

Polyhedral Cobaltadiselenaboranes: *Nido* Structures without Bridging Hydrogens

Amr A. A. Attia,^{1,2} Alexandru Lupan,*¹ and R. Bruce King*³

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

² *National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*

³ *Department of Chemistry and Center for Computational Quantum Chemistry, University of Georgia, Athens, Georgia, 30602, USA*

Supporting Information

Table S1A. Initial CpCoSe₂B₅H₅ structures.

Table S1B. Distance table for the lowest-lying CpCoSe₂B₅H₅ structures.

Table S1C. Energy ranking for all the CpCoSe₂B₅H₅ structures.

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Table S6. Orbital energies and HOMO/LUMO gaps.

Cartesian coordinates of all optimized structures (M06-L/6-311G(d,p)).

Complete Gaussian09 Reference (reference 24)

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 CpCoSe₂B₅H₅ structures, 291 structures:

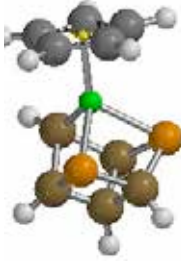
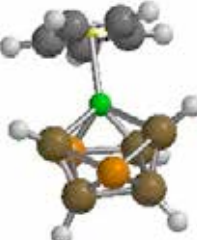
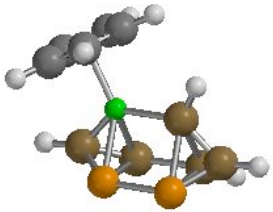
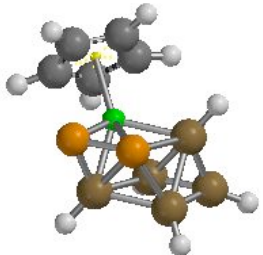
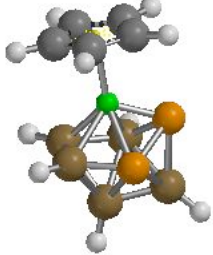
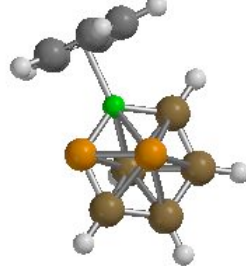
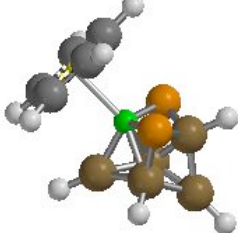
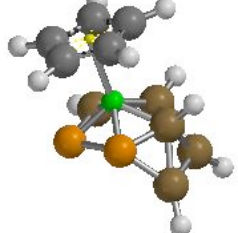

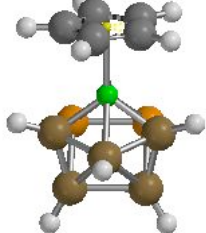
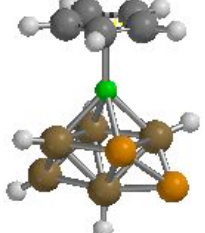
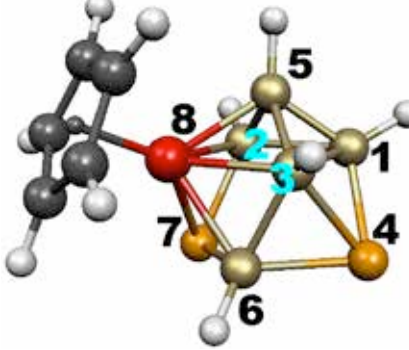
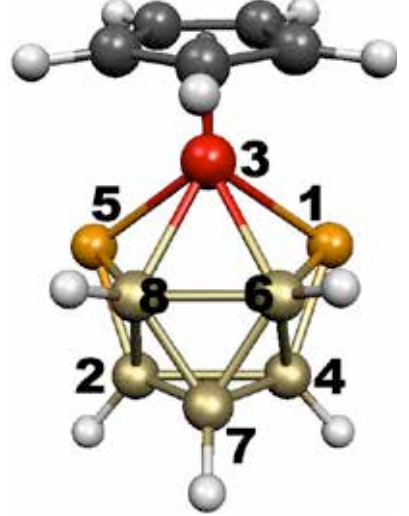
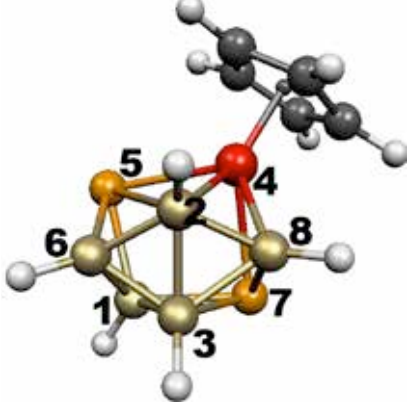
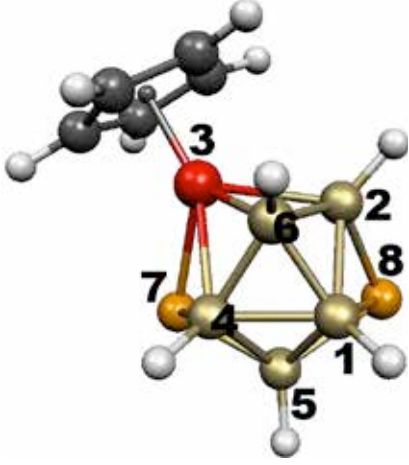
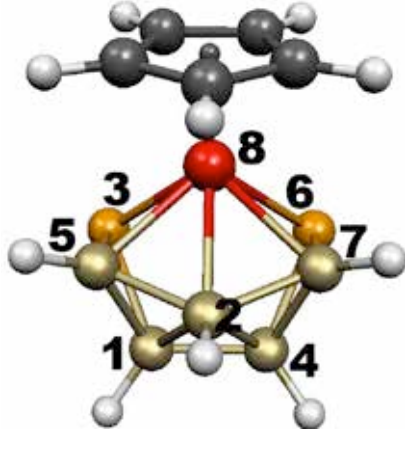
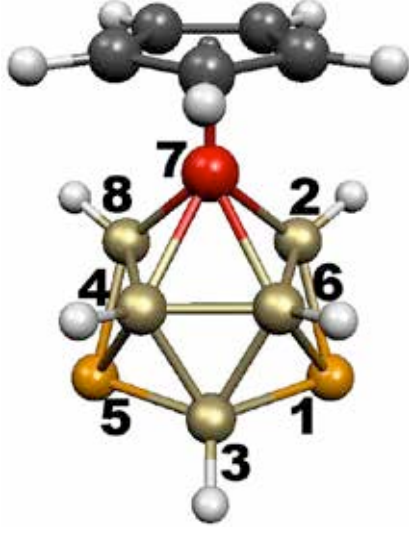
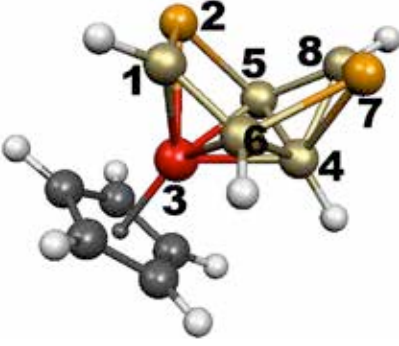
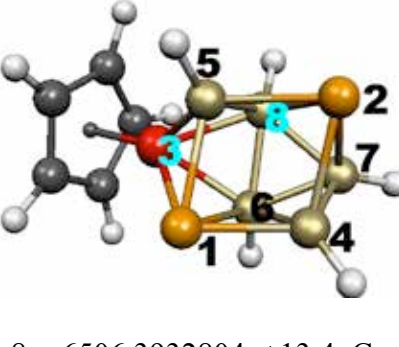
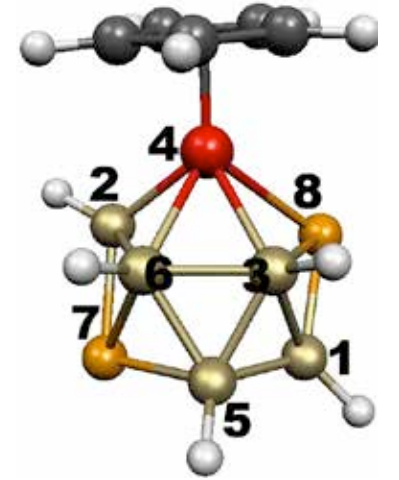
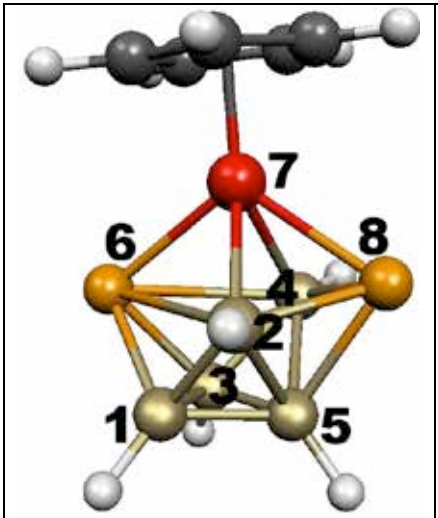
<p>Initial structures</p>	 <p>1. Cube 7</p>	 <p>2. Antiprism 11</p>
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Table S1B. Distance table for the lowest-lying CpCoSe₂B₅H₅ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -6506.4145852 0.0 C₁</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.050512</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.861402</td><td>2.710680</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Se</td><td>1.980502</td><td>3.289335</td><td>2.078780</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>1.650376</td><td>1.693784</td><td>1.712288</td><td>3.151374</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.792426</td><td>2.794028</td><td>1.896722</td><td>2.044669</td><td>2.912809</td></tr> <tr><td>7 Se</td><td>3.231661</td><td>1.970467</td><td>3.255014</td><td>3.282889</td><td>3.191196</td></tr> <tr><td>8 Co</td><td>3.075145</td><td>2.168051</td><td>2.130728</td><td>3.594855</td><td>2.007613</td></tr> <tr><td></td><td>6</td><td>7</td><td>8</td><td></td><td></td></tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Se</td><td>2.025828</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Co</td><td>2.101003</td><td>2.329242</td><td>0.000000</td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.050512	0.000000				3 B	1.861402	2.710680	0.000000			4 Se	1.980502	3.289335	2.078780	0.000000		5 B	1.650376	1.693784	1.712288	3.151374	0.000000	6 B	2.792426	2.794028	1.896722	2.044669	2.912809	7 Se	3.231661	1.970467	3.255014	3.282889	3.191196	8 Co	3.075145	2.168051	2.130728	3.594855	2.007613		6	7	8			6 B	0.000000					7 Se	2.025828	0.000000				8 Co	2.101003	2.329242	0.000000		
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5 B	1.839146	2.807352	3.180580	1.871647	0.000000																																																																										
6 B	1.723583	1.689726	1.948784	1.737928	2.927452																																																																										
7 Se	3.218342	3.358964	2.311389	2.040404	2.003495																																																																										
8 Se	2.075509	1.985136	3.547779	3.224485	2.032339																																																																										
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7 Se	3.254976	0.000000																																																																													
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	1	2	3	4	5
1 B	0.000000				
2 B	1.753134	0.000000			
3 B	1.779351	2.801317	0.000000		
4 B	2.787864	2.661208	1.753902	0.000000	
5 B	1.702524	1.916706	1.699061	1.915848	0.000000
6 Se	2.014553	2.639924	2.010922	2.609409	2.973085
7 Co	3.077395	2.133966	3.096061	2.139759	3.050404
8 Se	3.236131	2.043252	3.238480	2.041868	2.107366
	6	7	8		
6 Se	0.000000				
7 Co	2.327969	0.000000			
8 Se	3.762654	2.288832	0.000000		

