2872169	23.64
280	01b-PentaCapTriPri-Fe1P2C3	-2041.2872080	23.64
281	03a-TricapCubeB-Fe1C1P6	-2041.2872077	23.64
282	01a-PentaCapTriPri-Fe1C3P4	-2041.2871929	23.65
283	02a-TricapCubeA-Fe2C1P9	-2041.2871928	23.65
284	04a-Icos-1vx-Fe4C4P3	-2041.2871813	23.66
285	01b-PentaCapTriPri-Fe1P1C3	-2041.2868926	23.84
286	04a-Icos-1vx-Fe1C2P1	-2041.2868792	23.85
287	02a-TricapCubeA-Fe1C2P1_r-15	-2041.2868508	23.87
288	02b-TricapCubeA-Fe2P3C3	-2041.2868126	23.89
289	02a-TricapCubeA-Fe3C5P4	-2041.2866959	23.96
290	04b-Icos-1vx-Fe1P3C1	-2041.2857950	24.53
291	02b-TricapCubeA-Fe3P7C1	-2041.2857537	24.55

292	04a-Icos-1vx-Fe3C5P2	-2041.2857210	24.58
293	02a-TricapCubeA-Fe3C2P6	-2041.2857035	24.59
294	04a-Icos-1vx-Fe1C3P1	-2041.2856971	24.59
295	02a-TricapCubeA-Fe2C3P6	-2041.2856960	24.59
296	04a-Icos-1vx-Fe2C2P2	-2041.2856921	24.59
297	01b-PentaCapTriPri-Fe1P3C2	-2041.2856910	24.59
298	03a-TricapCubeB-Fe3C2P6	-2041.2856706	24.61
299	02b-TricapCubeA-Fe4P1C5	-2041.2856677	24.61
300	04a-Icos-1vx-Fe3C3P2	-2041.2856541	24.62
301	03a-TricapCubeB-Fe4C2P3	-2041.2856440	24.62
302	02a-TricapCubeA-Fe4C7P1	-2041.2856188	24.64
303	04a-Icos-1vx-Fe1C2P3	-2041.2856117	24.64
304	01a-PentaCapTriPri-Fe1C1P9	-2041.2856046	24.65
305	02a-TricapCubeA-Fe3C5P5	-2041.2855992	24.65
306	03a-TricapCubeB-Fe1C2P2	-2041.2855983	24.65
307	03b-TricapCubeB-Fe2P1C8	-2041.2855977	24.65
308	04b-Icos-1vx-Fe4P3C1	-2041.2855790	24.66
309	03b-TricapCubeB-Fe2P4C1	-2041.2855761	24.67
310	04a-Icos-1vx-Fe4C1P8	-2041.2855535	24.68
311	02a-TricapCubeA-Fe2C1P1	-2041.2855441	24.69
312	04a-Icos-1vx-Fe4C3P5	-2041.2855005	24.71
313	02a-TricapCubeA-Fe2C3P4	-2041.2854951	24.72
314	02b-TricapCubeA-Fe4P3C7	-2041.2854642	24.74
315	02b-TricapCubeA-Fe2P3C4	-2041.2854239	24.76
316	03b-TricapCubeB-Fe3P2C7	-2041.2854207	24.76
317	04a-Icos-1vx-Fe3C1P8	-2041.2854037	24.77
318	04b-Icos-1vx-Fe2P1C7	-2041.2853867	24.79
319	04a-Icos-1vx-Fe2C1P7	-2041.2853859	24.79
320	02b-TricapCubeA-Fe2P1C4	-2041.2853810	24.79
321	02b-TricapCubeA-Fe3P4C1	-2041.2853611	24.80
322	04a-Icos-1vx-Fe1C3P6	-2041.2851402	24.94
323	04b-Icos-1vx-Fe5P5C1	-2041.2844958	25.34
324	03a-TricapCubeB-Fe1C1P4	-2041.2844798	25.35
325	03a-TricapCubeB-Fe1C3P3	-2041.2844391	25.38
326	02a-TricapCubeA-Fe3C6P1	-2041.2844366	25.38
327	04b-Icos-1vx-Fe3P2C7	-2041.2844262	25.39
328	04a-Icos-1vx-Fe1C4P2	-2041.2844036	25.40
329	04a-Icos-1vx-Fe4C3P4	-2041.2844028	25.40
330	04a-Icos-1vx-Fe1C3P3	-2041.2842949	25.47
331	04a-Icos-1vx-Fe3C5P3	-2041.2842905	25.47
332	04a-Icos-1vx-Fe2C2P7	-2041.2842823	25.48
333	03b-TricapCubeB-Fe1P1C6	-2041.2842317	25.51

334	02b-TricapCubeA-Fe2P4C2	-2041.2842253	25.51
335	04b-Icos-1vx-Fe2P3C3	-2041.2842222	25.52
336	04b-Icos-1vx-Fe3P4C4	-2041.2842211	25.52
337	04a-Icos-1vx-Fe2C3P7	-2041.2842109	25.52
338	04b-Icos-1vx-Fe4P4C2	-2041.2838553	25.75
339	04b-Icos-1vx-Fe4P1C9	-2041.2838088	25.78
340	03a-TricapCubeB-Fe1C2P7	-2041.2837548	25.81
341	04b-Icos-1vx-Fe4P2C6	-2041.2837399	25.82
342	02a-TricapCubeA-Fe3C1P9	-2041.2836650	25.87
343	04b-Icos-1vx-Fe4P1C7	-2041.2831229	26.21
344	03a-TricapCubeB-Fe1C1P5	-2041.2831033	26.22
345	04b-Icos-1vx-Fe3P5C2	-2041.2830627	26.24
346	03b-TricapCubeB-Fe3P1C8	-2041.2830311	26.26
347	02b-TricapCubeA-Fe3P1C6	-2041.2830261	26.27
348	03b-TricapCubeB-Fe2P3C6	-2041.2830203	26.27
349	03b-TricapCubeB-Fe1P1C5	-2041.2830185	26.27
350	04a-Icos-1vx-Fe4C1P7	-2041.2829929	26.29
351	01a-PentaCapTriPri-Fe2C5P1	-2041.2829916	26.29
352	01b-PentaCapTriPri-Fe2P5C5	-2041.2829914	26.29
353	01a-PentaCapTriPri-Fe2C4P4	-2041.2829828	26.29
354	02a-TricapCubeA-Fe4C1P7	-2041.2829816	26.29
355	01a-PentaCapTriPri-Fe2C4P2	-2041.2829599	26.31
356	03a-TricapCubeB-Fe1C1P9	-2041.2829569	26.31
357	02a-TricapCubeA-Fe3C8P2	-2041.2829569	26.31
358	02b-TricapCubeA-Fe4P5C1	-2041.2829403	26.32
359	03a-TricapCubeB-Fe1C2P6	-2041.2828908	26.35
360	03a-TricapCubeB-Fe4C1P1	-2041.2819970	26.91
361	04b-Icos-1vx-Fe4P2C2	-2041.2818581	27.00
362	02a-TricapCubeA-Fe2C2P4	-2041.2818260	27.02
363	04a-Icos-1vx-Fe4C1P5	-2041.2817512	27.07
364	02b-TricapCubeA-Fe2P1C3	-2041.2817325	27.08
365	02b-TricapCubeA-Fe2P3C2	-2041.2817148	27.09
366	04a-Icos-1vx-Fe5C1P5	-2041.2816177	27.15
367	04b-Icos-1vx-Fe3P2C4	-2041.2815604	27.19
368	02b-TricapCubeA-Fe3P9C1	-2041.2814549	27.25
369	04b-Icos-1vx-Fe1P2C1	-2041.2814218	27.27
370	02a-TricapCubeA-Fe4C1P4	-2041.2814180	27.28
371	03b-TricapCubeB-Fe4P1C4	-2041.2813951	27.29
372	01a-PentaCapTriPri-Fe1C1P3	-2041.2813631	27.31
373	03a-TricapCubeB-Fe3C3P2	-2041.2807866	27.67
374	04a-Icos-1vx-Fe3C8P1	-2041.2807439	27.70
375	03a-TricapCubeB-Fe3C3P7	-2041.2807405	27.70

376	02b-TricapCubeA-Fe1P3C2	-2041.2807354	27.70
377	04b-Icos-1vx-Fe4P6C1	-2041.2807246	27.71
378	04b-Icos-1vx-Fe5P4C1	-2041.2807203	27.71
379	02a-TricapCubeA-Fe3C2P7	-2041.2807120	27.72
380	03b-TricapCubeB-Fe3P3C7	-2041.2807089	27.72
381	04a-Icos-1vx-Fe5C3P7	-2041.2806985	27.73
382	02b-TricapCubeA-Fe3P2C7	-2041.2806967	27.73
383	02b-TricapCubeA-Fe4P5C3	-2041.2806941	27.73
384	03a-TricapCubeB-Fe4C5P2	-2041.2806897	27.73
385	03b-TricapCubeB-Fe4P3C6	-2041.2806838	27.74
386	03a-TricapCubeB-Fe4C2P8	-2041.2806834	27.74
387	04a-Icos-1vx-Fe4C2P8	-2041.2806768	27.74
388	02a-TricapCubeA-Fe4C5P4	-2041.2806750	27.74
389	02b-TricapCubeA-Fe3P6C3	-2041.2806745	27.74
390	04a-Icos-1vx-Fe3C4P4	-2041.2806740	27.74
391	04a-Icos-1vx-Fe5C4P1	-2041.2806727	27.74
392	02b-TricapCubeA-Fe4P2C8	-2041.2806648	27.75
393	04a-Icos-1vx-Fe5C4P6	-2041.2806646	27.75
394	04b-Icos-1vx-Fe3P3C7	-2041.2806626	27.75
395	02a-TricapCubeA-Fe3C6P4	-2041.2806610	27.75
396	03a-TricapCubeB-Fe3C1P9	-2041.2805971	27.79
397	02a-TricapCubeA-Fe2C4P3	-2041.2805789	27.80
398	03a-TricapCubeB-Fe4C3P6	-2041.2803251	27.96
399	04b-Icos-1vx-Fe5P1C8	-2041.2803121	27.97
400	04b-Icos-1vx-Fe3P3C3	-2041.2802914	27.98
401	04a-Icos-1vx-Fe5C2P5	-2041.2800741	28.12
402	04a-Icos-1vx-Fe5C1P7	-2041.2799884	28.17
403	03b-TricapCubeB-Fe3P2C2	-2041.2799508	28.20
404	03b-TricapCubeB-Fe1P2C3	-2041.2795986	28.42
405	02a-TricapCubeA-Fe3C9P1	-2041.2795858	28.43
406	02a-TricapCubeA-Fe4C3P6	-2041.2792467	28.64
407	04a-Icos-1vx-Fe3C1P2	-2041.2792302	28.65
408	04b-Icos-1vx-Fe5P2C2	-2041.2791790	28.68
409	02b-TricapCubeA-Fe1P1C4	-2041.2784549	29.13
410	04a-Icos-1vx-Fe3C1P3	-2041.2784457	29.14
411	02a-TricapCubeA-Fe3C2P3	-2041.2784297	29.15
412	04b-Icos-1vx-Fe5P2C1	-2041.2784241	29.15
413	03b-TricapCubeB-Fe3P1C1	-2041.2784039	29.17
414	04b-Icos-1vx-Fe4P2C1	-2041.2783839	29.18
415	01b-PentaCapTriPri-Fe1P1C1	-2041.2783822	29.18
416	04b-Icos-1vx-Fe3P7C3	-2041.2783786	29.18
417	03a-TricapCubeB-Fe4C2P4	-2041.2783748	29.19