Table S1C. Energy ranking for all of the CpCoSe₂B₅H₅ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	10-DicapTrPrism-Co3Se5Se1	-6502.2230052	0.00
2	10-DicapTrPrism-Co1Se1Se6	-6502.2229716	0.02
3	11-DicapOh-Co1Se1Se4	-6502.2229702	0.02
4	11-DicapOh-Co2Se1Se3	-6502.2229682	0.02
5	08-Nido-Co2Se1Se1	-6502.2229628	0.03
6	06-Bipirhex-Co2Se2Se1	-6502.2229587	0.03
7	03-TrigPyr-CoSe1Se2	-6502.2229517	0.03
8	09-DicapTrPr-Co2Se1Se4	-6502.2229355	0.04
9	10-DicapTrPrism-Co2Se2Se5	-6502.2182724	2.97
10	04-AntiprTrig-CoSe1Se3	-6502.2182669	2.97
11	05-Bisdisph-Co1Se3Se1	-6502.2182652	2.97
12	08-Nido-Co1Se3Se4	-6502.2182646	2.97
13	02-Antipr-CoSe3Se2	-6502.2182635	2.98
14	11-DicapOh-Co1Se2Se1	-6502.2182633	2.98
15	10-DicapTrPrism-Co3Se2Se4	-6502.2182617	2.98
16	11-DicapOh-Co1Se2Se3	-6502.2182614	2.98
17	09-DicapTrPr-Co1Se2Se2	-6502.2182583	2.98
18	10-DicapTrPrism-Co2Se3Se4	-6502.2182572	2.98
19	09-DicapTrPr-Co3Se5Se2	-6502.2182561	2.98
20	06-Bipirhex-Co2Se2Se3	-6502.2182527	2.98
21	04-AntiprTrig-CoSe2Se3	-6502.2182505	2.98
22	08-Nido-Co2Se2Se2	-6502.2182433	2.99
23	01-Cube-CoSe1Se4	-6502.2182426	2.99
24	10-DicapTrPrism-Co3Se2Se3	-6502.2182422	2.99
25	08-Nido-Co1Se1Se2	-6502.2182388	2.99
26	05-Bisdisph-Co1Se2Se3	-6502.2182382	2.99
27	09-DicapTrPr-Co3Se4Se3	-6502.2182371	2.99
28	10-DicapTrPrism-Co3Se2Se1	-6502.2182350	2.99
29	04-AntiprTrig-CoSe2Se5	-6502.2182342	2.99
30	09-DicapTrPr-Co2Se3Se2	-6502.2182340	2.99
31	09-DicapTrPr-Co3Se2Se3	-6502.2182338	2.99
32	02-Antipr-CoSe1Se6	-6502.2182335	2.99
33	05-Bisdisph-Co1Se4Se1	-6502.2182329	2.99
34	07-Tdallcap-Co1Se3Se3	-6502.2182314	3.00
35	10-DicapTrPrism-Co1Se2Se5	-6502.2182265	3.00
36	10-DicapTrPrism-Co3Se4Se2	-6502.2182261	3.00
37	11-DicapOh-Co1Se1Se3	-6502.2182238	3.00
38	09-DicapTrPr-Co3Se1Se1	-6502.2182195	3.00
39	07-Tdallcap-Co2Se3Se1	-6502.2182172	3.00

40	09-DicapTrPr-Co1Se4Se1	-6502.2182148	3.01
41	09-DicapTrPr-Co3Se3Se3	-6502.2182130	3.01
42	09-DicapTrPr-Co1Se3Se1	-6502.2182093	3.01
43	09-DicapTrPr-Co2Se1Se1	-6502.2182072	3.01
44	09-DicapTrPr-Co3Se2Se1	-6502.2182062	3.01
45	10-DicapTrPrism-Co2Se1Se6	-6502.2181989	3.02
46	07-Tdallcap-Co2Se4Se1	-6502.2181966	3.02
47	09-DicapTrPr-Co2Se3Se3	-6502.2181907	3.02
48	09-DicapTrPr-Co3Se1Se5	-6502.2181901	3.02
49	07-Tdallcap-Co1Se2Se2	-6502.2181900	3.02
50	04-AntiprTrig-CoSe4Se1	-6502.2181851	3.02
51	09-DicapTrPr-Co2Se2Se5	-6502.2181842	3.03
52	11-DicapOh-Co3Se3Se3	-6502.2181792	3.03
53	01-Cube-CoSe2Se1	-6502.2181704	3.03
54	07-Tdallcap-Co1Se1Se6	-6502.2138330	5.76
55	09-DicapTrPr-Co1Se2Se4	-6502.2138317	5.76
56	02-Antipr-CoSe1Se3	-6502.2138306	5.76
57	08-Nido-Co2Se4Se1	-6502.2138259	5.76
58	10-DicapTrPrism-Co1Se1Se1	-6502.2138241	5.76
59	10-DicapTrPrism-Co2Se1Se2	-6502.2138223	5.76
60	11-DicapOh-Co1Se1Se5	-6502.2138218	5.76
61	08-Nido-Co2Se1Se6	-6502.2138210	5.76
62	09-DicapTrPr-Co2Se1Se6	-6502.2138207	5.76
63	09-DicapTrPr-Co2Se4Se2	-6502.2138204	5.76
64	10-DicapTrPrism-Co1Se2Se1	-6502.2138192	5.76
65	10-DicapTrPrism-Co3Se1Se5	-6502.2138162	5.77
66	05-Bisdisph-Co2Se1Se1	-6502.2138154	5.77
67	09-DicapTrPr-Co3Se1Se3	-6502.2138132	5.77
68	10-DicapTrPrism-Co3Se1Se4	-6502.2138104	5.77
69	05-Bisdisph-Co1Se1Se1	-6502.2138064	5.77
70	04-AntiprTrig-CoSe1Se2	-6502.2138061	5.77
71	09-DicapTrPr-Co2Se5Se2	-6502.2138010	5.78
72	07-Tdallcap-Co2Se1Se6	-6502.2137969	5.78
73	10-DicapTrPrism-Co2Se1Se4	-6502.2137948	5.78
74	09-DicapTrPr-Co1Se1Se6	-6502.2137928	5.78
75	11-DicapOh-Co3Se5Se1	-6502.2137896	5.78
76	07-Tdallcap-Co2Se1Se1	-6502.2137883	5.78
77	05-Bisdisph-Co1Se1Se2	-6502.2137858	5.79
78	10-DicapTrPrism-Co3Se1Se3	-6502.2137840	5.79
79	11-DicapOh-Co3Se2Se5	-6502.2137753	5.79
80	01-Cube-CoSe1Se1	-6502.2137701	5.80
81	10-DicapTrPrism-Co2Se2Se1	-6502.2137664	5.80
82	02-Antipr-CoSe1Se2	-6502.2137507	5.81

83	09-DicapTrPr-Co1Se2Se5	-6502.2137496	5.81
84	04-AntiprTrig-CoSe3Se2	-6502.2137490	5.81
85	10-DicapTrPrism-Co2Se1Se1	-6502.2051857	11.18
86	07-Tdallcap-Co2Se4Se2	-6502.2051498	11.20
87	08-Nido-Co1Se1Se5	-6502.2051488	11.21
88	09-DicapTrPr-Co1Se1Se1	-6502.2051478	11.21
89	10-DicapTrPrism-Co3Se6Se1	-6502.2051384	11.21
90	05-Bisdisph-Co1Se4Se3	-6502.2051339	11.21
91	07-Tdallcap-Co1Se1Se3	-6502.2051325	11.22
92	07-Tdallcap-Co1Se3Se2	-6502.2051325	11.22
93	07-Tdallcap-Co1Se1Se5	-6502.2051225	11.22
94	07-Tdallcap-Co2Se1Se2	-6502.2051161	11.23
95	07-Tdallcap-Co2Se1Se5	-6502.2050935	11.24
96	08-Nido-Co1Se1Se3	-6502.2030433	12.53
97	10-DicapTrPrism-Co2Se1Se5	-6502.2029873	12.56
98	05-Bisdisph-Co1Se3Se2	-6502.2029868	12.56
99	07-Tdallcap-Co2Se3Se2	-6502.2029808	12.57
100	09-DicapTrPr-Co2Se1Se2	-6502.2029735	12.57
101	10-DicapTrPrism-Co3Se4Se3	-6502.2029654	12.58
102	10-DicapTrPrism-Co1Se2Se4	-6502.2029605	12.58
103	10-DicapTrPrism-Co2Se3Se1	-6502.2029605	12.58
104	09-DicapTrPr-Co1Se3Se2	-6502.2029581	12.58
105	10-DicapTrPrism-Co2Se3Se2	-6502.2029576	12.58
106	09-DicapTrPr-Co3Se4Se2	-6502.2029525	12.58
107	07-Tdallcap-Co2Se1Se3	-6502.2029505	12.58
108	07-Tdallcap-Co2Se2Se3	-6502.2029505	12.58
109	07-Tdallcap-Co1Se1Se4	-6502.2029501	12.58
110	11-DicapOh-Co1Se1Se2	-6502.2029486	12.59
111	08-Nido-Co1Se3Se3	-6502.2029471	12.59
112	09-DicapTrPr-Co2Se2Se3	-6502.2029461	12.59
113	10-DicapTrPrism-Co3Se2Se2	-6502.2029421	12.59
114	10-DicapTrPrism-Co3Se3Se3	-6502.2029412	12.59
115	03-TrigPyr-CoSe2Se3	-6502.2029347	12.59
116	07-Tdallcap-Co1Se4Se1	-6502.2029342	12.59
117	05-Bisdisph-Co1Se1Se4	-6502.2029336	12.60
118	07-Tdallcap-Co1Se1Se2	-6502.2029329	12.60
119	10-DicapTrPrism-Co2Se2Se4	-6502.2029305	12.60
120	09-DicapTrPr-Co2Se2Se2	-6502.2029256	12.60
121	05-Bisdisph-Co2Se2Se2	-6502.2029251	12.60
122	09-DicapTrPr-Co1Se2Se3	-6502.2029250	12.60
123	10-DicapTrPrism-Co1Se3Se4	-6502.2029072	12.61
124	04-AntiprTrig-CoSe3Se1	-6502.2029041	12.61
125	11-DicapOh-Co2Se2Se3	-6502.2028999	12.62

126	02-Antipr-CoSe3Se3	-6502.2028930	12.62
127	07-Tdallcap-Co1Se2Se3	-6502.2028853	12.63
128	07-Tdallcap-Co2Se1Se4	-6502.2028522	12.65
129	05-Bisdisph-Co1Se4Se2	-6502.2005913	14.07
130	09-DicapTrPr-Co2Se5Se1	-6502.2005709	14.08
131	09-DicapTrPr-Co2Se3Se4	-6502.2005559	14.09
132	04-AntiprTrig-CoSe2Se2	-6502.2005489	14.09
133	02-Antipr-CoSe1Se5	-6502.2005451	14.09
134	08-Nido-Co2Se1Se2	-6502.2005416	14.10
135	11-DicapOh-Co2Se1Se4	-6502.2005269	14.11
136	08-Nido-Co2Se3Se1	-6502.2004957	14.13
137	08-Nido-Co2Se3Se4	-6502.2004885	14.13
138	10-DicapTrPrism-Co3Se3Se2	-6502.2004761	14.14
139	11-DicapOh-Co3Se4Se2	-6502.1989597	15.09
140	05-Bisdisph-Co2Se2Se5	-6502.1989566	15.09
141	10-DicapTrPrism-Co1Se2Se3	-6502.1989525	15.09
142	05-Bisdisph-Co2Se1Se2	-6502.1989520	15.09
143	08-Nido-Co2Se2Se1	-6502.1989419	15.10
144	10-DicapTrPrism-Co3Se1Se2	-6502.1989272	15.11
145	10-DicapTrPrism-Co3Se1Se1	-6502.1989254	15.11
146	10-DicapTrPrism-Co2Se2Se3	-6502.1989102	15.12
147	06-Bipirhex-Co1Se1Se2	-6502.1989097	15.12
148	10-DicapTrPrism-Co3Se4Se1	-6502.1955005	17.26
149	10-DicapTrPrism-Co2Se1Se3	-6502.1954396	17.30
150	05-Bisdisph-Co2Se4Se1	-6502.1954225	17.31
151	05-Bisdisph-Co2Se2Se4	-6502.1954188	17.31
152	10-DicapTrPrism-Co1Se1Se3	-6502.1954170	17.31
153	02-Antipr-CoSe2Se2	-6502.1954160	17.31
154	09-DicapTrPr-Co2Se6Se1	-6502.1953962	17.33
155	10-DicapTrPrism-Co1Se1Se4	-6502.1953841	17.33
156	09-DicapTrPr-Co2Se2Se4	-6502.1953812	17.33
157	10-DicapTrPrism-Co1Se3Se3	-6502.1953807	17.33
158	05-Bisdisph-Co2Se3Se2	-6502.1927158	19.01
159	11-DicapOh-Co1Se2Se2	-6502.1926963	19.02
160	04-AntiprTrig-CoSe2Se4	-6502.1926907	19.02
161	10-DicapTrPrism-Co3Se2Se5	-6502.1926904	19.02
162	02-Antipr-CoSe2Se1	-6502.1926901	19.02
163	10-DicapTrPrism-Co3Se3Se4	-6502.1926870	19.03
164	09-DicapTrPr-Co2Se2Se1	-6502.1926850	19.03
165	05-Bisdisph-Co1Se2Se2	-6502.1926831	19.03
166	11-DicapOh-Co3Se4Se3	-6502.1926781	19.03
167	09-DicapTrPr-Co2Se3Se1	-6502.1926684	19.04
168	06-Bipirhex-Co2Se3Se2	-6502.1926666	19.04