418	03b-TricapCubeB-Fe3P2C1	-2041.2783691	29.19
419	02b-TricapCubeA-Fe1P1C3	-2041.2783668	29.19
420	02b-TricapCubeA-Fe3P3C6	-2041.2783595	29.19
421	02a-TricapCubeA-Fe4C1P8	-2041.2783278	29.21
422	04b-Icos-1vx-Fe1P3C5	-2041.2783087	29.23
423	04a-Icos-1vx-Fe3C2P5	-2041.2782799	29.24
424	03b-TricapCubeB-Fe4P1C1	-2041.2782782	29.25
425	04b-Icos-1vx-Fe4P4C1	-2041.2782649	29.25
426	01b-PentaCapTriPri-Fe1P1C7	-2041.2782533	29.26
427	03a-TricapCubeB-Fe1C1P2	-2041.2782527	29.26
428	04a-Icos-1vx-Fe2C2P4	-2041.2782501	29.26
429	03b-TricapCubeB-Fe1P1C3	-2041.2782456	29.27
430	02b-TricapCubeA-Fe4P1C2	-2041.2782453	29.27
431	04b-Icos-1vx-Fe4P1C1	-2041.2782437	29.27
432	02a-TricapCubeA-Fe2C2P3	-2041.2782388	29.27
433	02a-TricapCubeA-Fe4C9P1	-2041.2782287	29.28
434	04b-Icos-1vx-Fe3P7C1	-2041.2782202	29.28
435	01a-PentaCapTriPri-Fe1C1P7	-2041.2782188	29.28
436	04a-Icos-1vx-Fe3C4P1	-2041.2782130	29.29
437	02a-TricapCubeA-Fe4C1P2	-2041.2782065	29.29
438	03b-TricapCubeB-Fe3P2C4	-2041.2782053	29.29
439	04b-Icos-1vx-Fe3P2C5	-2041.2781998	29.30
440	04b-Icos-1vx-Fe4P3C3	-2041.2781967	29.30
441	02b-TricapCubeA-Fe3P4C6	-2041.2781955	29.30
442	04a-Icos-1vx-Fe1C3P5	-2041.2781905	29.30
443	01b-PentaCapTriPri-Fe2P3C3	-2041.2781731	29.31
444	03b-TricapCubeB-Fe1P5C1	-2041.2781655	29.32
445	04a-Icos-1vx-Fe4C3P3	-2041.2781564	29.32
446	02b-TricapCubeA-Fe2P1C2	-2041.2781169	29.35
447	04b-Icos-1vx-Fe2P2C6	-2041.2780579	29.38
448	04b-Icos-1vx-Fe2P1C9	-2041.2779827	29.43
449	04a-Icos-1vx-Fe1C1P4	-2041.2775967	29.67
450	02b-TricapCubeA-Fe4P4C2	-2041.2775794	29.68
451	03b-TricapCubeB-Fe4P2C4	-2041.2775669	29.69
452	02a-TricapCubeA-Fe3C3P6	-2041.2775663	29.69
453	02b-TricapCubeA-Fe4P3C4	-2041.2775464	29.71
454	03b-TricapCubeB-Fe1P3C2	-2041.2775439	29.71
455	03b-TricapCubeB-Fe4P1C3	-2041.2775395	29.71
456	02a-TricapCubeA-Fe1C1P4	-2041.2775362	29.71
457	02a-TricapCubeA-Fe2C3P3	-2041.2775358	29.71
458	04b-Icos-1vx-Fe3P1C1	-2041.2775294	29.72
459	04a-Icos-1vx-Fe2C1P1	-2041.2775218	29.72

460	01a-PentaCapTriPri-Fe2C3P6	-2041.2775212	29.72
461	04b-Icos-1vx-Fe3P1C3	-2041.2775010	29.73
462	02a-TricapCubeA-Fe3C3P1	-2041.2774976	29.74
463	03b-TricapCubeB-Fe3P1C3	-2041.2774951	29.74
464	02b-TricapCubeA-Fe4P1C3	-2041.2774907	29.74
465	03b-TricapCubeB-Fe3P2C6	-2041.2764700	30.38
466	04a-Icos-1vx-Fe2C3P5	-2041.2764551	30.39
467	04a-Icos-1vx-Fe2C1P8	-2041.2763308	30.47
468	03b-TricapCubeB-Fe3P4C3	-2041.2758646	30.76
469	04b-Icos-1vx-Fe2P4C2_r-21	-2041.2757223	30.85
470	01a-PentaCapTriPri-Fe2C3P4	-2041.2755868	30.93
471	04b-Icos-1vx-Fe2P4C2_i-21	-2041.2755767	30.94
472	02a-TricapCubeA-Fe3C1P8	-2041.2755735	30.94
473	01a-PentaCapTriPri-Fe2C5P3	-2041.2754678	31.01
474	02a-TricapCubeA-Fe4C3P3	-2041.2754464	31.02
475	04b-Icos-1vx-Fe5P3C4	-2041.2749800	31.32
476	04b-Icos-1vx-Fe2P1C4	-2041.2740875	31.88
477	02a-TricapCubeA-Fe2C1P2	-2041.2740072	31.93
478	04a-Icos-1vx-Fe4C4P2	-2041.2739916	31.94
479	02b-TricapCubeA-Fe3P8C2	-2041.2739480	31.96
480	02b-TricapCubeA-Fe3P7C2	-2041.2735397	32.22
481	01a-PentaCapTriPri-Fe1C1P2	-2041.2734652	32.27
482	02a-TricapCubeA-Fe4C6P1	-2041.2734401	32.28
483	04a-Icos-1vx-Fe2C5P1	-2041.2730711	32.51
484	04a-Icos-1vx-Fe2C1P6	-2041.2730571	32.52
485	03a-TricapCubeB-Fe4C6P1	-2041.2730109	32.55
486	02b-TricapCubeA-Fe2P1C9	-2041.2729965	32.56
487	04b-Icos-1vx-Fe2P4C3	-2041.2729834	32.57
488	02b-TricapCubeA-Fe3P5C3	-2041.2726888	32.75
489	02b-TricapCubeA-Fe4P7C2	-2041.2726797	32.76
490	01a-PentaCapTriPri-Fe2C2P2	-2041.2726586	32.77
491	01a-PentaCapTriPri-Fe2C4P1	-2041.2719706	33.20
492	01b-PentaCapTriPri-Fe2P4C1	-2041.2719651	33.21
493	02a-TricapCubeA-Fe3C1P5	-2041.2707683	33.96
494	03a-TricapCubeB-Fe2C1P3	-2041.2707655	33.96
495	02a-TricapCubeA-Fe2C1P6	-2041.2707544	33.97
496	02b-TricapCubeA-Fe3P4C2	-2041.2707526	33.97
497	04a-Icos-1vx-Fe4C1P3	-2041.2707073	34.00
498	03a-TricapCubeB-Fe1C3P2	-2041.2707047	34.00
499	03b-TricapCubeB-Fe2P1C2	-2041.2706955	34.00
500	04a-Icos-1vx-Fe4C1P2	-2041.2706933	34.01
501	03b-TricapCubeB-Fe2P1C3	-2041.2706900	34.01

502	03a-TricapCubeB-Fe2C3P2	-2041.2706847	34.01
503	03a-TricapCubeB-Fe2C1P2	-2041.2706777	34.02
504	04b-Icos-1vx-Fe4P1C3	-2041.2706647	34.02
505	04b-Icos-1vx-Fe1P4C1	-2041.2705516	34.09
506	01b-PentaCapTriPri-Fe2P4C4	-2041.2705148	34.12
507	03b-TricapCubeB-Fe2P1C7	-2041.2701746	34.33
508	02a-TricapCubeA-Fe4C4P2	-2041.2701525	34.34
509	03a-TricapCubeB-Fe4C1P3	-2041.2701046	34.37
510	04a-Icos-1vx-Fe3C1P1	-2041.2700522	34.41
511	02b-TricapCubeA-Fe1P2C4	-2041.2698928	34.51
512	03a-TricapCubeB-Fe4C1P9	-2041.2698658	34.52
513	02a-TricapCubeA-Fe1C2P4	-2041.2698651	34.53
514	04b-Icos-1vx-Fe5P3C5	-2041.2698521	34.53
515	03a-TricapCubeB-Fe3C4P3	-2041.2698197	34.55
516	02a-TricapCubeA-Fe1C3P6	-2041.2698141	34.56
517	02a-TricapCubeA-Fe1C1P6	-2041.2698055	34.56
518	04a-Icos-1vx-Fe5C2P8	-2041.2697688	34.59
519	04b-Icos-1vx-Fe3P1C9	-2041.2697652	34.59
520	03a-TricapCubeB-Fe3C5P2	-2041.2696783	34.64
521	04a-Icos-1vx-Fe1C3P4	-2041.2696655	34.65
522	03a-TricapCubeB-Fe4C3P7	-2041.2696641	34.65
523	03b-TricapCubeB-Fe3P3C5	-2041.2696572	34.66
524	02b-TricapCubeA-Fe2P2C1	-2041.2696407	34.67
525	02a-TricapCubeA-Fe2C2P1	-2041.2696354	34.67
526	03b-TricapCubeB-Fe4P3C7	-2041.2696269	34.67
527	04b-Icos-1vx-Fe5P3C7	-2041.2696233	34.68
528	04a-Icos-1vx-Fe4C5P1	-2041.2696110	34.68
529	02a-TricapCubeA-Fe1C3P2	-2041.2695978	34.69
530	02b-TricapCubeA-Fe4P5C4	-2041.2695965	34.69
531	03b-TricapCubeB-Fe4P5C2	-2041.2695931	34.70
532	04a-Icos-1vx-Fe3C3P7	-2041.2695921	34.70
533	01b-PentaCapTriPri-Fe1P4C1	-2041.2695906	34.70
534	02b-TricapCubeA-Fe4P5C5	-2041.2695905	34.70
535	04b-Icos-1vx-Fe5P4C6	-2041.2695900	34.70
536	04b-Icos-1vx-Fe3P3C6	-2041.2695837	34.70
537	01b-PentaCapTriPri-Fe1P1C5	-2041.2695678	34.71
538	04b-Icos-1vx-Fe4P2C8	-2041.2695406	34.73
539	04a-Icos-1vx-Fe3C5P1	-2041.2693657	34.84
540	03b-TricapCubeB-Fe1P1C1	-2041.2693418	34.85
541	04b-Icos-1vx-Fe5P1C6	-2041.2693232	34.87
542	04a-Icos-1vx-Fe5C1P6	-2041.2692800	34.89
543	04a-Icos-1vx-Fe4C1P9	-2041.2691166	34.99

544	02b-TricapCubeA-Fe2P3C5	-2041.2690994	35.01
545	01b-PentaCapTriPri-Fe2P4C2	-2041.2690721	35.02
546	04a-Icos-1vx-Fe4C2P6	-2041.2690368	35.04
547	02a-TricapCubeA-Fe3C1P3	-2041.2686955	35.26
548	03b-TricapCubeB-Fe3P4C1	-2041.2685816	35.33
549	02a-TricapCubeA-Fe4C4P5	-2041.2685680	35.34
550	02a-TricapCubeA-Fe4C2P1	-2041.2685323	35.36
551	02a-TricapCubeA-Fe3C5P2	-2041.2685231	35.37
552	04b-Icos-1vx-Fe1P1C1	-2041.2684741	35.40
553	03a-TricapCubeB-Fe3C2P8	-2041.2679231	35.74
554	03b-TricapCubeB-Fe1P2C7	-2041.2679202	35.75
555	03a-TricapCubeB-Fe4C3P5	-2041.2678999	35.76
556	01a-PentaCapTriPri-Fe1C1P5	-2041.2678898	35.76
557	04a-Icos-1vx-Fe1C1P1	-2041.2678479	35.79
558	03b-TricapCubeB-Fe4P4C1_r-16	-2041.2678469	35.79
559	04b-Icos-1vx-Fe5P1C2	-2041.2677996	35.82
560	04a-Icos-1vx-Fe3C6P4	-2041.2677910	35.83
561	02a-TricapCubeA-Fe2C3P5	-2041.2675305	35.99
562	02b-TricapCubeA-Fe3P4C4	-2041.2674558	36.04
563	01b-PentaCapTriPri-Fe2P1C5	-2041.2673882	36.08
564	03a-TricapCubeB-Fe1C2P3	-2041.2673303	36.12
565	04a-Icos-1vx-Fe4C3P2	-2041.2669041	36.38
566	04b-Icos-1vx-Fe5P3C3	-2041.2668851	36.40
567	04a-Icos-1vx-Fe3C2P8	-2041.2668051	36.45
568	04b-Icos-1vx-Fe3P6C2	-2041.2667027	36.51
569	04a-Icos-1vx-Fe5C1P3	-2041.2666909	36.52
570	02b-TricapCubeA-Fe1P1C7	-2041.2666493	36.54
571	02b-TricapCubeA-Fe1P1C2	-2041.2666441	36.55
572	02b-TricapCubeA-Fe1P3C5	-2041.2666418	36.55
573	02b-TricapCubeA-Fe3P4C3	-2041.2665834	36.58
574	03a-TricapCubeB-Fe3C1P2	-2041.2663810	36.71
575	03b-TricapCubeB-Fe4P2C1	-2041.2663513	36.73
576	02b-TricapCubeA-Fe3P3C1	-2041.2662659	36.78
577	02b-TricapCubeA-Fe2P1C8	-2041.2657657	37.10
578	04b-Icos-1vx-Fe2P1C1	-2041.2657616	37.10
579	04a-Icos-1vx-Fe2C6P1	-2041.2657488	37.11
580	02b-TricapCubeA-Fe4P3C2	-2041.2657324	37.12
581	04b-Icos-1vx-Fe2P3C1	-2041.2657183	37.13
582	02a-TricapCubeA-Fe4C2P4	-2041.2651002	37.52
583	01b-PentaCapTriPri-Fe2P5C1	-2041.2650776	37.53
584	04b-Icos-1vx-Fe3P5C1	-2041.2645946	37.83
585	02a-TricapCubeA-Fe3C5P3	-2041.2643648	37.98

586	04a-Icos-1vx-Fe2C1P2	-2041.2642931	38.02
587	04a-Icos-1vx-Fe5C5P1	-2041.2640205	38.19
588	02b-TricapCubeA-Fe3P6C1	-2041.2639770	38.22
589	04a-Icos-1vx-Fe3C2P7	-2041.2639640	38.23
590	03b-TricapCubeB-Fe1P3C4	-2041.2639533	38.23
591	03b-TricapCubeB-Fe4P4C1_i-16	-2041.2631771	38.72
592	03a-TricapCubeB-Fe3C4P1	-2041.2630320	38.81
593	03b-TricapCubeB-Fe4P1C6	-2041.2626977	39.02
594	04b-Icos-1vx-Fe2P2C5	-2041.2626627	39.04
595	03b-TricapCubeB-Fe3P5C2	-2041.2626570	39.05
596	02b-TricapCubeA-Fe4P8C2	-2041.2626536	39.05
597	01a-PentaCapTriPri-Fe1C2P2	-2041.2626472	39.05
598	02b-TricapCubeA-Fe2P5C1	-2041.2626409	39.06
599	02b-TricapCubeA-Fe3P5C1	-2041.2625748	39.10
600	04a-Icos-1vx-Fe2C4P2	-2041.2624783	39.16
601	04a-Icos-1vx-Fe2C1P9	-2041.2624622	39.17
602	04a-Icos-1vx-Fe2C2P6	-2041.2624151	39.20
603	03b-TricapCubeB-Fe2P3C4	-2041.2620605	39.42
604	04b-Icos-1vx-Fe5P3C2	-2041.2613435	39.87
605	03a-TricapCubeB-Fe4C3P2	-2041.2613171	39.89
606	04b-Icos-1vx-Fe2P3C4	-2041.2612844	39.91
607	02a-TricapCubeA-Fe3C2P2	-2041.2612711	39.92
608	04a-Icos-1vx-Fe5C3P2	-2041.2612612	39.92
609	02a-TricapCubeA-Fe2C2P6	-2041.2612603	39.92
610	04a-Icos-1vx-Fe3C9P1	-2041.2612602	39.92
611	02b-TricapCubeA-Fe1P3C3	-2041.2612548	39.93
612	04b-Icos-1vx-Fe5P4C5	-2041.2612497	39.93
613	03b-TricapCubeB-Fe3P3C4	-2041.2612289	39.94
614	04a-Icos-1vx-Fe3C4P5	-2041.2612288	39.94
615	04a-Icos-1vx-Fe5C4P5	-2041.2612176	39.95
616	02b-TricapCubeA-Fe4P2C6	-2041.2612167	39.95
617	04b-Icos-1vx-Fe4P2C5	-2041.2612053	39.96
618	01b-PentaCapTriPri-Fe1P3C1	-2041.2612038	39.96
619	04b-Icos-1vx-Fe3P3C5	-2041.2611868	39.97
620	03a-TricapCubeB-Fe3C2P5	-2041.2609370	40.13
621	02a-TricapCubeA-Fe1C1P8	-2041.2609261	40.13
622	04a-Icos-1vx-Fe5C2P7	-2041.2609184	40.14
623	04a-Icos-1vx-Fe5C4P4	-2041.2609079	40.15
624	04a-Icos-1vx-Fe3C3P4	-2041.2608990	40.15
625	02a-TricapCubeA-Fe1C3P7	-2041.2608937	40.15
626	03a-TricapCubeB-Fe3C3P1	-2041.2608891	40.16
627	03a-TricapCubeB-Fe3C2P7	-2041.2606731	40.29

628	01b-PentaCapTriPri-Fe2P4C5	-2041.2605735	40.36
629	02a-TricapCubeA-Fe4C6P2	-2041.2604489	40.43
630	03b-TricapCubeB-Fe3P6C1	-2041.2604478	40.43
631	03a-TricapCubeB-Fe4C4P1	-2041.2604412	40.44
632	04b-Icos-1vx-Fe3P6C4	-2041.2604372	40.44
633	04a-Icos-1vx-Fe5C4P2	-2041.2604276	40.45
634	03a-TricapCubeB-Fe1C2P1	-2041.2603974	40.47
635	04a-Icos-1vx-Fe5C1P2	-2041.2603958	40.47
636	02b-TricapCubeA-Fe4P6C1	-2041.2603663	40.49
637	02b-TricapCubeA-Fe2P2C4	-2041.2602769	40.54
638	04a-Icos-1vx-Fe4C2P7	-2041.2602285	40.57
639	04b-Icos-1vx-Fe3P2C2	-2041.2602226	40.58
640	04b-Icos-1vx-Fe1P4C2	-2041.2602218	40.58
641	04b-Icos-1vx-Fe1P3C3	-2041.2601765	40.60
642	04a-Icos-1vx-Fe4C3P7	-2041.2601657	40.61
643	02a-TricapCubeA-Fe4C2P8	-2041.2601521	40.62
644	04b-Icos-1vx-Fe3P5C3	-2041.2601152	40.64
645	03a-TricapCubeB-Fe1C4P2	-2041.2601132	40.64
646	03a-TricapCubeB-Fe3C3P6	-2041.2595659	40.99
647	04b-Icos-1vx-Fe1P3C6	-2041.2595556	40.99
648	04b-Icos-1vx-Fe5P4C3	-2041.2595357	41.01
649	04a-Icos-1vx-Fe5C1P8	-2041.2595114	41.02
650	03a-TricapCubeB-Fe1C5P2	-2041.2592508	41.19
651	04b-Icos-1vx-Fe4P1C6	-2041.2592267	41.20
652	04a-Icos-1vx-Fe2C4P3	-2041.2591418	41.25
653	04a-Icos-1vx-Fe3C7P2	-2041.2591348	41.26
654	03b-TricapCubeB-Fe3P2C3	-2041.2591255	41.26
655	02a-TricapCubeA-Fe1C1P2	-2041.2591113	41.27
656	02a-TricapCubeA-Fe1C1P7	-2041.2590982	41.28
657	02a-TricapCubeA-Fe1C3P5	-2041.2590892	41.29
658	04a-Icos-1vx-Fe5C2P3	-2041.2590846	41.29
659	02b-TricapCubeA-Fe4P1C7	-2041.2590180	41.33
660	03b-TricapCubeB-Fe1P3C3	-2041.2589066	41.40
661	03a-TricapCubeB-Fe1C2P8	-2041.2587871	41.48
662	03a-TricapCubeB-Fe2C1P4	-2041.2587751	41.48
663	04b-Icos-1vx-Fe4P3C6	-2041.2587634	41.49
664	04a-Icos-1vx-Fe4C3P6	-2041.2587548	41.50
665	01a-PentaCapTriPri-Fe1C4P1	-2041.2587440	41.50
666	03a-TricapCubeB-Fe1C3P6	-2041.2587408	41.51
667	02a-TricapCubeA-Fe3C2P8	-2041.2580884	41.92
668	01a-PentaCapTriPri-Fe2C3P1	-2041.2580670	41.93
669	02a-TricapCubeA-Fe1C3P3	-2041.2579004	42.03

670	04a-Icos-1vx-Fe2C1P3	-2041.2577354	42.14
671	03a-TricapCubeB-Fe2C5P1	-2041.2575921	42.23
672	03a-TricapCubeB-Fe2C1P1	-2041.2575395	42.26
673	04a-Icos-1vx-Fe2C2P5_r-27	-2041.2575215	42.27
674	03a-TricapCubeB-Fe1C4P3	-2041.2574665	42.31
675	02b-TricapCubeA-Fe4P6C4	-2041.2574328	42.33
676	04b-Icos-1vx-Fe2P5C2	-2041.2574251	42.33
677	01b-PentaCapTriPri-Fe2P2C4	-2041.2570491	42.57
678	02b-TricapCubeA-Fe4P5C2	-2041.2570234	42.58
679	02a-TricapCubeA-Fe4C5P2_i-12	-2041.2570158	42.59
680	02b-TricapCubeA-Fe4P9C1	-2041.2570130	42.59
681	02a-TricapCubeA-Fe4C5P2_r-12	-2041.2569691	42.62
682	04a-Icos-1vx-Fe2C2P5_i-27	-2041.2569515	42.63
683	03a-TricapCubeB-Fe3C1P4	-2041.2568569	42.69
684	02a-TricapCubeA-Fe1C2P1_i-15	-2041.2567639	42.75
685	02b-TricapCubeA-Fe3P2C4	-2041.2566633	42.81
686	02b-TricapCubeA-Fe2P2C3	-2041.2566372	42.83
687	04b-Icos-1vx-Fe3P3C4	-2041.2565564	42.88
688	04a-Icos-1vx-Fe2C3P4	-2041.2563307	43.02
689	03b-TricapCubeB-Fe3P3C2	-2041.2562965	43.04
690	04b-Icos-1vx-Fe3P4C5	-2041.2562807	43.05
691	02a-TricapCubeA-Fe4C2P6	-2041.2562663	43.06
692	04b-Icos-1vx-Fe3P8C1	-2041.2562654	43.06
693	03b-TricapCubeB-Fe4P3C2	-2041.2562642	43.06
694	04b-Icos-1vx-Fe3P9C1	-2041.2562591	43.06
695	04a-Icos-1vx-Fe4C2P5	-2041.2562521	43.07
696	02b-TricapCubeA-Fe3P2C2	-2041.2562252	43.08
697	04a-Icos-1vx-Fe4C5P2	-2041.2562073	43.10
698	03a-TricapCubeB-Fe3C3P4	-2041.2561911	43.11
699	02b-TricapCubeA-Fe4P4C5	-2041.2545419	44.14
700	03b-TricapCubeB-Fe2P5C1	-2041.2545236	44.15
701	04a-Icos-1vx-Fe4C1P1	-2041.2545062	44.16
702	02a-TricapCubeA-Fe3C1P1	-2041.2544809	44.18
703	04a-Icos-1vx-Fe4C4P1	-2041.2544676	44.19
704	03a-TricapCubeB-Fe2C2P1	-2041.2543819	44.24
705	02b-TricapCubeA-Fe4P3C3	-2041.2540694	44.44
706	01b-PentaCapTriPri-Fe2P3C4	-2041.2539825	44.49
707	01b-PentaCapTriPri-Fe2P5C3	-2041.2538231	44.59
708	03a-TricapCubeB-Fe1C1P1	-2041.2534972	44.80
709	02b-TricapCubeA-Fe3P1C5	-2041.2534646	44.82
710	02b-TricapCubeA-Fe3P3C7	-2041.2531022	45.04
711	02b-TricapCubeA-Fe3P1C1	-2041.2529696	45.13