169	02-Antipr-CoSe3Se1	-6502.1926555	19.05
170	10-DicapTrPrism-Co1Se3Se1	-6502.1926554	19.05
171	05-Bisdisph-Co2Se2Se6	-6502.1926482	19.05
172	08-Nido-Co2Se3Se3	-6502.1918853	19.53
173	10-DicapTrPrism-Co1Se3Se2	-6502.1918566	19.55
174	05-Bisdisph-Co2Se1Se4	-6502.1860466	23.19
175	02-Antipr-CoSe1Se4	-6502.1860407	23.20
176	09-DicapTrPr-Co3Se1Se4	-6502.1860398	23.20
177	10-DicapTrPrism-Co1Se2Se2	-6502.1860351	23.20
178	08-Nido-Co2Se1Se5	-6502.1860315	23.20
179	10-DicapTrPrism-Co1Se1Se5	-6502.1860066	23.22
180	08-Nido-Co2Se4Se2	-6502.1859770	23.24
181	09-DicapTrPr-Co1Se1Se5	-6502.1840926	24.42
182	05-Bisdisph-Co1Se5Se1	-6502.1840805	24.43
183	08-Nido-Co1Se2Se5	-6502.1795477	27.27
184	08-Nido-Co1Se1Se6	-6502.1768745	28.95
185	10-DicapTrPrism-Co3Se5Se2	-6502.1768261	28.98
186	09-DicapTrPr-Co1Se1Se3	-6502.1759791	29.51
187	06-Bipirhex-Co2Se1Se3	-6502.1759219	29.55
188	11-DicapOh-Co3Se1Se2	-6502.1759199	29.55
189	09-DicapTrPr-Co3Se1Se6	-6502.1746292	30.36
190	09-DicapTrPr-Co3Se3Se2	-6502.1746085	30.37
191	11-DicapOh-Co3Se6Se1	-6502.1740217	30.74
192	07-Tdallcap-Co1Se1Se1	-6502.1739737	30.77
193	04-AntiprTrig-CoSe1Se1	-6502.1738666	30.84
194	09-DicapTrPr-Co1Se1Se4	-6502.1738582	30.84
195	01-Cube-CoSe1Se2	-6502.1738439	30.85
196	11-DicapOh-Co2Se1Se1	-6502.1738346	30.86
197	10-DicapTrPrism-Co3Se3Se1	-6502.1738275	30.86
198	05-Bisdisph-Co2Se2Se3	-6502.1732407	31.23
199	02-Antipr-CoSe1Se1	-6502.1732275	31.24
200	08-Nido-Co2Se3Se2	-6502.1724913	31.70
201	09-DicapTrPr-Co2Se4Se3	-6502.1724818	31.70
202	08-Nido-Co1Se1Se4	-6502.1724743	31.71
203	04-AntiprTrig-CoSe2Se1	-6502.1724691	31.71
204	09-DicapTrPr-Co2Se1Se5	-6502.1724605	31.72
205	03-TrigPyr-CoSe1Se3	-6502.1724541	31.72
206	08-Nido-Co2Se4Se3	-6502.1724521	31.72
207	09-DicapTrPr-Co2Se1Se3	-6502.1724482	31.73
208	08-Nido-Co1Se2Se1	-6502.1724414	31.73
209	11-DicapOh-Co3Se5Se2	-6502.1724403	31.73
210	06-Bipirhex-Co2Se1Se2	-6502.1723145	31.81
211	11-DicapOh-Co3Se2Se3	-6502.1722678	31.84

212	03-TrigPyr-CoSe1Se4	-6502.1722108	31.87
213	09-DicapTrPr-Co3Se3Se4	-6502.1703942	33.01
214	11-DicapOh-Co3Se3Se2	-6502.1703073	33.07
215	03-TrigPyr-CoSe2Se1	-6502.1694373	33.61
216	08-Nido-Co1Se3Se1	-6502.1660636	35.73
217	07-Tdallcap-Co1Se3Se1	-6502.1660606	35.73
218	06-Bipirhex-Co1Se1Se4	-6502.1660457	35.74
219	07-Tdallcap-Co2Se2Se1	-6502.1660389	35.75
220	07-Tdallcap-Co1Se2Se1	-6502.1660325	35.75
221	07-Tdallcap-Co2Se2Se2	-6502.1660085	35.77
222	05-Bisdisph-Co2Se3Se1	-6502.1658310	35.88
223	08-Nido-Co2Se1Se4	-6502.1658301	35.88
224	11-DicapOh-Co3Se2Se2	-6502.1658172	35.89
225	10-DicapTrPrism-Co1Se1Se2	-6502.1657692	35.92
226	06-Bipirhex-Co2Se1Se1	-6502.1644709	36.73
227	11-DicapOh-Co3Se1Se1	-6502.1644512	36.74
228	11-DicapOh-Co2Se2Se1	-6502.1637197	37.20
229	08-Nido-Co1Se1Se1	-6502.1628481	37.75
230	11-DicapOh-Co3Se1Se3	-6502.1628245	37.76
231	09-DicapTrPr-Co3Se1Se2	-6502.1628040	37.78
232	11-DicapOh-Co2Se2Se2	-6502.1627847	37.79
233	09-DicapTrPr-Co1Se1Se2	-6502.1621951	38.16
234	05-Bisdisph-Co1Se1Se3	-6502.1608422	39.01
235	08-Nido-Co1Se2Se4	-6502.1608067	39.03
236	11-DicapOh-Co1Se1Se1	-6502.1608022	39.03
237	06-Bipirhex-Co1Se1Se1	-6502.1607590	39.06
238	08-Nido-Co1Se2Se2	-6502.1559611	42.07
239	05-Bisdisph-Co2Se1Se3	-6502.1557042	42.23
240	11-DicapOh-Co3Se1Se5	-6502.1556953	42.24
241	10-DicapTrPrism-Co3Se1Se6	-6502.1556876	42.24
242	10-DicapTrPrism-Co2Se2Se2	-6502.1551622	42.57
243	09-DicapTrPr-Co3Se2Se4	-6502.1551416	42.59
244	01-Cube-CoSe1Se3	-6502.1551377	42.59
245	06-Bipirhex-Co1Se1Se3	-6502.1551197	42.60
246	04-AntiprTrig-CoSe1Se4	-6502.1550953	42.61
247	11-DicapOh-Co3Se2Se4	-6502.1550880	42.62
248	03-TrigPyr-CoSe2Se2	-6502.1550033	42.67
249	09-DicapTrPr-Co3Se3Se1	-6502.1539735	43.32
250	09-DicapTrPr-Co3Se5Se1	-6502.1531210	43.85
251	11-DicapOh-Co3Se2Se1	-6502.1530758	43.88
252	11-DicapOh-Co2Se1Se2	-6502.1530511	43.90
253	11-DicapOh-Co3Se4Se1	-6502.1520762	44.51
254	06-Bipirhex-Co2Se2Se2	-6502.1519890	44.56

255	09-DicapTrPr-Co3Se2Se5	-6502.1518963	44.62
256	09-DicapTrPr-Co3Se4Se1	-6502.1508665	45.27
257	11-DicapOh-Co1Se1Se6	-6502.1504695	45.52
258	08-Nido-Co1Se3Se2	-6502.1502884	45.63
259	03-TrigPyr-CoSe4Se1	-6502.1502778	45.64
260	03-TrigPyr-CoSe1Se5	-6502.1502464	45.66
261	08-Nido-Co1Se2Se3	-6502.1502413	45.66
262	09-DicapTrPr-Co1Se2Se1	-6502.1466411	47.92
263	03-TrigPyr-CoSe1Se1	-6502.1463196	48.12
264	03-TrigPyr-CoSe1Se6	-6502.1438974	49.64
265	09-DicapTrPr-Co3Se6Se1	-6502.1426790	50.41
266	11-DicapOh-Co3Se1Se4	-6502.1420086	50.83
267	11-DicapOh-Co3Se3Se1	-6502.1414508	51.18
268	11-DicapOh-Co3Se3Se4	-6502.1411862	51.34
269	10-DicapTrPrism-Co2Se3Se3	-6502.1405161	51.76
270	05-Bisdisph-Co1Se2Se1	-6502.1404736	51.79
271	08-Nido-Co2Se1Se3	-6502.1374072	53.71
272	09-DicapTrPr-Co2Se4Se1	-6502.1361119	54.53
273	06-Bipirhex-Co2Se2Se4	-6502.1334797	56.18
274	06-Bipirhex-Co2Se3Se1	-6502.1326151	56.72
275	11-DicapOh-Co3Se1Se6	-6502.1314864	57.43
276	04-AntiprTrig-CoSe3Se3	-6502.1299256	58.41
277	06-Bipirhex-Co2Se1Se4	-6502.1268017	60.37
278	05-Bisdisph-Co2Se2Se1	-6502.1258017	61.00
279	01-Cube-CoSe2Se2	-6502.1223573	63.16
280	03-TrigPyr-CoSe3Se1	-6502.1184648	65.60
281	03-TrigPyr-CoSe3Se2	-6502.0931377	81.49
282	09-DicapTrPr-Co3Se2Se2	-6502.0853685	86.37

Table S2A. Initial CpCoSe₂B₆H₆ structures, 215 structures.

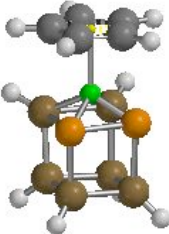
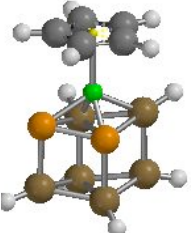

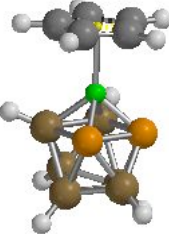
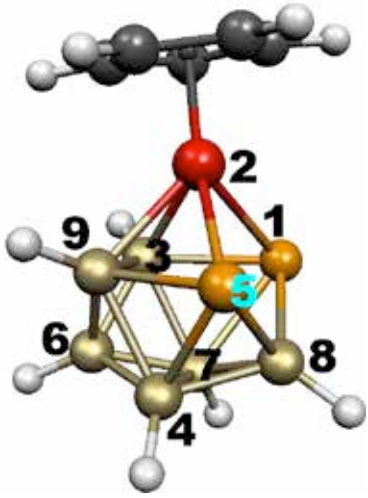
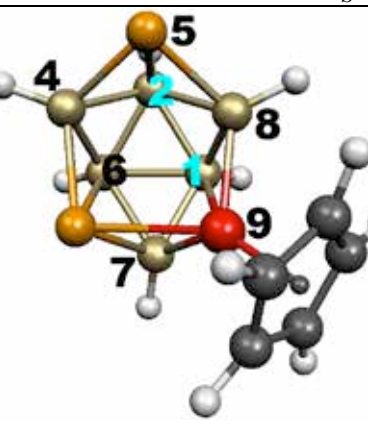
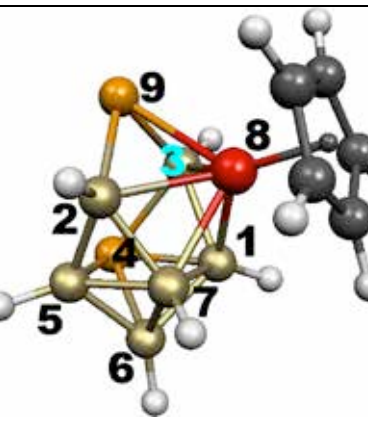
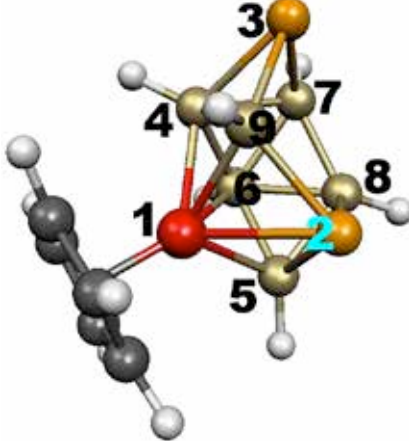
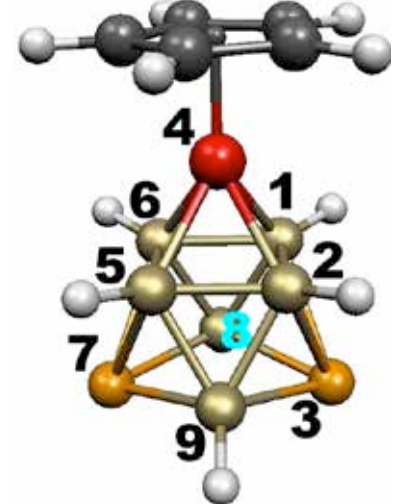
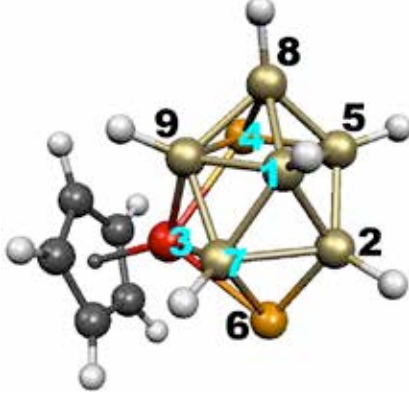
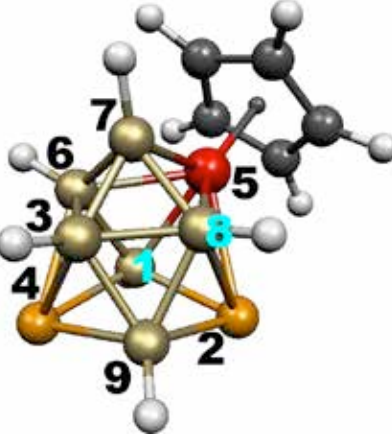
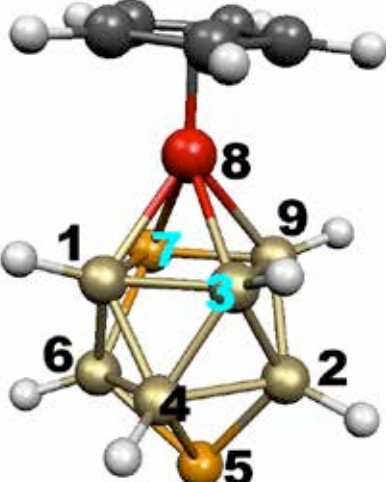
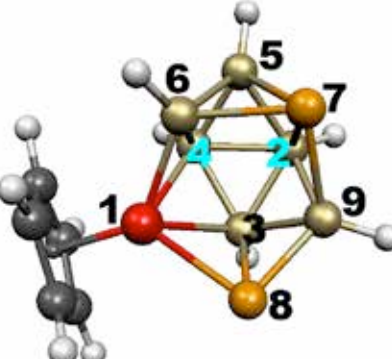
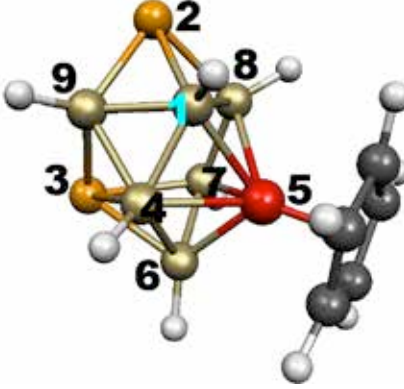
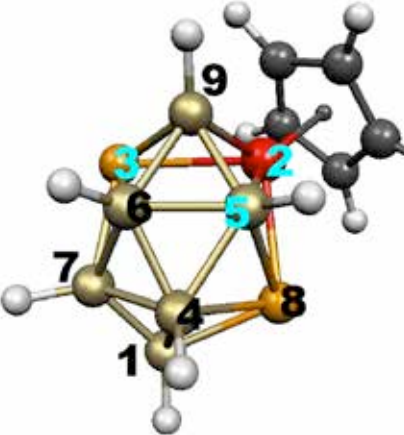
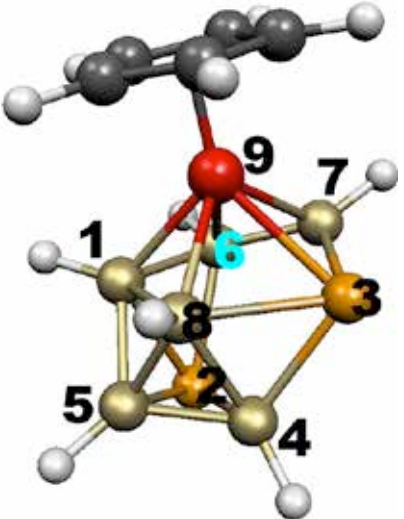
Initial structures
 <p>1. Capped cube 43 structures</p>
 <p>2. Pressed capped cube 67 structures</p>
 <p>3. Tl₉⁹⁻-like structure 79 structures</p>
 <p>4. Tricapped trigonal prism 26 structures</p>