712	01b-PentaCapTriPri-Fe2P1C2	-2041.2528452	45.21
713	04a-Icos-1vx-Fe3C3P6	-2041.2527649	45.26
714	03b-TricapCubeB-Fe2P2C3	-2041.2527635	45.26
715	04a-Icos-1vx-Fe1C2P2	-2041.2527634	45.26
716	03b-TricapCubeB-Fe2P1C5	-2041.2527388	45.27
717	03b-TricapCubeB-Fe2P2C6	-2041.2527041	45.29
718	03a-TricapCubeB-Fe2C3P3	-2041.2524321	45.46
719	01b-PentaCapTriPri-Fe1P3C4	-2041.2524182	45.47
720	02b-TricapCubeA-Fe4P2C4	-2041.2517565	45.89
721	02a-TricapCubeA-Fe2C1P8	-2041.2513696	46.13
722	04b-Icos-1vx-Fe2P6C1	-2041.2512716	46.19
723	02a-TricapCubeA-Fe4C1P3	-2041.2510972	46.30
724	04b-Icos-1vx-Fe1P1C4	-2041.2510065	46.36
725	03b-TricapCubeB-Fe1P2C6	-2041.2509267	46.41
726	02a-TricapCubeA-Fe4C5P1	-2041.2508794	46.44
727	03b-TricapCubeB-Fe4P2C2	-2041.2508528	46.46
728	02a-TricapCubeA-Fe3C1P6	-2041.2508441	46.46
729	03b-TricapCubeB-Fe1P1C9	-2041.2508225	46.47
730	01a-PentaCapTriPri-Fe1C1P4	-2041.2507904	46.49
731	03b-TricapCubeB-Fe2P5C2	-2041.2505417	46.65
732	03b-TricapCubeB-Fe2P1C6	-2041.2505036	46.67
733	04b-Icos-1vx-Fe3P1C2	-2041.2503957	46.74
734	02b-TricapCubeA-Fe4P2C1	-2041.2503951	46.74
735	03b-TricapCubeB-Fe2P2C2	-2041.2501562	46.89
736	03b-TricapCubeB-Fe2P3C3	-2041.2501113	46.92
737	02a-TricapCubeA-Fe4C3P4	-2041.2500730	46.95
738	03b-TricapCubeB-Fe2P2C1	-2041.2500534	46.96
739	01b-PentaCapTriPri-Fe1P1C2	-2041.2497922	47.12
740	04a-Icos-1vx-Fe1C4P1	-2041.2496271	47.22
741	02a-TricapCubeA-Fe3C4P5	-2041.2487901	47.75
742	01b-PentaCapTriPri-Fe2P4C3	-2041.2487685	47.76
743	03b-TricapCubeB-Fe1P3C7	-2041.2480928	48.19
744	01b-PentaCapTriPri-Fe2P2C2	-2041.2480172	48.24
745	03b-TricapCubeB-Fe1P2C2	-2041.2474869	48.57
746	02b-TricapCubeA-Fe3P2C1	-2041.2474688	48.58
747	03b-TricapCubeB-Fe1P1C2_r-39	-2041.2470492	48.84
748	03a-TricapCubeB-Fe2C4P2	-2041.2469624	48.90
749	03a-TricapCubeB-Fe2C3P7	-2041.2469165	48.93
750	03b-TricapCubeB-Fe1P2C1	-2041.2469165	48.93
751	03a-TricapCubeB-Fe2C2P7	-2041.2468837	48.95
752	01a-PentaCapTriPri-Fe2C5P5	-2041.2468557	48.96
753	01b-PentaCapTriPri-Fe2P1C1	-2041.2467787	49.01

754	01a-PentaCapTriPri-Fe2C3P7	-2041.2466694	49.08
755	04b-Icos-1vx-Fe4P5C1	-2041.2466576	49.09
756	04b-Icos-1vx-Fe1P2C4	-2041.2464355	49.23
757	03a-TricapCubeB-Fe4C3P1	-2041.2461668	49.40
758	04a-Icos-1vx-Fe1C2P4	-2041.2460915	49.44
759	03a-TricapCubeB-Fe4C1P6	-2041.2460600	49.46
760	04b-Icos-1vx-Fe1P4C3	-2041.2460091	49.50
761	04a-Icos-1vx-Fe1C4P3	-2041.2460083	49.50
762	03a-TricapCubeB-Fe2C1P7	-2041.2460030	49.50
763	03b-TricapCubeB-Fe2P1C4	-2041.2459785	49.51
764	04b-Icos-1vx-Fe5P1C3	-2041.2459717	49.52
765	03a-TricapCubeB-Fe2C2P2	-2041.2459613	49.53
766	02a-TricapCubeA-Fe3C4P3	-2041.2455367	49.79
767	02b-TricapCubeA-Fe3P1C7_i-43	-2041.2455194	49.80
768	01a-PentaCapTriPri-Fe2C3P5	-2041.2451650	50.03
769	03a-TricapCubeB-Fe3C1P3	-2041.2450060	50.12
770	03a-TricapCubeB-Fe1C1P3	-2041.2448003	50.25
771	04b-Icos-1vx-Fe3P4C1	-2041.2447421	50.29
772	01a-PentaCapTriPri-Fe2C1P1	-2041.2446727	50.33
773	04b-Icos-1vx-Fe2P1C5	-2041.2445600	50.40
774	02b-TricapCubeA-Fe4P3C6	-2041.2440440	50.73
775	02a-TricapCubeA-Fe2C1P7	-2041.2440279	50.74
776	04a-Icos-1vx-Fe3C2P1	-2041.2439471	50.79
777	02a-TricapCubeA-Fe3C2P4_r-21	-2041.2439010	50.82
778	03b-TricapCubeB-Fe4P2C6	-2041.2438400	50.86
779	02a-TricapCubeA-Fe3C3P2	-2041.2437536	50.91
780	02a-TricapCubeA-Fe3C2P4_i-21	-2041.2437523	50.91
781	01a-PentaCapTriPri-Fe2C1P6	-2041.2436647	50.97
782	01b-PentaCapTriPri-Fe2P2C3	-2041.2433288	51.18
783	01a-PentaCapTriPri-Fe2C2P4	-2041.2432510	51.23
784	04b-Icos-1vx-Fe1P3C4	-2041.2431904	51.26
785	03b-TricapCubeB-Fe1P4C3	-2041.2431803	51.27
786	02a-TricapCubeA-Fe4C6P4	-2041.2431684	51.28
787	02a-TricapCubeA-Fe3C5P1	-2041.2431612	51.28
788	01b-PentaCapTriPri-Fe2P3C7	-2041.2428843	51.46
789	04b-Icos-1vx-Fe4P3C4	-2041.2425380	51.67
790	03b-TricapCubeB-Fe3P3C3	-2041.2423337	51.80
791	01a-PentaCapTriPri-Fe2C1P5	-2041.2413337	52.43
792	02a-TricapCubeA-Fe4C2P3	-2041.2412624	52.47
793	03a-TricapCubeB-Fe4C2P5	-2041.2412093	52.51
794	04b-Icos-1vx-Fe4P2C4	-2041.2411780	52.53
795	02b-TricapCubeA-Fe1P2C1	-2041.2411202	52.56

796	04b-Icos-1vx-Fe2P1C2	-2041.2403653	53.04
797	02a-TricapCubeA-Fe3C4P6	-2041.2400405	53.24
798	03a-TricapCubeB-Fe4C1P2	-2041.2392076	53.76
799	02a-TricapCubeA-Fe3C1P2	-2041.2391431	53.80
800	02b-TricapCubeA-Fe3P5C2	-2041.2391295	53.81
801	04a-Icos-1vx-Fe2C5P2	-2041.2386405	54.12
802	02a-TricapCubeA-Fe4C7P3	-2041.2385398	54.18
803	04a-Icos-1vx-Fe3C8P2	-2041.2383103	54.33
804	03a-TricapCubeB-Fe4C2P1	-2041.2382704	54.35
805	04b-Icos-1vx-Fe5P3C1	-2041.2379082	54.58
806	04b-Icos-1vx-Fe3P8C2	-2041.2378495	54.62
807	02b-TricapCubeA-Fe4P7C3	-2041.2378099	54.64
808	02b-TricapCubeA-Fe2P4C1	-2041.2378054	54.64
809	03a-TricapCubeB-Fe1C5P1	-2041.2375889	54.78
810	04a-Icos-1vx-Fe2C2P1	-2041.2375706	54.79
811	04a-Icos-1vx-Fe3C3P1	-2041.2373108	54.95
812	03a-TricapCubeB-Fe1C2P5	-2041.2372627	54.98
813	03b-TricapCubeB-Fe3P1C4	-2041.2372159	55.01
814	02a-TricapCubeA-Fe2C4P2	-2041.2369917	55.15
815	04a-Icos-1vx-Fe2C2P8	-2041.2369870	55.16
816	04b-Icos-1vx-Fe2P3C7	-2041.2369669	55.17
817	04b-Icos-1vx-Fe2P2C8	-2041.2369639	55.17
818	04b-Icos-1vx-Fe2P2C7	-2041.2369527	55.18
819	04a-Icos-1vx-Fe2C3P3	-2041.2369418	55.19
820	01a-PentaCapTriPri-Fe2C2P5	-2041.2368493	55.24
821	03a-TricapCubeB-Fe1C3P4	-2041.2368395	55.25
822	01b-PentaCapTriPri-Fe1P2C2	-2041.2367716	55.29
823	02a-TricapCubeA-Fe4C5P3	-2041.2361113	55.71
824	03b-TricapCubeB-Fe1P2C5	-2041.2361104	55.71
825	01b-PentaCapTriPri-Fe2P6C1	-2041.2360561	55.74
826	02b-TricapCubeA-Fe2P2C6	-2041.2360505	55.74
827	04a-Icos-1vx-Fe4C6P1	-2041.2360362	55.75
828	02a-TricapCubeA-Fe3C6P3	-2041.2360127	55.77
829	02a-TricapCubeA-Fe3C2P5	-2041.2358781	55.85
830	02b-TricapCubeA-Fe4P1C9	-2041.2358677	55.86
831	02a-TricapCubeA-Fe3C1P4	-2041.2358327	55.88
832	02b-TricapCubeA-Fe3P1C4	-2041.2358243	55.89
833	01a-PentaCapTriPri-Fe2C2P3	-2041.2358075	55.90
834	04a-Icos-1vx-Fe3C7P3	-2041.2356461	56.00
835	02b-TricapCubeA-Fe1P2C2	-2041.2354567	56.12
836	03b-TricapCubeB-Fe4P3C4	-2041.2351767	56.29
837	03a-TricapCubeB-Fe1C2P4	-2041.2349461	56.44

838	04b-Icos-1vx-Fe1P2C2	-2041.2346735	56.61
839	04b-Icos-1vx-Fe3P2C6	-2041.2345119	56.71
840	03a-TricapCubeB-Fe2C1P6	-2041.2345012	56.72
841	03b-TricapCubeB-Fe4P2C5	-2041.2337528	57.19
842	02a-TricapCubeA-Fe4C3P2	-2041.2337041	57.22
843	04a-Icos-1vx-Fe4C2P1	-2041.2336911	57.23
844	02b-TricapCubeA-Fe3P2C3	-2041.2336139	57.27
845	01a-PentaCapTriPri-Fe2C2P1	-2041.2334307	57.39
846	02b-TricapCubeA-Fe2P3C6	-2041.2333245	57.46
847	02b-TricapCubeA-Fe4P1C4	-2041.2332836	57.48
848	01b-PentaCapTriPri-Fe2P3C5	-2041.2326051	57.91
849	01b-PentaCapTriPri-Fe2P5C2	-2041.2311852	58.80
850	01b-PentaCapTriPri-Fe2P2C5	-2041.2310239	58.90
851	03b-TricapCubeB-Fe1P2C8	-2041.2307056	59.10
852	03b-TricapCubeB-Fe1P1C2_i-39	-2041.2305808	59.18
853	02b-TricapCubeA-Fe3P2C5	-2041.2305557	59.19
854	04a-Icos-1vx-Fe5C3P1	-2041.2301546	59.44
855	02b-TricapCubeA-Fe3P5C4	-2041.2299257	59.59
856	02a-TricapCubeA-Fe3C8P1	-2041.2299125	59.60
857	04b-Icos-1vx-Fe5P4C2	-2041.2297964	59.67
858	03a-TricapCubeB-Fe3C6P1	-2041.2297765	59.68
859	04b-Icos-1vx-Fe3P2C1	-2041.2297652	59.69
860	03b-TricapCubeB-Fe4P1C2	-2041.2297067	59.73
861	03a-TricapCubeB-Fe2C1P9	-2041.2290050	60.17
862	01a-PentaCapTriPri-Fe2C5P2	-2041.2288738	60.25
863	01a-PentaCapTriPri-Fe2C3P2	-2041.2284198	60.53
864	04b-Icos-1vx-Fe2P1C8	-2041.2283297	60.59
865	04b-Icos-1vx-Fe2P3C5_i-13	-2041.2277517	60.95
866	02a-TricapCubeA-Fe1C1P3	-2041.2275194	61.10
867	04a-Icos-1vx-Fe5C2P1	-2041.2275047	61.11
868	03a-TricapCubeB-Fe3C2P1	-2041.2274620	61.13
869	03a-TricapCubeB-Fe3C1P1	-2041.2274569	61.14
870	04a-Icos-1vx-Fe4C2P4	-2041.2273964	61.18
871	02b-TricapCubeA-Fe4P2C3	-2041.2273531	61.20
872	04b-Icos-1vx-Fe3P3C1	-2041.2272961	61.24
873	01a-PentaCapTriPri-Fe2C1P2	-2041.2271671	61.32
874	01a-PentaCapTriPri-Fe2C6P1	-2041.2258629	62.14
875	03b-TricapCubeB-Fe1P4C2	-2041.2258086	62.17
876	03b-TricapCubeB-Fe2P3C5	-2041.2257130	62.23
877	02a-TricapCubeA-Fe4C2P5	-2041.2254859	62.37
878	02b-TricapCubeA-Fe3P7C3	-2041.2247078	62.86
879	04b-Icos-1vx-Fe4P5C2	-2041.2243584	63.08

880	01b-PentaCapTriPri-Fe1P3C3	-2041.2243190	63.11
881	01a-PentaCapTriPri-Fe1C3P3	-2041.2242871	63.13
882	01b-PentaCapTriPri-Fe2P3C1	-2041.2242212	63.17
883	02a-TricapCubeA-Fe4C7P2	-2041.2237168	63.48
884	04a-Icos-1vx-Fe3C2P6	-2041.2237147	63.49
885	02b-TricapCubeA-Fe3P1C2	-2041.2236268	63.54
886	01a-PentaCapTriPri-Fe2C3P3	-2041.2235791	63.57
887	02b-TricapCubeA-Fe3P3C5	-2041.2230671	63.89
888	03b-TricapCubeB-Fe4P6C1	-2041.2227872	64.07
889	03b-TricapCubeB-Fe2P1C1	-2041.2227048	64.12
890	02a-TricapCubeA-Fe3C2P1	-2041.2220833	64.51
891	03a-TricapCubeB-Fe2C4P3	-2041.2217689	64.71
892	03a-TricapCubeB-Fe2C3P4	-2041.2217614	64.71
893	02a-TricapCubeA-Fe3C3P5	-2041.2215329	64.85
894	03b-TricapCubeB-Fe1P2C4	-2041.2202599	65.65
895	02b-TricapCubeA-Fe3P2C6	-2041.2192918	66.26
896	02b-TricapCubeA-Fe3P3C3	-2041.2181069	67.00
897	03b-TricapCubeB-Fe1P6C1	-2041.2172290	67.56
898	01a-PentaCapTriPri-Fe1C2P1	-2041.2168527	67.79
899	04a-Icos-1vx-Fe5C2P2	-2041.2150633	68.91
900	03b-TricapCubeB-Fe2P6C1	-2041.2141138	69.51
901	03b-TricapCubeB-Fe2P2C5	-2041.2140039	69.58
902	03b-TricapCubeB-Fe3P1C2	-2041.2139392	69.62
903	04b-Icos-1vx-Fe2P2C4	-2041.2135591	69.86
904	03a-TricapCubeB-Fe4C3P4	-2041.2130176	70.20
905	02b-TricapCubeA-Fe3P2C8	-2041.2124886	70.53
906	03a-TricapCubeB-Fe2C6P1	-2041.2091265	72.64
907	03a-TricapCubeB-Fe2C2P5	-2041.2090418	72.69
908	01a-PentaCapTriPri-Fe2C4P6	-2041.2082500	73.19
909	03a-TricapCubeB-Fe1C6P1	-2041.2067183	74.15
910	02a-TricapCubeA-Fe3C3P3	-2041.2065131	74.28
911	02a-TricapCubeA-Fe3C7P3	-2041.2056774	74.80
912	03a-TricapCubeB-Fe2C3P1	-2041.2051783	75.12
913	03a-TricapCubeB-Fe2C3P6	-2041.2051594	75.13
914	03b-TricapCubeB-Fe2P3C1	-2041.2051422	75.14
915	03b-TricapCubeB-Fe2P2C4	-2041.2033642	76.26
916	02a-TricapCubeA-Fe3C4P4	-2041.2026042	76.73
917	02a-TricapCubeA-Fe2C1P5	-2041.2021831	77.00
918	01b-PentaCapTriPri-Fe1P2C1	-2041.2010676	77.70
919	03b-TricapCubeB-Fe2P3C2	-2041.1968899	80.32
920	01a-PentaCapTriPri-Fe1C3P1	-2041.1947200	81.68
921	01b-PentaCapTriPri-Fe2P1C4	-2041.1946943	81.70

922	04a-Icos-1vx-Fe3C7P1	-2041.1944616	81.84
923	01a-PentaCapTriPri-Fe2C1P3	-2041.1937933	82.26
924	02a-TricapCubeA-Fe3C4P2	-2041.1894288	85.00
925	02b-TricapCubeA-Fe3P6C4	-2041.1875753	86.16
926	04b-Icos-1vx-Fe2P3C6	-2041.1827757	89.18
927	04a-Icos-1vx-Fe2C3P6	-2041.1827093	89.22
928	01b-PentaCapTriPri-Fe2P4C6	-2041.1803776	90.68
929	02a-TricapCubeA-Fe4C8P2	-2041.1766253	93.04
930	02b-TricapCubeA-Fe2P4C3	-2041.1750046	94.05
931	01b-PentaCapTriPri-Fe2P3C2	-2041.1740024	94.68
932	01a-PentaCapTriPri-Fe1C1P1	-2041.1730575	95.27
933	01b-PentaCapTriPri-Fe2P1C3	-2041.1705343	96.86
934	02b-TricapCubeA-Fe4P8C1	-2041.1667870	99.21
935	01b-PentaCapTriPri-Fe2P1C6	-2041.1619009	102.27
936	01b-PentaCapTriPri-Fe2P3C6	-2041.1613984	102.59
937	02b-TricapCubeA-Fe1P3C1	-2041.1507641	109.26
938	02a-TricapCubeA-Fe1C3P1	-2041.1507584	109.27

Table S5A. Initial $CpFeCHPHB_9H_9$ structures, 304 in all.

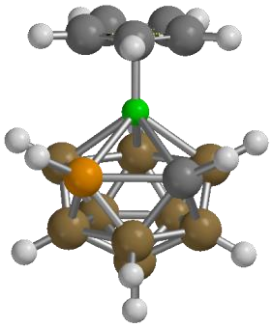
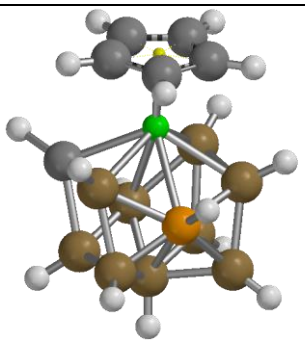
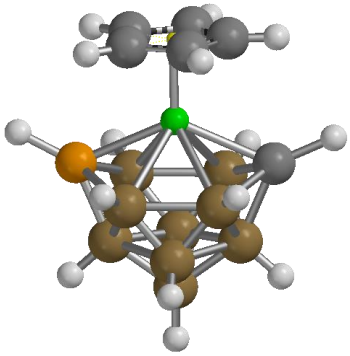
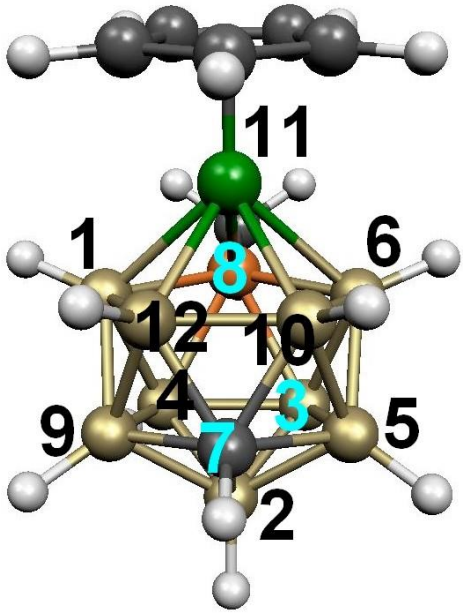
 Icosahedron 18
 Cubeoctahedron 110
 Anticubeoctahedron 176

Table S5B. Distance table for the lowest-lying $CpFeCHPCH_3B_9H_9$ 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.

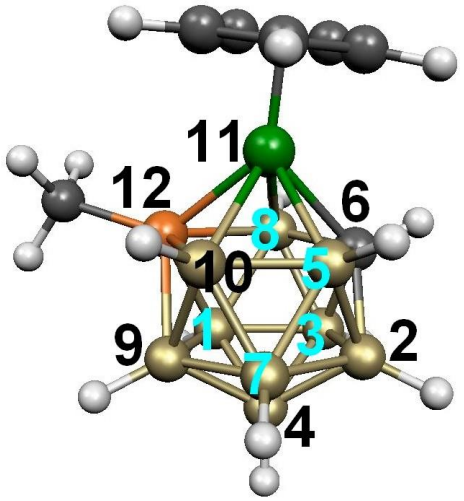


1. -2106.13477850 0.0
C_S H/L 3.17

		1	2	3	4	5
1	B	0.000000				
2	B	2.919404	0.000000			
3	B	3.050288	1.746854	0.000000		
4	B	1.883695	1.746791	1.854900	0.000000	
5	B	3.457189	1.768423	1.752662	2.895354	0.000000
6	B	3.103100	2.919500	1.883849	3.050380	1.751201
7	C	2.745212	1.679179	2.722261	2.722221	1.681293
8	P	1.984806	3.022159	1.970692	1.970737	3.015029
9	B	1.751200	1.768344	2.895348	1.752612	2.863400
10	B	2.933325	2.875426	2.906151	3.426851	1.781301
11	Fe	2.137921	3.853364	3.364205	3.364153	3.291705
12	B	1.756902	2.875339	3.426848	2.905939	2.874791

		6	7	8	9	10
7	C	2.745182	0.000000			
8	P	1.984856	3.356851	0.000000		
9	B	3.457179	1.681257	3.015044	0.000000	
10	B	1.757011	1.698931	2.997504	2.874663	0.000000
11	Fe	2.137961	3.151228	2.101469	3.291625	2.064474
12	B	2.933367	1.698988	2.997444	1.781082	1.778100

		11	12
12	B	2.064472	0.000000

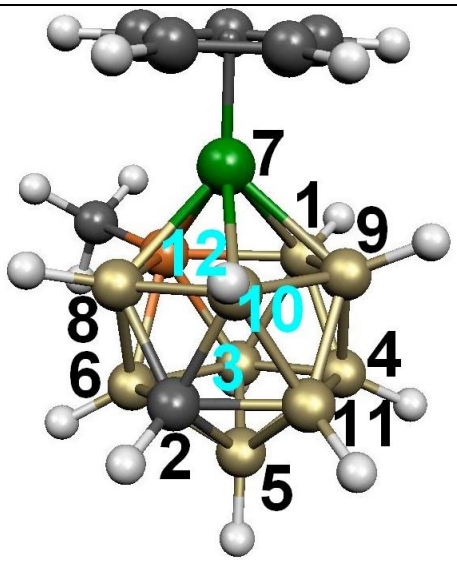


2. -2106.12909080 +3.6
C_1 H/L 2.95

		1	2	3	4	5
1	B	0.000000				
2	B	2.848156	0.000000			
3	B	1.749813	1.750844	0.000000		
4	B	1.762640	1.758188	1.765706	0.000000	
5	B	3.399906	1.772903	2.858914	2.878103	0.000000
6	C	2.765004	1.687003	1.697783	2.748769	1.691423
7	B	2.899515	1.757212	2.861880	1.777790	1.786536
8	B	1.870538	2.847827	1.756171	2.916986	2.873148
9	B	1.857141	2.849962	2.892553	1.753972	2.897813
10	B	3.035550	2.881699	3.459440	2.931144	1.764567
11	Fe	3.344934	3.290517	3.298756	3.874685	2.066651
12	P	1.967035	3.531224	3.041727	3.042466	2.993734

		6	7	8	9	10
7	B	2.749014	0.000000			
8	B	1.665306	3.432728	0.000000		
9	B	3.277834	1.755947	3.034280	0.000000	
10	B	2.824687	1.760690	3.069404	1.876916	0.000000
11	Fe	2.040825	3.313294	2.095279	3.374374	2.158096
12	P	2.909544	3.023642	2.000081	1.964566	1.972168