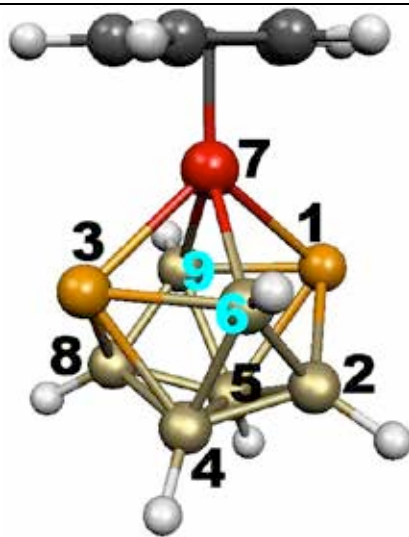
Table S2B. Distance table for the lowest-lying CpCoSe₂B₆H₆ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -6531.8871054 0.0 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 Se</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Co</td><td>2.352837</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>2.129942</td><td>2.120060</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.183805</td><td>3.351334</td><td>2.641395</td><td>0.000000</td><td></td></tr> <tr><td>5 Se</td><td>3.145552</td><td>2.352868</td><td>3.208503</td><td>2.145821</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.234671</td><td>3.290181</td><td>1.689139</td><td>1.678917</td><td>3.234541</td></tr> <tr><td>7 B</td><td>2.146358</td><td>3.351710</td><td>1.938912</td><td>1.758330</td><td>3.183807</td></tr> <tr><td>8 B</td><td>2.059509</td><td>3.064007</td><td>2.894639</td><td>1.806660</td><td>2.059438</td></tr> <tr><td>9 B</td><td>3.208538</td><td>2.120039</td><td>1.830490</td><td>1.938582</td><td>2.129963</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td></td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.678937</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.900293</td><td>1.806688</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.689071</td><td>2.641538</td><td>2.894680</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 Se	0.000000					2 Co	2.352837	0.000000				3 B	2.129942	2.120060	0.000000			4 B	3.183805	3.351334	2.641395	0.000000		5 Se	3.145552	2.352868	3.208503	2.145821	0.000000	6 B	3.234671	3.290181	1.689139	1.678917	3.234541	7 B	2.146358	3.351710	1.938912	1.758330	3.183807	8 B	2.059509	3.064007	2.894639	1.806660	2.059438	9 B	3.208538	2.120039	1.830490	1.938582	2.129963		6	7	8	9		6 B	0.000000					7 B	1.678937	0.000000				8 B	2.900293	1.806688	0.000000			9 B	1.689071	2.641538	2.894680	0.000000	
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 <p>10. -6531.8593560 +17.4 C₁</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Se</td><td>2.054155</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Se</td><td>3.127581</td><td>3.330232</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.754619</td><td>3.255172</td><td>2.175556</td><td>0.000000</td><td></td></tr> <tr><td>5 Co</td><td>2.053555</td><td>3.605623</td><td>3.295642</td><td>2.058609</td><td>0.000000</td></tr> <tr><td>6 B</td><td>3.033493</td><td>4.159923</td><td>2.046166</td><td>1.871256</td><td>1.925978</td></tr> <tr><td>7 B</td><td>2.855678</td><td>3.199311</td><td>2.142838</td><td>2.664656</td><td>2.113339</td></tr> <tr><td>8 B</td><td>1.985241</td><td>2.044170</td><td>3.086869</td><td>2.886708</td><td>2.106926</td></tr> <tr><td>9 B</td><td>1.813869</td><td>1.999671</td><td>2.074498</td><td>1.806386</td><td>3.257057</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th></th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.750037</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>2.953878</td><td>1.683353</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.136213</td><td>3.042573</td><td>2.792882</td><td>0.000000</td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Se	2.054155	0.000000				3 Se	3.127581	3.330232	0.000000			4 B	1.754619	3.255172	2.175556	0.000000		5 Co	2.053555	3.605623	3.295642	2.058609	0.000000	6 B	3.033493	4.159923	2.046166	1.871256	1.925978	7 B	2.855678	3.199311	2.142838	2.664656	2.113339	8 B	1.985241	2.044170	3.086869	2.886708	2.106926	9 B	1.813869	1.999671	2.074498	1.806386	3.257057		6	7	8	9		6 B	0.000000					7 B	1.750037	0.000000				8 B	2.953878	1.683353	0.000000			9 B	3.136213	3.042573	2.792882	0.000000	
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13. -6531.8500740 +23.2 C₂

	1	2	3	4	5	
1 Se	0.000000					
2 B	2.038330	0.000000				
3 Se	3.643733	3.161303	0.000000			
4 B	3.101237	1.704121	2.156302	0.000000		
5 B	2.162489	1.790354	3.106275	1.706853	0.000000	
6 B	2.660575	1.719564	2.028977	1.935668	2.803733	
7 Co	2.311045	3.078189	2.310799	3.293698	3.296135	
8 B	3.156141	2.898955	2.040834	1.792410	1.704399	
9 B	2.025288	2.949094	2.690232	2.809806	1.933028	
	6	7	8	9		
6 B	0.000000					
7 Co	2.143803	0.000000				
8 B	2.944688	3.060532	0.000000			
9 B	3.036614	2.147860	1.719686	0.000000		

Table S2C. Energy ranking for all of the CpCoSe₂B₆H₆ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	4-TricTrPrism-Co2Se1Se4	-6527.6855582	0.00
2	1-CapCube-Co2Se2Se1	-6527.6855566	0.00
3	4-TricTrPrism-Co2Se2Se2	-6527.6855334	0.02
4	3-Tl99-Co4Se1Se1	-6527.6855320	0.02
5	3-Tl99-Co3Se6Se2	-6527.6855292	0.02
6	2-PressCapCube-Co2Se1Se4	-6527.6855284	0.02
7	4-TricTrPrism-Co2Se1Se1	-6527.6855263	0.02
8	3-Tl99-Co4Se1Se6	-6527.6855249	0.02
9	3-Tl99-Co3Se1Se5	-6527.6855221	0.02
10	1-CapCube-Co2Se3Se2	-6527.6855097	0.03
11	3-Tl99-Co2Se3Se1	-6527.6855086	0.03
12	3-Tl99-Co3Se1Se4	-6527.6855027	0.03
13	4-TricTrPrism-Co1Se1Se1	-6527.6855025	0.03
14	1-CapCube-Co3Se5Se2	-6527.6854973	0.04
15	3-Tl99-Co4Se2Se1	-6527.6854904	0.04
16	3-Tl99-Co1Se1Se1	-6527.6854800	0.05
17	2-PressCapCube-Co1Se1Se2	-6527.6854769	0.05
18	2-PressCapCube-Co1Se2Se3	-6527.6766882	5.57
19	1-CapCube-Co1Se1Se4	-6527.6766783	5.57
20	3-Tl99-Co1Se1Se3	-6527.6766680	5.58
21	2-PressCapCube-Co3Se2Se4	-6527.6766586	5.58
22	2-PressCapCube-Co5Se1Se4	-6527.6766576	5.59
23	3-Tl99-Co3Se5Se1	-6527.6766451	5.59
24	3-Tl99-Co3Se1Se7	-6527.6697137	9.94
25	3-Tl99-Co3Se4Se3	-6527.6697081	9.95
26	3-Tl99-Co2Se3Se4	-6527.6696953	9.95
27	2-PressCapCube-Co5Se2Se4	-6527.6696526	9.98
28	2-PressCapCube-Co1Se1Se4	-6527.6696488	9.98
29	3-Tl99-Co2Se2Se1	-6527.6696486	9.98
30	2-PressCapCube-Co5Se3Se3	-6527.6696427	9.99
31	2-PressCapCube-Co5Se3Se2	-6527.6696406	9.99
32	3-Tl99-Co2Se3Se2	-6527.6696298	10.00
33	2-PressCapCube-Co2Se2Se4	-6527.6696246	10.00
34	2-PressCapCube-Co2Se2Se3	-6527.6695952	10.02
35	4-TricTrPrism-Co2Se4Se1	-6527.6695877	10.02
36	2-PressCapCube-Co3Se1Se5	-6527.6693614	10.16
37	2-PressCapCube-Co5Se1Se5	-6527.6693369	10.18
38	3-Tl99-Co3Se1Se6	-6527.6693165	10.19
39	3-Tl99-Co2Se1Se3	-6527.6693032	10.20
40	2-PressCapCube-Co2Se1Se1	-6527.6693030	10.20