		11	12
12	P	2.117358	0.000000

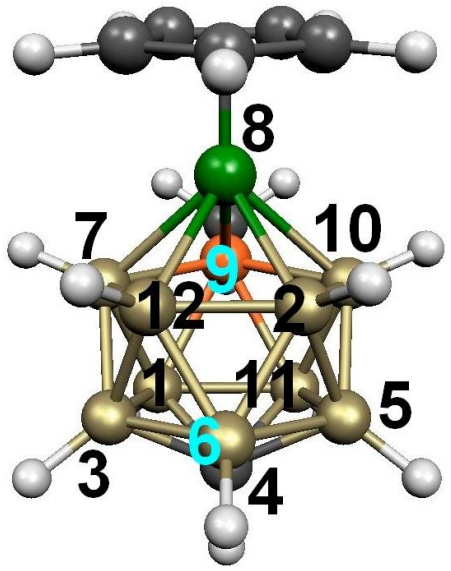


3. -2106.12494590 +6.2
C_1 H/L 3.04

		1	2	3	4	5
1	B	0.000000				
2	C	3.292870	0.000000			
3	B	1.881684	2.759542	0.000000		
4	B	1.757891	2.739750	1.758002	0.000000	
5	B	2.912453	1.696709	1.750275	1.758707	0.000000
6	B	3.027164	1.663750	1.840881	2.885137	1.751706
7	Fe	2.152663	3.158521	3.364720	3.321980	3.857828
8	B	3.078295	1.677314	3.033495	3.452264	2.919242
9	B	1.762573	2.750894	2.917020	1.798055	2.876459
10	B	2.922785	1.717541	3.427657	2.880781	2.879039
11	B	2.867092	1.686460	2.857099	1.765176	1.755475
12	P	1.982688	2.900208	1.972803	3.034701	3.044916

		6	7	8	9	10
6	B	0.000000				
7	Fe	3.333253	0.000000			
8	B	1.868680	2.099600	0.000000		
9	B	3.416665	2.096829	2.924055	0.000000	
10	B	2.898893	2.064723	1.760656	1.768220	0.000000
11	B	2.840593	3.283463	2.861606	1.769964	1.764666
12	P	1.974621	2.092825	1.989661	3.019668	3.020275

		11	12
11	B	0.000000	
12	P	3.531869	0.000000

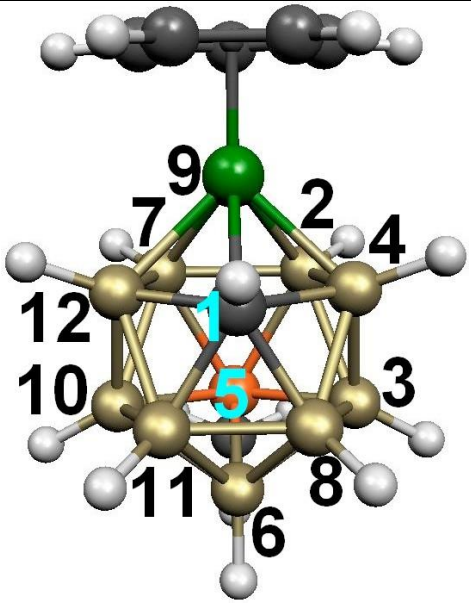


4. -2106.11976760 +9.4
C_S H/L 3.02

		1	2	3	4	5
1	B	0.000000				
2	B	3.418399	0.000000			
3	B	1.747547	2.881071	0.000000		
4	C	1.669102	2.742217	1.690695	0.000000	
5	B	2.891190	1.784192	2.867900	1.690762	0.000000
6	B	2.845760	1.771377	1.759498	1.682033	1.759497
7	B	1.860579	2.943065	1.753822	2.780013	3.459829
8	Fe	3.339261	2.090475	3.302681	3.692992	3.302626
9	P	1.974997	3.019760	3.038001	2.905211	3.038028
10	B	3.032934	1.768602	3.459850	2.780082	1.753875
11	B	1.849700	2.895731	2.891133	1.669094	1.747627
12	B	2.895681	1.784200	1.784221	2.742152	2.880977

		6	7	8	9	10
6	B	0.000000				
7	B	2.875069	0.000000			
8	Fe	3.290852	2.138754	0.000000		
9	P	3.535636	1.990087	2.082377	0.000000	
10	B	2.875120	3.101400	2.138654	1.990084	0.000000
11	B	2.845773	3.032906	3.339274	1.975020	1.860681
12	B	1.771289	1.768631	2.090530	3.019757	2.943029

		11	12
12	B	3.418369	0.000000

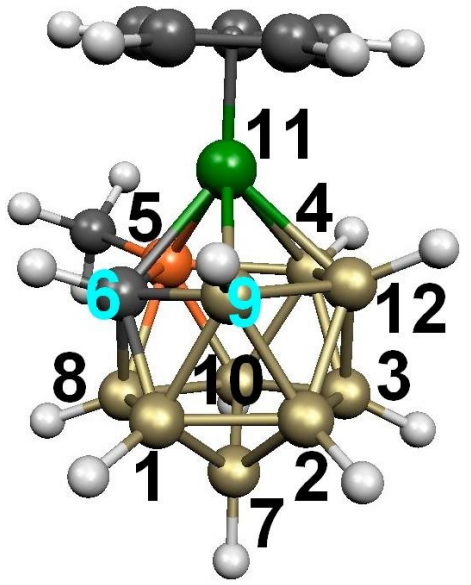


5. -2106.10367930 +19.5
C_S H/L 3.04

		1	2	3	4	5
1	C	0.000000				
2	B	2.788089	0.000000			
3	B	2.745485	1.912868	0.000000		
4	B	1.689684	1.777262	1.774062	0.000000	
5	P	3.359001	1.969653	1.949840	2.999104	0.000000
6	B	2.739626	3.085260	1.873212	2.920495	1.970338
7	B	2.788109	1.906600	3.070347	2.931501	1.969760
8	B	1.688868	2.947874	1.747379	1.788840	2.992185
9	Fe	2.009860	2.010747	3.295810	2.029024	3.369069
10	B	2.745449	3.070113	3.025000	3.430732	1.949739
11	B	1.688832	3.471280	2.895711	2.867766	2.992124
12	B	1.689557	2.931448	3.430838	2.850500	2.999228

		6	7	8	9	10
6	B	0.000000				
7	B	3.085315	0.000000			
8	B	1.739002	3.471419	0.000000		
9	Fe	3.885245	2.010825	3.264111	0.000000	
10	B	1.873168	1.912754	2.895703	3.295788	0.000000
11	B	1.738985	2.947783	1.762600	3.264069	1.747334
12	B	2.920542	1.777329	2.867759	2.029054	1.774190

		11	12
11	B	0.000000	
12	B	1.788740	0.000000

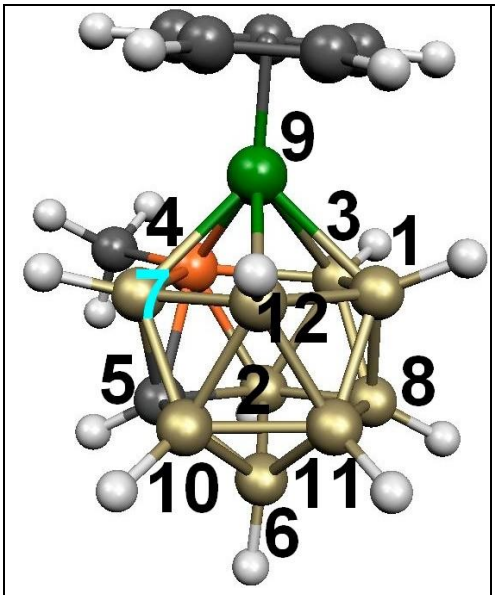


6. -2106.09886950 +22.5
C_1 H/L 2.94

		1	2	3	4	5
1	B	0.000000				
2	B	1.759363	0.000000			
3	B	2.866464	1.761672	0.000000		
4	B	3.471740	2.881192	1.758414	0.000000	
5	P	3.076565	3.550906	3.020010	1.970072	0.000000
6	C	1.661706	2.735076	3.302259	2.985008	1.983709
7	B	1.766933	1.763962	1.770952	2.931412	3.051129
8	B	1.754745	2.848722	2.884352	3.026384	1.970086
9	B	1.783244	1.775604	2.878496	2.937426	3.038499
10	B	2.901895	2.864551	1.761548	1.885357	1.947762
11	Fe	3.286807	3.303711	3.327119	2.167749	2.076306
12	B	2.880636	1.779940	1.791911	1.755618	3.007138

		6	7	8	9	10
6	C	0.000000				
7	B	2.777925	0.000000			
8	B	1.756573	1.761433	0.000000		
9	B	1.667052	2.875965	2.871806	0.000000	
10	B	2.909554	1.760345	1.842068	3.422692	0.000000
11	Fe	2.054024	3.857340	3.284027	2.074952	3.349154
12	B	2.800497	2.884170	3.396723	1.777975	2.908082

		11	12
12	B	2.112131	0.000000

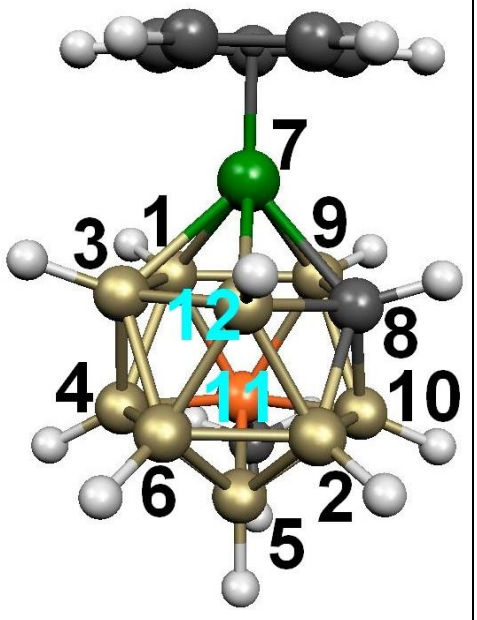


7. -2106.09670600 +23.9
C_1 H/L 3.01

		1	2	3	4	5
1	B	0.000000				
2	B	2.890742	0.000000			
3	B	1.764097	1.868420	0.000000		
4	P	2.991764	1.972897	1.970879	0.000000	
5	C	3.250583	1.749152	2.901941	1.934481	0.000000
6	B	2.866964	1.761699	2.926214	3.075590	1.681024
7	B	2.914872	3.003591	3.087784	1.989503	1.783541
8	B	1.793802	1.752677	1.758678	3.035533	2.754041
9	Fe	2.106969	3.346285	2.161468	2.054985	3.219857
10	B	2.872017	2.880436	3.464761	3.058328	1.673382
11	B	1.772566	2.855569	2.885721	3.549372	2.724012
12	B	1.780305	3.411384	2.947770	3.014005	2.763356

		6	7	8	9	10
6	B	0.000000				
7	B	2.911623	0.000000			
8	B	1.762744	3.447634	0.000000		
9	Fe	3.876370	2.120596	3.333263	0.000000	
10	B	1.762893	1.755395	2.868805	3.313068	0.000000
11	B	1.751995	2.873648	1.770362	3.318437	1.764606
12	B	2.873020	1.754832	2.892133	2.100136	1.783396

		11	12
12	B	1.780203	0.000000



8. -2106.09320800 +26.1
C_1 H/L 3.07

		1	2	3	4	5
1	B	0.000000				
2	B	3.472865	0.000000			
3	B	1.772105	2.888354	0.000000		
4	B	1.908597	2.901564	1.770917	0.000000	
5	B	3.081962	1.741334	2.927631	1.873424	0.000000
6	B	2.948397	1.763000	1.797452	1.758585	1.744928
7	Fe	2.015522	3.262999	2.071719	3.310166	3.883500
8	C	2.837524	1.704657	2.787623	3.302949	2.787288
9	B	1.906917	2.929437	2.926101	3.063515	3.075460
10	B	3.063858	1.739652	3.435669	3.010434	1.854599
11	P	1.976166	3.005767	3.011623	1.950891	1.974163
12	B	2.882574	1.778898	1.775209	2.873913	2.873220

		6	7	8	9	10
6	B	0.000000				
7	Fe	3.278888	0.000000			
8	C	2.759966	2.007620	0.000000		
9	B	3.454950	1.959942	1.689312	0.000000	
10	B	2.883500	3.276339	1.674694	1.910276	0.000000
11	P	3.006816	3.369645	2.884459	1.988982	1.950001
12	B	1.783881	2.029716	1.699703	2.849883	2.852263