41	1-CapCube-Co3Se4Se2	-6527.6692998	10.20
42	1-CapCube-Co1Se1Se2	-6527.6692956	10.21
43	3-Tl99-Co2Se1Se1	-6527.6692897	10.21
44	4-TricTrPrism-Co2Se1Se6	-6527.6692865	10.21
45	1-CapCube-Co2Se2Se3	-6527.6692820	10.21
46	3-Tl99-Co4Se1Se3	-6527.6692791	10.22
47	2-PressCapCube-Co3Se1Se4	-6527.6692680	10.22
48	2-PressCapCube-Co1Se1Se1	-6527.6692661	10.22
49	3-Tl99-Co4Se2Se2	-6527.6692542	10.23
50	2-PressCapCube-Co3Se1Se1	-6527.6692470	10.24
51	1-CapCube-Co2Se1Se4	-6527.6645957	13.15
52	2-PressCapCube-Co2Se5Se1	-6527.6645544	13.18
53	3-Tl99-Co3Se4Se2	-6527.6645503	13.18
54	3-Tl99-Co4Se3Se4	-6527.6645369	13.19
55	2-PressCapCube-Co2Se3Se2	-6527.6645197	13.20
56	1-CapCube-Co2Se2Se4	-6527.6644466	13.25
57	1-CapCube-Co3Se6Se1	-6527.6584536	17.01
58	4-TricTrPrism-Co2Se2Se3	-6527.6584439	17.01
59	4-TricTrPrism-Co2Se2Se4	-6527.6584411	17.02
60	3-Tl99-Co4Se1Se4	-6527.6584386	17.02
61	3-Tl99-Co1Se1Se5	-6527.6584320	17.02
62	2-PressCapCube-Co5Se1Se1	-6527.6584289	17.02
63	2-PressCapCube-Co3Se1Se3	-6527.6584280	17.02
64	2-PressCapCube-Co3Se3Se2	-6527.6584252	17.03
65	3-Tl99-Co1Se2Se1	-6527.6584198	17.03
66	3-Tl99-Co3Se5Se3	-6527.6584084	17.04
67	3-Tl99-Co3Se4Se4	-6527.6584077	17.04
68	2-PressCapCube-Co2Se1Se3	-6527.6584016	17.04
69	3-Tl99-Co1Se1Se6	-6527.6584000	17.04
70	1-CapCube-Co2Se3Se1	-6527.6583974	17.04
71	2-PressCapCube-Co3Se6Se1	-6527.6583945	17.05
72	3-Tl99-Co2Se1Se4	-6527.6583883	17.05
73	2-PressCapCube-Co2Se6Se1	-6527.6583866	17.05
74	3-Tl99-Co4Se1Se7	-6527.6583822	17.05
75	4-TricTrPrism-Co1Se2Se1	-6527.6583808	17.05
76	1-CapCube-Co3Se1Se5	-6527.6583769	17.06
77	3-Tl99-Co4Se2Se4	-6527.6583748	17.06
78	1-CapCube-Co2Se6Se1	-6527.6583737	17.06
79	4-TricTrPrism-Co1Se1Se6	-6527.6583350	17.08
80	4-TricTrPrism-Co2Se1Se7	-6527.6583213	17.09
81	4-TricTrPrism-Co2Se2Se1	-6527.6560102	18.54
82	3-Tl99-Co3Se6Se1	-6527.6560027	18.55
83	4-TricTrPrism-Co2Se1Se2	-6527.6559830	18.56

84	3-Tl99-Co3Se3Se1	-6527.6538238	19.91
85	4-TricTrPrism-Co1Se1Se4	-6527.6538052	19.93
86	3-Tl99-Co3Se3Se2	-6527.6537826	19.94
87	4-TricTrPrism-Co2Se2Se6	-6527.6537825	19.94
88	3-Tl99-Co4Se2Se5	-6527.6526685	20.64
89	3-Tl99-Co3Se1Se2	-6527.6526343	20.66
90	2-PressCapCube-Co2Se5Se2	-6527.6521473	20.97
91	3-Tl99-Co3Se7Se1	-6527.6521388	20.97
92	4-TricTrPrism-Co1Se1Se2	-6527.6521242	20.98
93	2-PressCapCube-Co1Se3Se2	-6527.6521240	20.98
94	3-Tl99-Co2Se1Se2	-6527.6502811	22.14
95	3-Tl99-Co3Se3Se3	-6527.6502506	22.16
96	2-PressCapCube-Co1Se4Se1	-6527.6502463	22.16
97	1-CapCube-Co1Se2Se2	-6527.6502443	22.16
98	4-TricTrPrism-Co1Se2Se2	-6527.6502382	22.16
99	4-TricTrPrism-Co2Se3Se1	-6527.6502327	22.17
100	3-Tl99-Co4Se4Se1	-6527.6502249	22.17
101	3-Tl99-Co1Se2Se2	-6527.6502038	22.19
102	4-TricTrPrism-Co1Se3Se1	-6527.6501993	22.19
103	3-Tl99-Co3Se2Se3	-6527.6501977	22.19
104	2-PressCapCube-Co1Se2Se2	-6527.6501693	22.21
105	2-PressCapCube-Co5Se4Se2	-6527.6500113	22.31
106	4-TricTrPrism-Co2Se2Se5	-6527.6499978	22.31
107	3-Tl99-Co2Se3Se5	-6527.6499300	22.36
108	2-PressCapCube-Co1Se3Se3	-6527.6477364	23.73
109	1-CapCube-Co2Se2Se2	-6527.6477106	23.75
110	2-PressCapCube-Co2Se5Se3	-6527.6477002	23.76
111	3-Tl99-Co2Se2Se2	-6527.6476579	23.78
112	1-CapCube-Co3Se4Se1	-6527.6462079	24.69
113	1-CapCube-Co3Se3Se3	-6527.6462001	24.70
114	3-Tl99-Co3Se2Se5	-6527.6461524	24.73
115	1-CapCube-Co3Se2Se3	-6527.6408850	28.03
116	1-CapCube-Co3Se2Se1	-6527.6408459	28.06
117	2-PressCapCube-Co5Se1Se2	-6527.6408339	28.07
118	3-Tl99-Co1Se3Se1	-6527.6408335	28.07
119	2-PressCapCube-Co3Se3Se1	-6527.6408236	28.07
120	3-Tl99-Co4Se3Se3	-6527.6408151	28.08
121	2-PressCapCube-Co3Se1Se2	-6527.6408131	28.08
122	3-Tl99-Co1Se1Se7	-6527.6408000	28.09
123	1-CapCube-Co3Se1Se2	-6527.6407985	28.09
124	3-Tl99-Co2Se2Se3	-6527.6407965	28.09
125	3-Tl99-Co1Se3Se2	-6527.6407781	28.10
126	2-PressCapCube-Co5Se1Se3	-6527.6379805	29.86

127	3-Tl99-Co2Se4Se4	-6527.6378719	29.92
128	2-PressCapCube-Co5Se2Se3	-6527.6378549	29.93
129	2-PressCapCube-Co2Se4Se1	-6527.6378539	29.94
130	2-PressCapCube-Co3Se5Se2	-6527.6373994	30.22
131	2-PressCapCube-Co5Se6Se1	-6527.6373154	30.27
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134	3-Tl99-Co1Se2Se3	-6527.6317733	33.75
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154	3-Tl99-Co2Se4Se2	-6527.6305616	34.51
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156	1-CapCube-Co1Se1Se5	-6527.6305192	34.54
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158	2-PressCapCube-Co3Se4Se2	-6527.6277576	36.27
159	3-Tl99-Co1Se1Se2	-6527.6256741	37.58
160	3-Tl99-Co4Se1Se5	-6527.6247884	38.13
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162	3-Tl99-Co3Se4Se1	-6527.6242980	38.44
163	1-CapCube-Co3Se2Se4	-6527.6242537	38.47
164	4-TricTrPrism-Co2Se1Se5	-6527.6234649	38.96
165	3-Tl99-Co2Se4Se1	-6527.6219176	39.94
166	2-PressCapCube-Co5Se4Se1	-6527.6218953	39.95
167	3-Tl99-Co3Se2Se1	-6527.6218609	39.97
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176	4-TricTrPrism-Co2Se1Se3	-6527.6105017	47.10
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178	3-Tl99-Co3Se1Se1	-6527.6103934	47.17
179	2-PressCapCube-Co2Se3Se3	-6527.6101569	47.32
180	2-PressCapCube-Co1Se2Se1	-6527.6101431	47.32
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186	1-CapCube-Co2Se5Se1	-6527.6091158	47.97
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188	2-PressCapCube-Co3Se2Se2	-6527.6084827	48.37
189	2-PressCapCube-Co2Se2Se1	-6527.6084654	48.38
190	3-Tl99-Co3Se3Se4	-6527.6078973	48.73
191	2-PressCapCube-Co5Se2Se2	-6527.6048150	50.67
192	1-CapCube-Co3Se3Se2	-6527.6047998	50.68
193	3-Tl99-Co4Se3Se5	-6527.6047810	50.69
194	4-TricTrPrism-Co1Se2Se3	-6527.6042013	51.05
195	2-PressCapCube-Co1Se1Se3	-6527.5986658	54.53
196	2-PressCapCube-Co5Se5Se3	-6527.5982100	54.81
197	2-PressCapCube-Co3Se2Se1	-6527.5949432	56.86
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199	3-Tl99-Co3Se2Se4	-6527.5912182	59.20
200	3-Tl99-Co3Se3Se5	-6527.5903055	59.77
201	2-PressCapCube-Co5Se5Se1	-6527.5859944	62.48
202	2-PressCapCube-Co5Se2Se1	-6527.5849297	63.15
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208	2-PressCapCube-Co2Se2Se2	-6527.5715785	71.52
209	1-CapCube-Co3Se3Se1	-6527.5651320	75.57
210	3-Tl99-Co2Se5Se3	-6527.5645090	75.96
211	2-PressCapCube-Co1Se3Se1	-6527.5621454	77.44
212	2-PressCapCube-Co3Se5Se3	-6527.5471031	86.88

Table S3A. Initial CpCoSe₂B₇H₇ structures, 317 structures.


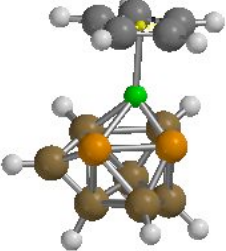
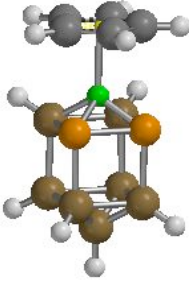
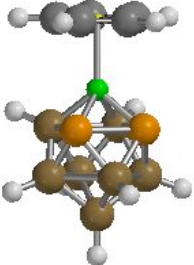
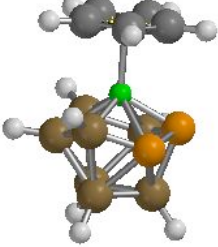
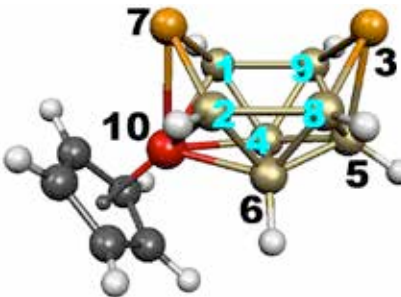
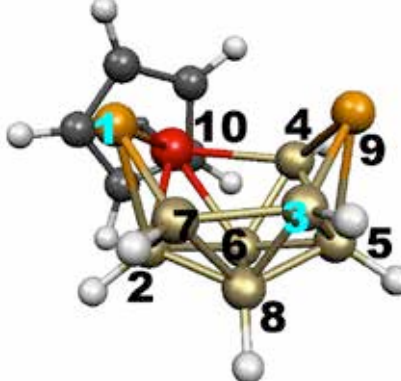
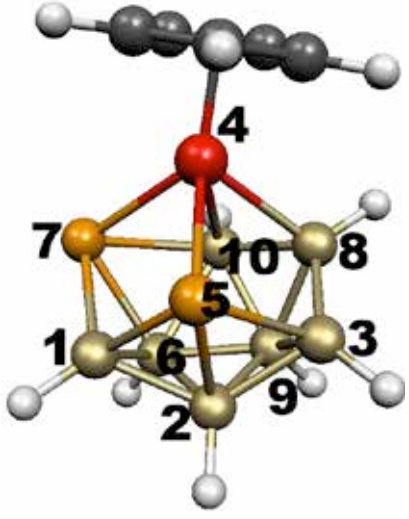
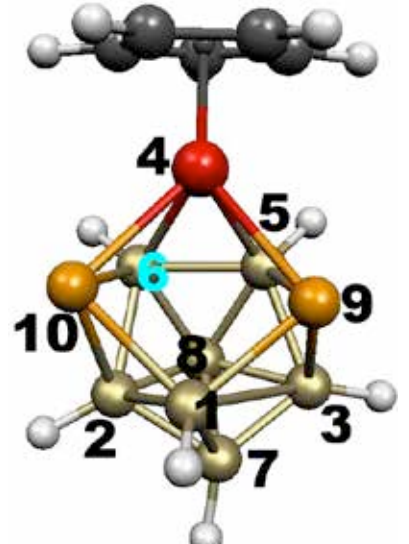
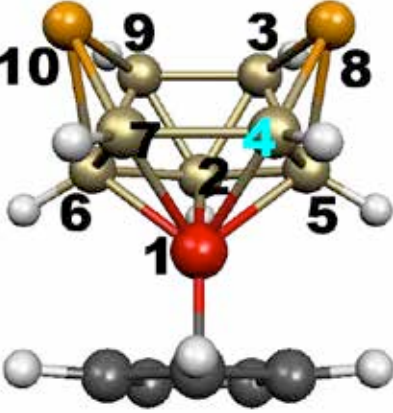
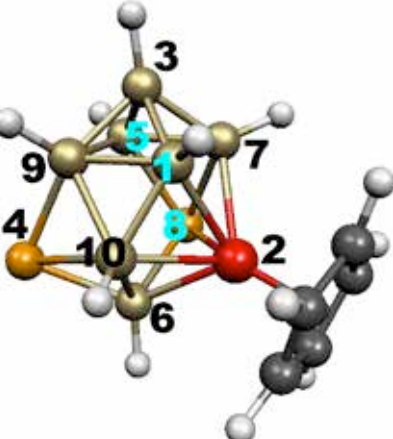
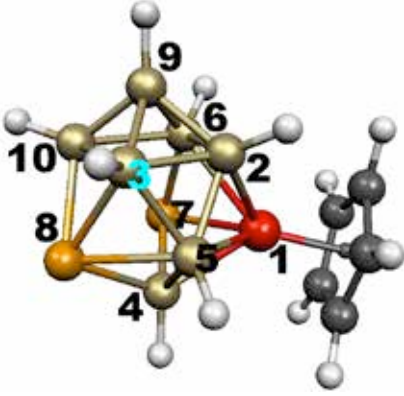
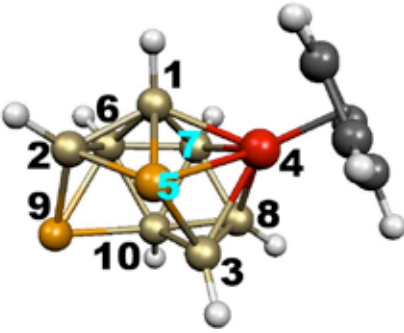
<p>Initial structures</p>	 <p>1. Tetracapped trigonal prism (C_{2v}) 98 structures</p>
 <p>2. Tetracapped trigonal prism (C_{3v}) 84 structures</p>	 <p>3. Bicapped cube 31 structures</p>
 <p>4. Bicapped square antiprism 32 structures</p>	 <p>5. Isocloso structure 72 structures</p>