		11	12
12	B	3.506905	0.000000

Table S5C. Energy ranking for all of the $CpFeCHPHB_9H_9$ optimized structures:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	03a-AnticubeOh-Fe3C5P2	-2066.8120894	0.00
2	03a-AnticubeOh-Fe1C3P3_r-261	-2066.8120862	0.00
3	02a-CubeOh-Fe2C4P4	-2066.8120832	0.00
4	03a-AnticubeOh-Fe2C2P7	-2066.8120816	0.00
5	03b-AnticubeOh-Fe3P2C8	-2066.8120802	0.01
6	01a-Icos-Fe1C1P5	-2066.8120796	0.01
7	02a-CubeOh-Fe2C3P6	-2066.8120796	0.01
8	03a-AnticubeOh-Fe1C1P2	-2066.8120794	0.01
9	03b-AnticubeOh-Fe2P3C3_r-55	-2066.8120787	0.01
10	02a-CubeOh-Fe2C1P10	-2066.8120786	0.01
11	03b-AnticubeOh-Fe3P3C6	-2066.8120786	0.01
12	02a-CubeOh-Fe1C1P5	-2066.8120777	0.01
13	03b-AnticubeOh-Fe2P4C2_r-56	-2066.8120742	0.01
14	02b-CubeOh-Fe2P2C8	-2066.8120601	0.02
15	03a-AnticubeOh-Fe3C1P9	-2066.8098554	1.40
16	03a-AnticubeOh-Fe3C3P7	-2066.8098540	1.40
17	03b-AnticubeOh-Fe3P3C5_r-50	-2066.8098511	1.40
18	03b-AnticubeOh-Fe1P1C1_r-248	-2066.8098509	1.40
19	03a-AnticubeOh-Fe3C3P5	-2066.8098502	1.41
20	03b-AnticubeOh-Fe2P3C2	-2066.8098502	1.41
21	02a-CubeOh-Fe1C1P4	-2066.8098500	1.41
22	03b-AnticubeOh-Fe3P2C6	-2066.8098498	1.41
23	03a-AnticubeOh-Fe1C2P1	-2066.8098492	1.41
24	03a-AnticubeOh-Fe2C1P2	-2066.8098491	1.41
25	03b-AnticubeOh-Fe2P2C2	-2066.8098490	1.41
26	02b-CubeOh-Fe1P1C4	-2066.8098488	1.41
27	02a-CubeOh-Fe1C2P1	-2066.8098488	1.41
28	03b-AnticubeOh-Fe2P1C2	-2066.8098483	1.41
29	03a-AnticubeOh-Fe2C3P2_r-248	-2066.8098482	1.41
30	03b-AnticubeOh-Fe2P3C1	-2066.8098481	1.41
31	03b-AnticubeOh-Fe2P1C5	-2066.8098479	1.41
32	03b-AnticubeOh-Fe3P1C8	-2066.8098478	1.41
33	02a-CubeOh-Fe1C1P1	-2066.8098475	1.41
34	02b-CubeOh-Fe1P2C1	-2066.8098469	1.41
35	01a-Icos-Fe1C1P2	-2066.8098463	1.41
36	02b-CubeOh-Fe1P1C1	-2066.8098461	1.41
37	03b-AnticubeOh-Fe1P2C1	-2066.8098459	1.41
38	03b-AnticubeOh-Fe3P1C9	-2066.8098454	1.41
39	03a-AnticubeOh-Fe3C1P8	-2066.8098442	1.41

40	03a-AnticubeOh-Fe3C2P6	-2066.8098439	1.41
41	01b-Icos-Fe1P1C2	-2066.8098115	1.43
42	02a-CubeOh-Fe2C1P9	-2066.8098111	1.43
43	03b-AnticubeOh-Fe3P3C5_i-50	-2066.8080278	2.55
44	02a-CubeOh-Fe2C2P1	-2066.8017239	6.50
45	02b-CubeOh-Fe2P4C6	-2066.8017239	6.50
46	03a-AnticubeOh-Fe1C2P9	-2066.8017192	6.51
47	02a-CubeOh-Fe2C4P1	-2066.8017183	6.51
48	02a-CubeOh-Fe2C3P8	-2066.8017167	6.51
49	03a-AnticubeOh-Fe3C1P6	-2066.8017165	6.51
50	01b-Icos-Fe1P1C4	-2066.8017165	6.51
51	03b-AnticubeOh-Fe3P2C4	-2066.8017162	6.51
52	02b-CubeOh-Fe2P1C8	-2066.8017153	6.51
53	03a-AnticubeOh-Fe2C2P2	-2066.8017133	6.51
54	03b-AnticubeOh-Fe3P3C2	-2066.8017132	6.51
55	03b-AnticubeOh-Fe2P2C6	-2066.8017125	6.51
56	02a-CubeOh-Fe2C2P6	-2066.8017124	6.51
57	02a-CubeOh-Fe1C1P3	-2066.8017122	6.51
58	03b-AnticubeOh-Fe3P3C4	-2066.8017112	6.51
59	02a-CubeOh-Fe2C3P2	-2066.8017110	6.51
60	02a-CubeOh-Fe1C2P5	-2066.7960833	10.04
61	03b-AnticubeOh-Fe2P1C4	-2066.7960600	10.06
62	03a-AnticubeOh-Fe3C4P6	-2066.7960574	10.06
63	03b-AnticubeOh-Fe3P3C1	-2066.7960568	10.06
64	01b-Icos-Fe1P1C6	-2066.7960563	10.06
65	02a-CubeOh-Fe2C6P1	-2066.7960561	10.06
66	03a-AnticubeOh-Fe3C1P3	-2066.7960558	10.06
67	03b-AnticubeOh-Fe2P3C4	-2066.7960551	10.06
68	03b-AnticubeOh-Fe3P3C8	-2066.7960530	10.06
69	03a-AnticubeOh-Fe2C3P3	-2066.7829356	18.29
70	03b-AnticubeOh-Fe2P2C7	-2066.7829139	18.31
71	03a-AnticubeOh-Fe2C1P5	-2066.7829115	18.31
72	03a-AnticubeOh-Fe3C2P8	-2066.7829108	18.31
73	03a-AnticubeOh-Fe3C3P6	-2066.7829108	18.31
74	03b-AnticubeOh-Fe3P1C10	-2066.7829107	18.31
75	03b-AnticubeOh-Fe3P4C4	-2066.7829107	18.31
76	01b-Icos-Fe1P1C5	-2066.7829086	18.31
77	02b-CubeOh-Fe1P2C4	-2066.7829078	18.31
78	02b-CubeOh-Fe2P5C1	-2066.7829075	18.31
79	02a-CubeOh-Fe1C2P4	-2066.7829074	18.31
80	03a-AnticubeOh-Fe2C4P2	-2066.7829054	18.31
81	02b-CubeOh-Fe2P4C4	-2066.7829041	18.31

82	01b-Icos-Fe1P1C1	-2066.7780930	21.33
83	03a-AnticubeOh-Fe3C1P5	-2066.7780731	21.35
84	03b-AnticubeOh-Fe3P1C5	-2066.7780712	21.35
85	02a-CubeOh-Fe2C1P7	-2066.7780702	21.35
86	02b-CubeOh-Fe1P1C2	-2066.7780693	21.35
87	02b-CubeOh-Fe2P1C2	-2066.7780692	21.35
88	02b-CubeOh-Fe2P1C7	-2066.7780691	21.35
89	03b-AnticubeOh-Fe1P1C5	-2066.7780683	21.35
90	03a-AnticubeOh-Fe1C1P5	-2066.7780682	21.35
91	03b-AnticubeOh-Fe2P1C6	-2066.7780681	21.35
92	03b-AnticubeOh-Fe3P1C7	-2066.7780678	21.35
93	03b-AnticubeOh-Fe3P3C3	-2066.7780670	21.35
94	03a-AnticubeOh-Fe3C3P3	-2066.7780661	21.35
95	02a-CubeOh-Fe1C1P2	-2066.7780660	21.35
96	03b-AnticubeOh-Fe3P2C1	-2066.7780659	21.35
97	03a-AnticubeOh-Fe3C1P7	-2066.7780628	21.35
98	02a-CubeOh-Fe2C1P2	-2066.7780610	21.35
99	01a-Icos-Fe1C1P1	-2066.7780437	21.36
100	02a-CubeOh-Fe2C1P8	-2066.7731118	24.46
101	01a-Icos-Fe1C1P4	-2066.7731071	24.46
102	03a-AnticubeOh-Fe2C1P3	-2066.7731071	24.46
103	02b-CubeOh-Fe1P2C2	-2066.7731059	24.46
104	02b-CubeOh-Fe2P1C5	-2066.7731052	24.46
105	03a-AnticubeOh-Fe3C3P2	-2066.7731048	24.46
106	03a-AnticubeOh-Fe3C3P4	-2066.7731042	24.46
107	02b-CubeOh-Fe2P3C2	-2066.7731039	24.46
108	02b-CubeOh-Fe1P1C3	-2066.7731031	24.46
109	02b-CubeOh-Fe2P2C6	-2066.7731015	24.47
110	02b-CubeOh-Fe2P2C1	-2066.7730982	24.47
111	01b-Icos-Fe1P1C3	-2066.7723507	24.94
112	03b-AnticubeOh-Fe2P1C3	-2066.7723504	24.94
113	03a-AnticubeOh-Fe3C1P2	-2066.7723502	24.94
114	03a-AnticubeOh-Fe2C1P6	-2066.7723496	24.94
115	03a-AnticubeOh-Fe3C6P1	-2066.7723494	24.94
116	02a-CubeOh-Fe2C3P1	-2066.7723493	24.94
117	03b-AnticubeOh-Fe1P2C4	-2066.7723486	24.94
118	03b-AnticubeOh-Fe1P2C5	-2066.7723486	24.94
119	02a-CubeOh-Fe2C3P3	-2066.7723484	24.94
120	02b-CubeOh-Fe2P1C1	-2066.7723464	24.94
121	02a-CubeOh-Fe1C3P2	-2066.7723451	24.94
122	03a-AnticubeOh-Fe3C4P2	-2066.7723397	24.94
123	02a-CubeOh-Fe1C1P7	-2066.7723329	24.95

124	01a-Icos-Fe1C2P2	-2066.7657284	29.09
125	02a-CubeOh-Fe2C2P4	-2066.7657238	29.10
126	01b-Icos-Fe1P2C2	-2066.7657237	29.10
127	03a-AnticubeOh-Fe2C2P9	-2066.7657235	29.10
128	02b-CubeOh-Fe2P2C4	-2066.7657230	29.10
129	02b-CubeOh-Fe2P4C5	-2066.7657229	29.10
130	03b-AnticubeOh-Fe3P5C1	-2066.7657227	29.10
131	03b-AnticubeOh-Fe2P2C8	-2066.7657220	29.10
132	02a-CubeOh-Fe2C4P5	-2066.7657218	29.10
133	03a-AnticubeOh-Fe3C4P1	-2066.7657218	29.10
134	03b-AnticubeOh-Fe1P3C4_r-366	-2066.7657216	29.10
135	02b-CubeOh-Fe2P2C7	-2066.7657215	29.10
136	02a-CubeOh-Fe2C2P7	-2066.7657211	29.10
137	03a-AnticubeOh-Fe3C5P1	-2066.7657209	29.10
138	03a-AnticubeOh-Fe2C2P8	-2066.7657205	29.10
139	03b-AnticubeOh-Fe3P4C1	-2066.7657205	29.10
140	02a-CubeOh-Fe2C2P9	-2066.7657185	29.10
141	03b-AnticubeOh-Fe2P2C9	-2066.7657163	29.10
142	03b-AnticubeOh-Fe3P4C6	-2066.7561176	35.12
143	03a-AnticubeOh-Fe2C2P4	-2066.7561175	35.12
144	02b-CubeOh-Fe2P1C6_r-101	-2066.7561174	35.12
145	03a-AnticubeOh-Fe3C3P8	-2066.7561166	35.12
146	02b-CubeOh-Fe1P2C5	-2066.7561166	35.12
147	01a-Icos-Fe1C1P6	-2066.7561158	35.12
148	03b-AnticubeOh-Fe3P1C3	-2066.7561135	35.13
149	03a-AnticubeOh-Fe3C3P1	-2066.7561086	35.13
150	03a-AnticubeOh-Fe1C2P8	-2066.7561084	35.13
151	03b-AnticubeOh-Fe2P2C4	-2066.7438233	42.84
152	03a-AnticubeOh-Fe1C3P4_r-401	-2066.7379492	46.52
153	02b-CubeOh-Fe1P2C3_r-20	-2066.7361297	47.67
154	03b-AnticubeOh-Fe3P1C4	-2066.7361279	47.67
155	01a-Icos-Fe1C1P3	-2066.7361270	47.67
156	02b-CubeOh-Fe1P1C7	-2066.7361238	47.67
157	02b-CubeOh-Fe2P3C3	-2066.7361152	47.68
158	02a-CubeOh-Fe2C1P1	-2066.7357497	47.90
159	03a-AnticubeOh-Fe1C2P4	-2066.7357422	47.91
160	02b-CubeOh-Fe2P3C5	-2066.7354069	48.12
161	03a-AnticubeOh-Fe1C2P2	-2066.7353860	48.13
162	03b-AnticubeOh-Fe1P2C2	-2066.7353841	48.13
163	02a-CubeOh-Fe2C3P5	-2066.7353840	48.13
164	03a-AnticubeOh-Fe1C1P1	-2066.7353809	48.14
165	02b-CubeOh-Fe2P1C9	-2066.7353794	48.14

166	03a-AnticubeOh-Fe1C2P6	-2066.7332535	49.47
167	03b-AnticubeOh-Fe1P2C6	-2066.7332509	49.47
168	03a-AnticubeOh-Fe1C1P6	-2066.7332502	49.47
169	03b-AnticubeOh-Fe1P1C6	-2066.7332499	49.47
170	02b-CubeOh-Fe2P3C7	-2066.7332488	49.47
171	02a-CubeOh-Fe2C3P7	-2066.7332450	49.48
172	03a-AnticubeOh-Fe3C2P4	-2066.7332364	49.48
173	02a-CubeOh-Fe2C2P2	-2066.7331723	49.52
174	02b-CubeOh-Fe2P4C2	-2066.7331723	49.52
175	02b-CubeOh-Fe2P2C3	-2066.7331714	49.52
176	01a-Icos-Fe1C2P1	-2066.7331713	49.52
177	02b-CubeOh-Fe2P2C2	-2066.7331713	49.52
178	02a-CubeOh-Fe2C4P2	-2066.7331703	49.52
179	01b-Icos-Fe1P2C1	-2066.7331703	49.52
180	02a-CubeOh-Fe2C2P3	-2066.7331657	49.53
181	03b-AnticubeOh-Fe3P3C7	-2066.7297114	51.69
182	03a-AnticubeOh-Fe3C4P7	-2066.7297006	51.70
183	03b-AnticubeOh-Fe3P4C7	-2066.7297006	51.70
184	01a-Icos-Fe1C2P3	-2066.7297005	51.70
185	02a-CubeOh-Fe2C4P3	-2066.7296994	51.70
186	02b-CubeOh-Fe2P5C2	-2066.7296930	51.71
187	02a-CubeOh-Fe2C4P6	-2066.7281474	52.68
188	03a-AnticubeOh-Fe1C2P7	-2066.7281451	52.68
189	03b-AnticubeOh-Fe1P3C1	-2066.7281435	52.68
190	02b-CubeOh-Fe2P3C8	-2066.7281344	52.68
191	02b-CubeOh-Fe1P1C5	-2066.7274503	53.11
192	03a-AnticubeOh-Fe3C1P10	-2066.7258216	54.13
193	02a-CubeOh-Fe1C1P6	-2066.7258199	54.14
194	03b-AnticubeOh-Fe1P1C4	-2066.7258195	54.14
195	03a-AnticubeOh-Fe3C4P4	-2066.7258193	54.14
196	02a-CubeOh-Fe2C1P6	-2066.7258155	54.14
197	02a-CubeOh-Fe2C3P4	-2066.7258098	54.14
198	03a-AnticubeOh-Fe2C3P1	-2066.7215408	56.82
199	03a-AnticubeOh-Fe3C2P1	-2066.7200843	57.74
200	03a-AnticubeOh-Fe3C1P4	-2066.7199032	57.85
201	03a-AnticubeOh-Fe2C3P2_i-248	-2066.7196043	58.04
202	03b-AnticubeOh-Fe1P1C1_i-248	-2066.7195974	58.04
203	03a-AnticubeOh-Fe2C2P5	-2066.7189495	58.45
204	02b-CubeOh-Fe2P2C9	-2066.7172684	59.50
205	03b-AnticubeOh-Fe1P1C7	-2066.7170070	59.67
206	03b-AnticubeOh-Fe1P2C9	-2066.7170067	59.67
207	02b-CubeOh-Fe2P1C4	-2066.7170053	59.67

208	03a-AnticubeOh-Fe3C4P3	-2066.7158759	60.38
209	02b-CubeOh-Fe2P4C3	-2066.7158708	60.38
210	01b-Icos-Fe1P2C3	-2066.7158700	60.38
211	03b-AnticubeOh-Fe1P2C8	-2066.7156384	60.52
212	03a-AnticubeOh-Fe3C2P9	-2066.7156324	60.53
213	03a-AnticubeOh-Fe3C4P5	-2066.7156324	60.53
214	02b-CubeOh-Fe2P3C4	-2066.7150149	60.92
215	03a-AnticubeOh-Fe2C3P4_r-349	-2066.7150148	60.92
216	03a-AnticubeOh-Fe2C1P4	-2066.7150138	60.92
217	03a-AnticubeOh-Fe1C1P4	-2066.7150132	60.92
218	02b-CubeOh-Fe1P1C6	-2066.7150127	60.92
219	02b-CubeOh-Fe2P4C1	-2066.7146898	61.12
220	02a-CubeOh-Fe2C4P7	-2066.7136686	61.76
221	02a-CubeOh-Fe1C2P2	-2066.7131511	62.09
222	03b-AnticubeOh-Fe1P2C3	-2066.7131426	62.09
223	02a-CubeOh-Fe2C2P8	-2066.7122255	62.67
224	02b-CubeOh-Fe2P3C6	-2066.7122243	62.67
225	03b-AnticubeOh-Fe1P2C7	-2066.7115488	63.09
226	03a-AnticubeOh-Fe1C1P7	-2066.7115431	63.09
227	03a-AnticubeOh-Fe1C3P1	-2066.7115393	63.10
228	03b-AnticubeOh-Fe3P4C2	-2066.7109411	63.47
229	02a-CubeOh-Fe2C1P4	-2066.7091381	64.60
230	02a-CubeOh-Fe2C1P3	-2066.7081335	65.23
231	02b-CubeOh-Fe1P3C2	-2066.7073345	65.74
232	02b-CubeOh-Fe2P3C1	-2066.7073330	65.74
233	03b-AnticubeOh-Fe3P1C2	-2066.7073330	65.74
234	02b-CubeOh-Fe2P1C3	-2066.7073180	65.75
235	03a-AnticubeOh-Fe1C3P2	-2066.7059974	66.57
236	02b-CubeOh-Fe2P1C6_i-101	-2066.7049953	67.20
237	02b-CubeOh-Fe2P1C10	-2066.7048678	67.28
238	03b-AnticubeOh-Fe1P3C3	-2066.7048648	67.29
239	03b-AnticubeOh-Fe1P1C2	-2066.7048566	67.29
240	02b-CubeOh-Fe1P3C3	-2066.7041019	67.76
241	03b-AnticubeOh-Fe3P1C1	-2066.7021344	69.00
242	03a-AnticubeOh-Fe1C2P5	-2066.7015495	69.37
243	02b-CubeOh-Fe2P6C1	-2066.6991215	70.89
244	03a-AnticubeOh-Fe3C2P7	-2066.6982527	71.43
245	03b-AnticubeOh-Fe3P2C7	-2066.6982500	71.44
246	03a-AnticubeOh-Fe3C1P1	-2066.6977446	71.75
247	02b-CubeOh-Fe1P3C4	-2066.6969330	72.26
248	03b-AnticubeOh-Fe3P5C2	-2066.6955957	73.10
249	03a-AnticubeOh-Fe2C3P5	-2066.6950245	73.46

250	03a-AnticubeOh-Fe3C2P5	-2066.6948478	73.57
251	03b-AnticubeOh-Fe3P2C5	-2066.6948474	73.57
252	02b-CubeOh-Fe1P3C1	-2066.6947056	73.66
253	02a-CubeOh-Fe1C3P4	-2066.6944098	73.85
254	03b-AnticubeOh-Fe3P2C9	-2066.6942526	73.94
255	03b-AnticubeOh-Fe3P4C5	-2066.6942514	73.95
256	02a-CubeOh-Fe2C5P2	-2066.6942493	73.95
257	02a-CubeOh-Fe1C3P3	-2066.6930730	74.69
258	03a-AnticubeOh-Fe2C4P4	-2066.6905567	76.26
259	03a-AnticubeOh-Fe2C2P1	-2066.6904854	76.31
260	03b-AnticubeOh-Fe2P2C1	-2066.6904853	76.31
261	03a-AnticubeOh-Fe1C2P3	-2066.6890503	77.21
262	02a-CubeOh-Fe2C1P5	-2066.6887739	77.38
263	02a-CubeOh-Fe1C3P1	-2066.6885438	77.53
264	02b-CubeOh-Fe1P2C3_i-20	-2066.6862922	78.94
265	03b-AnticubeOh-Fe1P3C5	-2066.6822020	81.51
266	02b-CubeOh-Fe2P2C5	-2066.6821975	81.51
267	03a-AnticubeOh-Fe1C1P3	-2066.6811491	82.17
268	03a-AnticubeOh-Fe2C1P1	-2066.6802342	82.74
269	03b-AnticubeOh-Fe2P1C1	-2066.6802332	82.74
270	03b-AnticubeOh-Fe1P4C2	-2066.6797123	83.07
271	03b-AnticubeOh-Fe1P3C2	-2066.6792564	83.36
272	03b-AnticubeOh-Fe1P4C1	-2066.6780033	84.14
273	03a-AnticubeOh-Fe1C4P1	-2066.6780025	84.14
274	03b-AnticubeOh-Fe2P3C3_i-55	-2066.6737009	86.84
275	03b-AnticubeOh-Fe2P4C4_i-83	-2066.6736938	86.85
276	03b-AnticubeOh-Fe1P1C3_r-38	-2066.6700138	89.16
277	03b-AnticubeOh-Fe1P1C3_i-38	-2066.6691589	89.69
278	03b-AnticubeOh-Fe3P1C6	-2066.6686431	90.02
279	03a-AnticubeOh-Fe1C3P5	-2066.6679305	90.46
280	03a-AnticubeOh-Fe2C3P4_i-349	-2066.6678721	90.50
281	03b-AnticubeOh-Fe2P4C3	-2066.6665034	91.36
282	03a-AnticubeOh-Fe2C4P3	-2066.6665000	91.36
283	03a-AnticubeOh-Fe3C2P2	-2066.6662901	91.49
284	03a-AnticubeOh-Fe3C2P3	-2066.6660579	91.64
285	03b-AnticubeOh-Fe3P4C3	-2066.6660563	91.64
286	03a-AnticubeOh-Fe2C2P6	-2066.6655434	91.96
287	02a-CubeOh-Fe2C2P5	-2066.6624875	93.88
288	03a-AnticubeOh-Fe1C4P2	-2066.6624868	93.88
289	02a-CubeOh-Fe1C2P3	-2066.6587999	96.19
290	03b-AnticubeOh-Fe3P2C3	-2066.6569255	97.37
291	03b-AnticubeOh-Fe2P2C3	-2066.6556361	98.18

292	03b-AnticubeOh-Fe2P4C2_i-56	-2066.6556336	98.18
293	02b-CubeOh-Fe2P4C7	-2066.6556320	98.18
294	02a-CubeOh-Fe2C5P1	-2066.6550659	98.54
295	03b-AnticubeOh-Fe2P3C5	-2066.6525376	100.12
296	03a-AnticubeOh-Fe1C3P3_i-261	-2066.6493882	102.10
297	03b-AnticubeOh-Fe3P2C2	-2066.6469913	103.60
298	03b-AnticubeOh-Fe3P6C1	-2066.6403239	107.79
299	03a-AnticubeOh-Fe2C2P3	-2066.6397708	108.13
300	03a-AnticubeOh-Fe2C4P1	-2066.6397646	108.14
301	03b-AnticubeOh-Fe2P2C5	-2066.6206265	120.15
302	03a-AnticubeOh-Fe1C3P4_i-401	-2066.6142929	124.12
303	03b-AnticubeOh-Fe1P3C4_i-366	-2066.6134193	124.67
304	03b-AnticubeOh-Fe2P4C4_r-83	-2066.5933599	137.26