Table 3B. Distance table for the lowest-lying CpCoSe₂B₇H₇ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -6557.3506350 0.0 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>2.875427</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Se</td><td>3.263064</td><td>3.263040</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>1.755998</td><td>2.876564</td><td>3.144643</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>2.990977</td><td>2.990939</td><td>2.078342</td><td>1.767014</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.876586</td><td>1.756012</td><td>3.144644</td><td>1.805342</td><td>1.766981</td></tr> <tr><td>7 Se</td><td>1.989424</td><td>1.989431</td><td>3.548465</td><td>3.178129</td><td>3.865066</td></tr> <tr><td>8 B</td><td>3.416059</td><td>1.850864</td><td>1.988454</td><td>2.853799</td><td>1.837521</td></tr> <tr><td>9 B</td><td>1.850936</td><td>3.416075</td><td>1.988450</td><td>1.722904</td><td>1.837528</td></tr> <tr><td>10 Co</td><td>2.095397</td><td>2.095388</td><td>4.300400</td><td>2.083850</td><td>3.350561</td></tr> <tr> <th></th> <th>6</th> <th>7</th> <th>8</th> <th>9</th> <th>10</th> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 Se</td><td>3.178153</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 B</td><td>1.722898</td><td>3.224707</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>2.853810</td><td>3.224757</td><td>2.866943</td><td>0.000000</td><td></td></tr> <tr><td>10 Co</td><td>2.083856</td><td>2.325595</td><td>3.346155</td><td>3.346202</td><td>0.000000</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	2.875427	0.000000				3 Se	3.263064	3.263040	0.000000			4 B	1.755998	2.876564	3.144643	0.000000		5 B	2.990977	2.990939	2.078342	1.767014	0.000000	6 B	2.876586	1.756012	3.144644	1.805342	1.766981	7 Se	1.989424	1.989431	3.548465	3.178129	3.865066	8 B	3.416059	1.850864	1.988454	2.853799	1.837521	9 B	1.850936	3.416075	1.988450	1.722904	1.837528	10 Co	2.095397	2.095388	4.300400	2.083850	3.350561		6	7	8	9	10	6 B	0.000000					7 Se	3.178153	0.000000				8 B	1.722898	3.224707	0.000000			9 B	2.853810	3.224757	2.866943	0.000000		10 Co	2.083856	2.325595	3.346155	3.346202	0.000000
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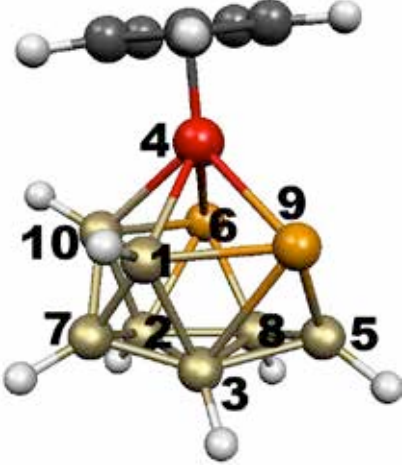
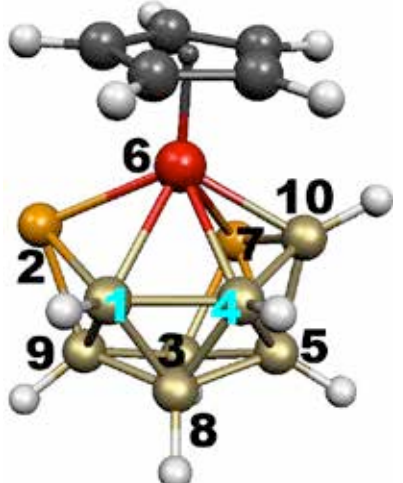
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Table S3C. Energy ranking for all of the CpCoSe₂B₇H₇ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	2-TetrTriPri2-Co1Se7Se1	-6553.13534170	0.00
2	4-BicapSqAntipr-Co2Se1Se2	-6553.13534150	0.00
3	5-Isocloso-Co3Se4Se1	-6553.13533340	0.01
4	3-BicapCub-Co2Se1Se4	-6553.13532950	0.01
5	2-TetrTriPri2-Co2Se4Se1	-6553.13532350	0.01
6	2-TetrTriPri2-Co2Se1Se1	-6553.13532050	0.01
7	3-BicapCub-Co2Se3Se1	-6553.13531440	0.02
8	3-BicapCub-Co1Se1Se6	-6553.13531210	0.02
9	5-Isocloso-Co2Se2Se4	-6553.13529670	0.03
10	1-TetrTriPri1-Co3Se4Se1	-6553.13529130	0.03
11	2-TetrTriPri2-Co2Se2Se7	-6553.13529120	0.03
12	1-TetrTriPri1-Co2Se4Se1	-6553.13528930	0.03
13	5-Isocloso-Co3Se2Se1	-6553.13527520	0.04
14	4-BicapSqAntipr-Co1Se2Se3	-6553.13527020	0.04
15	1-TetrTriPri1-Co2Se4Se2	-6553.13521860	0.08
16	1-TetrTriPri1-Co3Se4Se2	-6553.13521860	0.08
17	4-BicapSqAntipr-Co2Se4Se1	-6553.13520270	0.09
18	5-Isocloso-Co2Se1Se6	-6553.12439700	6.87
19	5-Isocloso-Co1Se1Se6	-6553.12437410	6.88
20	5-Isocloso-Co2Se1Se4	-6553.12437240	6.88
21	2-TetrTriPri2-Co3Se1Se2	-6553.12437130	6.88
22	5-Isocloso-Co3Se1Se7	-6553.12436250	6.89
23	3-BicapCub-Co2Se1Se6	-6553.12435570	6.89
24	5-Isocloso-Co3Se3Se4	-6553.12435540	6.89
25	1-TetrTriPri1-Co1Se1Se6	-6553.12435200	6.90
26	2-TetrTriPri2-Co1Se1Se1	-6553.12434100	6.90
27	2-TetrTriPri2-Co1Se4Se2	-6553.12433340	6.91
28	4-BicapSqAntipr-Co2Se2Se5	-6553.12432970	6.91
29	5-Isocloso-Co1Se1Se4	-6553.12432150	6.92
30	1-TetrTriPri1-Co2Se1Se5	-6553.12430530	6.93
31	1-TetrTriPri1-Co3Se2Se5	-6553.12430530	6.93
32	4-BicapSqAntipr-Co2Se2Se3	-6553.12430100	6.93
33	2-TetrTriPri2-Co2Se1Se3	-6553.12339840	7.49
34	4-BicapSqAntipr-Co1Se1Se1	-6553.12338530	7.50
35	2-TetrTriPri2-Co1Se2Se5	-6553.12336690	7.51
36	3-BicapCub-Co1Se1Se1	-6553.12237930	8.13
37	2-TetrTriPri2-Co1Se2Se1	-6553.12057800	9.26
38	2-TetrTriPri2-Co1Se2Se2	-6553.12054000	9.29
39	2-TetrTriPri2-Co1Se6Se2	-6553.12053280	9.29

40	2-TetrTriPri2-Co3Se2Se3	-6553.12053200	9.29
41	5-Isocloso-Co2Se2Se3	-6553.12052980	9.29
42	4-BicapSqAntipr-Co2Se1Se1	-6553.12051130	9.31
43	3-BicapCub-Co1Se1Se4	-6553.12050130	9.31
44	1-TetrTriPri1-Co2Se1Se1	-6553.12049660	9.32
45	5-Isocloso-Co1Se2Se7	-6553.12048900	9.32
46	4-BicapSqAntipr-Co1Se1Se3	-6553.12048180	9.32
47	2-TetrTriPri2-Co1Se6Se3	-6553.12048130	9.33
48	5-Isocloso-Co1Se2Se2	-6553.12046310	9.34
49	5-Isocloso-Co3Se3Se2	-6553.11465660	12.98
50	5-Isocloso-Co3Se2Se2	-6553.11465470	12.98
51	2-TetrTriPri2-Co2Se2Se1	-6553.11464220	12.99
52	5-Isocloso-Co2Se1Se7	-6553.11463960	12.99
53	5-Isocloso-Co2Se3Se4	-6553.11463790	12.99
54	5-Isocloso-Co3Se1Se2	-6553.11463170	13.00
55	2-TetrTriPri2-Co2Se3Se4	-6553.11462120	13.00
56	5-Isocloso-Co2Se3Se1	-6553.11458200	13.03
57	4-BicapSqAntipr-Co2Se3Se4	-6553.11454600	13.05
58	2-TetrTriPri2-Co3Se3Se6	-6553.11160530	14.90
59	2-TetrTriPri2-Co3Se4Se4	-6553.11159030	14.90
60	2-TetrTriPri2-Co2Se1Se8	-6553.11158910	14.91
61	1-TetrTriPri1-Co2Se2Se2	-6553.11158420	14.91
62	1-TetrTriPri1-Co3Se1Se4	-6553.11158420	14.91
63	4-BicapSqAntipr-Co2Se1Se7	-6553.11158040	14.91
64	3-BicapCub-Co2Se2Se1	-6553.11157420	14.91
65	2-TetrTriPri2-Co3Se2Se6	-6553.11157000	14.92
66	2-TetrTriPri2-Co3Se1Se1	-6553.11047710	15.60
67	1-TetrTriPri1-Co2Se4Se3	-6553.11047410	15.60
68	1-TetrTriPri1-Co3Se4Se3	-6553.11047410	15.60
69	2-TetrTriPri2-Co2Se1Se6	-6553.11044540	15.62
70	2-TetrTriPri2-Co2Se1Se2	-6553.11037500	15.67
71	5-Isocloso-Co3Se3Se1	-6553.11035350	15.68
72	5-Isocloso-Co2Se1Se5	-6553.10863270	16.76
73	4-BicapSqAntipr-Co2Se2Se1	-6553.10862360	16.77
74	1-TetrTriPri1-Co1Se1Se2	-6553.10858830	16.79
75	2-TetrTriPri2-Co1Se2Se6	-6553.10858460	16.79
76	2-TetrTriPri2-Co1Se6Se1	-6553.10857490	16.80
77	2-TetrTriPri2-Co2Se1Se7	-6553.10853790	16.82
78	2-TetrTriPri2-Co2Se1Se4	-6553.10590080	18.47
79	1-TetrTriPri1-Co2Se3Se1	-6553.10589660	18.48
80	1-TetrTriPri1-Co3Se3Se1	-6553.10589660	18.48
81	2-TetrTriPri2-Co2Se2Se3	-6553.10589650	18.48
82	4-BicapSqAntipr-Co2Se1Se8	-6553.10589080	18.48

83	5-Isocloso-Co3Se1Se3	-6553.10585470	18.50
84	5-Isocloso-Co2Se4Se2	-6553.10391180	19.72
85	4-BicapSqAntipr-Co1Se1Se5	-6553.10390940	19.72
86	5-Isocloso-Co2Se5Se1	-6553.10390760	19.73
87	5-Isocloso-Co1Se4Se2	-6553.10388950	19.74
88	2-TetrTriPri2-Co3Se1Se5	-6553.10388930	19.74
89	5-Isocloso-Co1Se1Se2	-6553.10387180	19.75
90	1-TetrTriPri1-Co2Se6Se1	-6553.10271790	20.47
91	1-TetrTriPri1-Co2Se7Se1	-6553.10271790	20.47
92	1-TetrTriPri1-Co3Se6Se2	-6553.10271790	20.47
93	5-Isocloso-Co3Se2Se3	-6553.10104110	21.52
94	2-TetrTriPri2-Co2Se3Se6	-6553.10101980	21.54
95	1-TetrTriPri1-Co1Se2Se3	-6553.10101550	21.54
96	4-BicapSqAntipr-Co2Se3Se5	-6553.10101030	21.54
97	2-TetrTriPri2-Co1Se7Se2	-6553.10097200	21.57
98	3-BicapCub-Co2Se4Se1	-6553.10097080	21.57
99	1-TetrTriPri1-Co2Se5Se3	-6553.10095680	21.58
100	1-TetrTriPri1-Co3Se5Se2	-6553.10095680	21.58
101	3-BicapCub-Co2Se2Se2	-6553.10094590	21.58
102	1-TetrTriPri1-Co1Se2Se4	-6553.10090630	21.61
103	1-TetrTriPri1-Co1Se3Se5	-6553.10090100	21.61
104	2-TetrTriPri2-Co1Se3Se5	-6553.10088970	21.62
105	2-TetrTriPri2-Co3Se4Se3	-6553.10087740	21.63
106	2-TetrTriPri2-Co3Se2Se7	-6553.10086870	21.63
107	2-TetrTriPri2-Co2Se3Se5	-6553.10084650	21.65
108	5-Isocloso-Co2Se1Se3	-6553.09935610	22.58
109	1-TetrTriPri1-Co2Se1Se3	-6553.09931430	22.61
110	1-TetrTriPri1-Co3Se2Se2	-6553.09931430	22.61
111	2-TetrTriPri2-Co1Se1Se4	-6553.09931070	22.61
112	3-BicapCub-Co2Se1Se1	-6553.09931010	22.61
113	5-Isocloso-Co3Se1Se1	-6553.09927230	22.63
114	4-BicapSqAntipr-Co2Se1Se6	-6553.09922780	22.66
115	1-TetrTriPri1-Co1Se4Se2	-6553.09917880	22.69
116	2-TetrTriPri2-Co3Se2Se1	-6553.09910550	22.74
117	1-TetrTriPri1-Co1Se1Se5	-6553.09909720	22.74
118	3-BicapCub-Co2Se3Se2	-6553.09697520	24.08
119	2-TetrTriPri2-Co2Se3Se3	-6553.09696000	24.09
120	1-TetrTriPri1-Co1Se1Se7	-6553.09695510	24.09
121	2-TetrTriPri2-Co2Se5Se1	-6553.09694200	24.10
122	5-Isocloso-Co1Se2Se5	-6553.09693810	24.10
123	2-TetrTriPri2-Co1Se5Se2	-6553.09692700	24.11
124	4-BicapSqAntipr-Co2Se3Se3	-6553.09692650	24.11
125	1-TetrTriPri1-Co1Se3Se2	-6553.09692470	24.11

126	4-BicapSqAntipr-Co2Se5Se1	-6553.09692300	24.11
127	5-Isocloso-Co3Se5Se1	-6553.09692020	24.11
128	5-Isocloso-Co1Se5Se1	-6553.09688460	24.13
129	5-Isocloso-Co1Se3Se4	-6553.09688270	24.13
130	5-Isocloso-Co1Se3Se6	-6553.09688070	24.14
131	5-Isocloso-Co3Se2Se6	-6553.09687970	24.14
132	5-Isocloso-Co1Se3Se3	-6553.09687780	24.14
133	2-TetrTriPri2-Co1Se3Se6	-6553.09687760	24.14
134	5-Isocloso-Co2Se2Se6	-6553.09659270	24.32
135	2-TetrTriPri2-Co1Se8Se1	-6553.09656520	24.33
136	4-BicapSqAntipr-Co2Se1Se5	-6553.09656400	24.33
137	2-TetrTriPri2-Co1Se3Se1	-6553.09654320	24.35
138	3-BicapCub-Co1Se2Se1	-6553.09653700	24.35
139	4-BicapSqAntipr-Co1Se2Se1	-6553.09653140	24.35
140	5-Isocloso-Co2Se2Se1	-6553.09653050	24.35
141	1-TetrTriPri1-Co2Se1Se2	-6553.09580540	24.81
142	1-TetrTriPri1-Co3Se2Se1	-6553.09580540	24.81
143	5-Isocloso-Co1Se2Se3	-6553.09514600	25.22
144	4-BicapSqAntipr-Co2Se2Se2	-6553.09511400	25.24
145	5-Isocloso-Co1Se1Se1	-6553.09508020	25.26
146	1-TetrTriPri1-Co1Se2Se1	-6553.09507160	25.27
147	5-Isocloso-Co1Se1Se3	-6553.09506790	25.27
148	5-Isocloso-Co2Se2Se2	-6553.09378230	26.08
149	5-Isocloso-Co3Se2Se5	-6553.09124120	27.67
150	3-BicapCub-Co2Se6Se1	-6553.09122570	27.68
151	2-TetrTriPri2-Co1Se3Se2	-6553.09122150	27.69
152	3-BicapCub-Co2Se5Se1	-6553.09121530	27.69
153	2-TetrTriPri2-Co1Se1Se8	-6553.09120860	27.69
154	5-Isocloso-Co3Se1Se8	-6553.09115830	27.73
155	1-TetrTriPri1-Co2Se1Se4	-6553.09082250	27.94
156	1-TetrTriPri1-Co3Se2Se3	-6553.09082250	27.94
157	1-TetrTriPri1-Co2Se2Se6	-6553.09078260	27.96
158	1-TetrTriPri1-Co3Se1Se6	-6553.09078260	27.96
159	3-BicapCub-Co2Se1Se3	-6553.09077070	27.97
160	2-TetrTriPri2-Co1Se2Se3	-6553.08985400	28.54
161	2-TetrTriPri2-Co1Se1Se6	-6553.08983550	28.56
162	1-TetrTriPri1-Co1Se4Se3	-6553.08982770	28.56
163	5-Isocloso-Co2Se4Se1	-6553.08982550	28.56
164	1-TetrTriPri1-Co1Se1Se8	-6553.08978320	28.59
165	2-TetrTriPri2-Co3Se3Se4	-6553.08908860	29.02
166	4-BicapSqAntipr-Co2Se1Se4	-6553.08907120	29.04
167	4-BicapSqAntipr-Co2Se4Se2	-6553.08907050	29.04
168	3-BicapCub-Co1Se1Se5	-6553.08906650	29.04

169	2-TetrTriPri2-Co3Se1Se4	-6553.08906530	29.04
170	5-Isocloso-Co1Se2Se6	-6553.08906450	29.04
171	2-TetrTriPri2-Co1Se1Se3	-6553.08905960	29.04
172	2-TetrTriPri2-Co1Se3Se4	-6553.08905960	29.04
173	5-Isocloso-Co2Se2Se5	-6553.08905690	29.04
174	2-TetrTriPri2-Co1Se4Se4	-6553.08904120	29.05
175	4-BicapSqAntipr-Co2Se2Se7	-6553.08903890	29.06
176	2-TetrTriPri2-Co3Se2Se5	-6553.08903650	29.06
177	5-Isocloso-Co1Se4Se1	-6553.08902840	29.06
178	5-Isocloso-Co2Se1Se8	-6553.08902500	29.06
179	2-TetrTriPri2-Co1Se2Se7	-6553.08901500	29.07
180	5-Isocloso-Co1Se1Se8	-6553.08900970	29.07
181	4-BicapSqAntipr-Co2Se2Se4	-6553.08869070	29.27
182	5-Isocloso-Co1Se1Se7	-6553.08868670	29.28
183	2-TetrTriPri2-Co1Se5Se1	-6553.08867680	29.28
184	4-BicapSqAntipr-Co2Se3Se2	-6553.08866490	29.29
185	5-Isocloso-Co2Se3Se3	-6553.08864830	29.30
186	4-BicapSqAntipr-Co2Se2Se6	-6553.08863970	29.31
187	2-TetrTriPri2-Co1Se2Se4	-6553.08863710	29.31
188	1-TetrTriPri1-Co1Se3Se1	-6553.08863190	29.31
189	5-Isocloso-Co1Se3Se5	-6553.08860250	29.33
190	5-Isocloso-Co1Se3Se2	-6553.08857860	29.34
191	5-Isocloso-Co1Se1Se5	-6553.08857360	29.35
192	3-BicapCub-Co2Se3Se3	-6553.08852990	29.38
193	2-TetrTriPri2-Co2Se2Se6	-6553.08558820	31.22
194	2-TetrTriPri2-Co1Se1Se7	-6553.08555750	31.24
195	2-TetrTriPri2-Co1Se4Se3	-6553.08554940	31.25
196	1-TetrTriPri1-Co1Se1Se3	-6553.08552080	31.26
197	5-Isocloso-Co3Se3Se5	-6553.08411360	32.15
198	3-BicapCub-Co2Se1Se5	-6553.08402900	32.20
199	1-TetrTriPri1-Co2Se2Se3	-6553.08401680	32.21
200	1-TetrTriPri1-Co3Se1Se3	-6553.08401680	32.21
201	1-TetrTriPri1-Co1Se3Se3	-6553.08400540	32.21
202	5-Isocloso-Co3Se1Se5	-6553.08373380	32.38
203	1-TetrTriPri1-Co2Se6Se3	-6553.08372740	32.39
204	1-TetrTriPri1-Co2Se8Se1	-6553.08372740	32.39
205	1-TetrTriPri1-Co3Se6Se3	-6553.08372740	32.39
206	2-TetrTriPri2-Co3Se5Se1	-6553.08372280	32.39
207	2-TetrTriPri2-Co1Se1Se5	-6553.08370590	32.40
208	2-TetrTriPri2-Co3Se3Se3	-6553.08370260	32.40
209	3-BicapCub-Co2Se4Se3	-6553.08368600	32.41
210	2-TetrTriPri2-Co1Se4Se1	-6553.08367380	32.42
211	3-BicapCub-Co1Se1Se2	-6553.08253960	33.13

212	4-BicapSqAntipr-Co1Se1Se2	-6553.08253100	33.14
213	2-TetrTriPri2-Co3Se3Se5	-6553.08251020	33.15
214	1-TetrTriPri1-Co2Se3Se4	-6553.08249660	33.16
215	3-BicapCub-Co2Se1Se2	-6553.08132550	33.90
216	2-TetrTriPri2-Co3Se4Se1	-6553.08091460	34.15
217	2-TetrTriPri2-Co3Se1Se3	-6553.08055740	34.38
218	1-TetrTriPri1-Co1Se3Se4	-6553.08051890	34.40
219	5-Isocloso-Co3Se1Se4	-6553.08051120	34.41
220	1-TetrTriPri1-Co1Se2Se7	-6553.08050290	34.41
221	2-TetrTriPri2-Co2Se1Se5	-6553.08049480	34.42
222	5-Isocloso-Co3Se3Se6	-6553.08049360	34.42
223	3-BicapCub-Co2Se2Se5	-6553.08049180	34.42
224	2-TetrTriPri2-Co2Se3Se1	-6553.08048560	34.42
225	1-TetrTriPri1-Co1Se4Se4	-6553.08047510	34.43
226	3-BicapCub-Co2Se5Se2	-6553.08047190	34.43
227	5-Isocloso-Co3Se2Se7	-6553.08046730	34.43
228	2-TetrTriPri2-Co2Se4Se2	-6553.08043870	34.45
229	5-Isocloso-Co3Se4Se2	-6553.08043100	34.46
230	1-TetrTriPri1-Co2Se3Se6	-6553.07603770	37.21
231	1-TetrTriPri1-Co3Se3Se6	-6553.07603640	37.22
232	3-BicapCub-Co1Se2Se2	-6553.07580520	37.36
233	4-BicapSqAntipr-Co1Se2Se2	-6553.07579810	37.36
234	5-Isocloso-Co2Se3Se6	-6553.07575460	37.39
235	5-Isocloso-Co2Se2Se7	-6553.07574940	37.40
236	5-Isocloso-Co2Se3Se2	-6553.07570260	37.42
237	4-BicapSqAntipr-Co2Se3Se6	-6553.07570020	37.43
238	2-TetrTriPri2-Co1Se5Se3	-6553.07569390	37.43
239	4-BicapSqAntipr-Co2Se1Se3	-6553.07567170	37.44
240	2-TetrTriPri2-Co2Se2Se5	-6553.07240580	39.49
241	5-Isocloso-Co3Se2Se4	-6553.07052930	40.67
242	1-TetrTriPri1-Co2Se7Se2	-6553.07051580	40.68
243	1-TetrTriPri1-Co3Se7Se2	-6553.07051490	40.68
244	3-BicapCub-Co2Se4Se2	-6553.07050260	40.69
245	5-Isocloso-Co3Se3Se3	-6553.07035460	40.78
246	1-TetrTriPri1-Co3Se4Se5	-6553.06895030	41.66
247	1-TetrTriPri1-Co2Se4Se5	-6553.06894860	41.66
248	1-TetrTriPri1-Co1Se2Se5	-6553.06892500	41.68
249	1-TetrTriPri1-Co1Se1Se4	-6553.06888490	41.70
250	1-TetrTriPri1-Co1Se4Se5	-6553.06887440	41.71
251	3-BicapCub-Co2Se5Se3	-6553.06860410	41.88
252	2-TetrTriPri2-Co3Se2Se2	-6553.06793030	42.30
253	5-Isocloso-Co1Se3Se1	-6553.06790010	42.32
254	5-Isocloso-Co1Se2Se1	-6553.06786960	42.34

255	1-TetrTriPri1-Co1Se2Se6	-6553.06786260	42.34
256	4-BicapSqAntipr-Co2Se3Se1	-6553.06785550	42.35
257	5-Isocloso-Co1Se2Se4	-6553.06780130	42.38
258	2-TetrTriPri2-Co3Se2Se4	-6553.06212050	45.95
259	1-TetrTriPri1-Co1Se2Se2	-6553.06202930	46.00
260	4-BicapSqAntipr-Co1Se1Se4	-6553.06009290	47.22
261	1-TetrTriPri1-Co2Se1Se8	-6553.05946630	47.61
262	1-TetrTriPri1-Co3Se2Se4	-6553.05946630	47.61
263	1-TetrTriPri1-Co2Se6Se2	-6553.05911580	47.83
264	1-TetrTriPri1-Co3Se6Se1	-6553.05911580	47.83
265	5-Isocloso-Co2Se1Se1	-6553.05788270	48.61
266	2-TetrTriPri2-Co2Se2Se2	-6553.05731400	48.96
267	1-TetrTriPri1-Co2Se2Se4	-6553.05596630	49.81
268	1-TetrTriPri1-Co3Se1Se5	-6553.05596630	49.81
269	1-TetrTriPri1-Co3Se1Se7	-6553.05596630	49.81
270	3-BicapCub-Co1Se1Se3	-6553.05487420	50.49
271	1-TetrTriPri1-Co3Se2Se6	-6553.05359750	51.30
272	1-TetrTriPri1-Co2Se1Se6	-6553.05357030	51.31
273	1-TetrTriPri1-Co3Se3Se2	-6553.05221040	52.17
274	1-TetrTriPri1-Co2Se3Se2	-6553.05220910	52.17
275	2-TetrTriPri2-Co3Se3Se1	-6553.05214580	52.21
276	1-TetrTriPri1-Co2Se1Se7	-6553.05164590	52.52
277	1-TetrTriPri1-Co3Se2Se7	-6553.05164590	52.52
278	2-TetrTriPri2-Co2Se2Se4	-6553.05078100	53.06
279	2-TetrTriPri2-Co2Se3Se2	-6553.05077550	53.07
280	5-Isocloso-Co2Se1Se2	-6553.04980680	53.67
281	2-TetrTriPri2-Co1Se1Se2	-6553.04938860	53.94
282	2-TetrTriPri2-Co1Se4Se5	-6553.04935220	53.96
283	1-TetrTriPri1-Co2Se5Se4	-6553.04834600	54.59
284	1-TetrTriPri1-Co3Se5Se4	-6553.04834600	54.59
285	3-BicapCub-Co2Se2Se4	-6553.04832180	54.61
286	3-BicapCub-Co1Se2Se3	-6553.04819010	54.69
287	1-TetrTriPri1-Co2Se5Se2	-6553.04764420	55.03
288	1-TetrTriPri1-Co3Se5Se3	-6553.04763450	55.04
289	1-TetrTriPri1-Co1Se3Se6	-6553.04700320	55.43
290	2-TetrTriPri2-Co3Se3Se2	-6553.04561510	56.31
291	1-TetrTriPri1-Co3Se3Se4	-6553.04538850	56.45
292	2-TetrTriPri2-Co3Se4Se5	-6553.04384640	57.42
293	1-TetrTriPri1-Co2Se2Se7	-6553.04290050	58.01
294	1-TetrTriPri1-Co3Se1Se8	-6553.04290050	58.01
295	2-TetrTriPri2-Co1Se5Se4	-6553.03677790	61.85
296	2-TetrTriPri2-Co1Se3Se3	-6553.03674690	61.87
297	5-Isocloso-Co3Se1Se6	-6553.03635040	62.12

298	1-TetrTriPri1-Co1Se1Se1	-6553.03238400	64.61
299	1-TetrTriPri1-Co3Se1Se1	-6553.02910280	66.67
300	1-TetrTriPri1-Co3Se3Se5	-6553.02660800	68.23
301	1-TetrTriPri1-Co2Se3Se5	-6553.02651710	68.29
302	3-BicapCub-Co2Se2Se3	-6553.02593460	68.66
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314	1-TetrTriPri1-Co3Se8Se1	-6553.00293550	83.09
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316	1-TetrTriPri1-Co2Se3Se3	-6552.99588710	87.51
317	1-TetrTriPri1-Co2Se2Se5	-6552.97424710	101.09

Table S4A. Initial CpCoSe₂B₈H₈ structures, 120 structures.

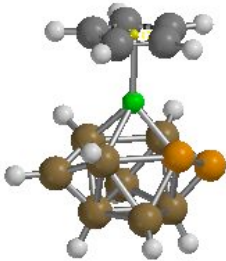
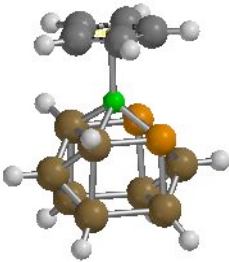
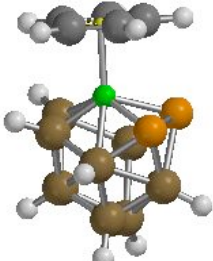
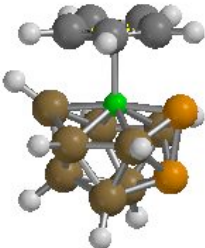
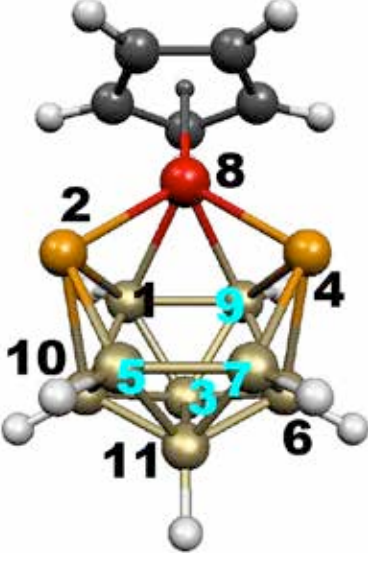
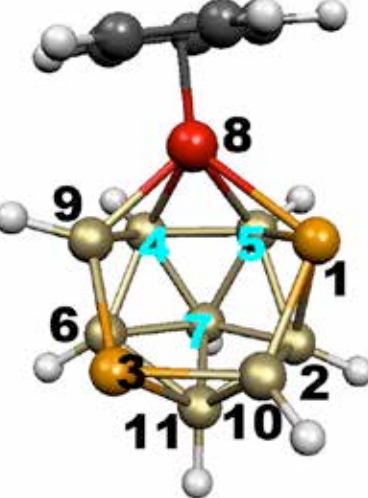
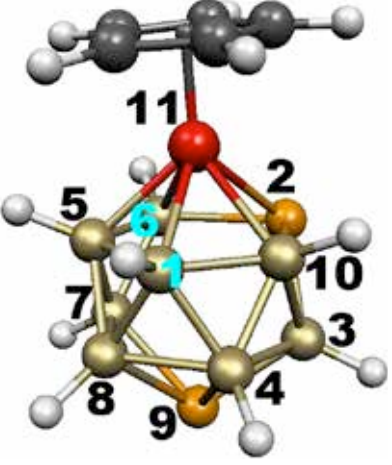
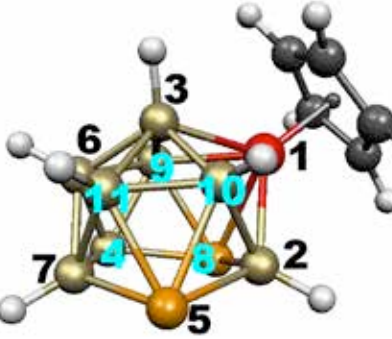
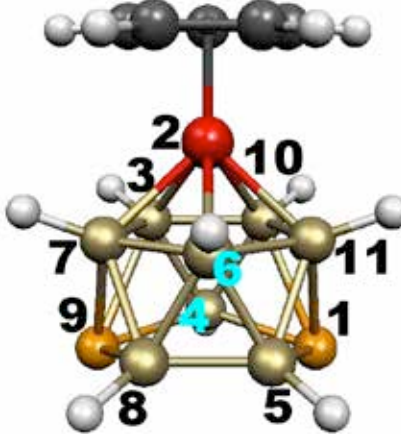
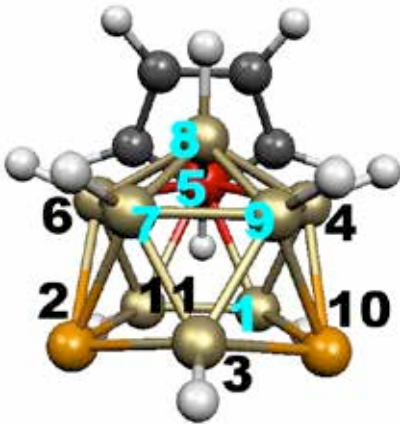

1. Pentacapped trigonal prism 54 structures

2. Tricapped cubeA (C _{2v}) 139 structures

2b. Tricapped cubeA (C _{3v}) 124 structures

4. Edge-coalesced icosahedrons (icosahedron without a vertex) 163 structures

Table S4B. Distance table for the lowest-lying CpCoSe₂B₈H₈ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity only the atoms forming the cluster framework are presented.

 <p>1. -6582.8292076 0.0 C_s</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 Se</td><td>2.121775</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 B</td><td>1.744191</td><td>3.195756</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 Se</td><td>3.252640</td><td>3.397625</td><td>3.195714</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.024699</td><td>2.040606</td><td>2.894301</td><td>3.170333</td><td>0.000000</td></tr> <tr><td>6 B</td><td>2.939124</td><td>3.766280</td><td>1.761177</td><td>2.103939</td><td>2.889037</td></tr> <tr><td>7 B</td><td>3.499728</td><td>3.170261</td><td>2.894294</td><td>2.040643</td><td>1.732573</td></tr> <tr><td>8 Co</td><td>2.108663</td><td>2.334326</td><td>3.299203</td><td>2.334361</td><td>3.553249</td></tr> <tr><td>9 B</td><td>1.788851</td><td>3.252640</td><td>1.744177</td><td>2.121724</td><td>3.499735</td></tr> <tr><td>10 B</td><td>1.870970</td><td>2.103971</td><td>1.761177</td><td>3.766292</td><td>1.835894</td></tr> <tr><td>11 B</td><td>2.913134</td><td>3.177265</td><td>1.780701</td><td>3.177275</td><td>1.746476</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>6 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>7 B</td><td>1.835872</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Co</td><td>3.454720</td><td>3.553243</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>1.871018</td><td>3.024699</td><td>2.108670</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.872089</td><td>2.889049</td><td>3.454681</td><td>2.939093</td><td>0.000000</td></tr> <tr><td>11 B</td><td>1.739730</td><td>1.746483</td><td>3.983485</td><td>2.913137</td><td>1.739752</td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 Se	2.121775	0.000000				3 B	1.744191	3.195756	0.000000			4 Se	3.252640	3.397625	3.195714	0.000000		5 B	3.024699	2.040606	2.894301	3.170333	0.000000	6 B	2.939124	3.766280	1.761177	2.103939	2.889037	7 B	3.499728	3.170261	2.894294	2.040643	1.732573	8 Co	2.108663	2.334326	3.299203	2.334361	3.553249	9 B	1.788851	3.252640	1.744177	2.121724	3.499735	10 B	1.870970	2.103971	1.761177	3.766292	1.835894	11 B	2.913134	3.177265	1.780701	3.177275	1.746476		6	7	8	9	10	6 B	0.000000					7 B	1.835872	0.000000				8 Co	3.454720	3.553243	0.000000			9 B	1.871018	3.024699	2.108670	0.000000		10 B	2.872089	2.889049	3.454681	2.939093	0.000000	11 B	1.739730	1.746483	3.983485	2.913137	1.739752
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4 B	1.911375	3.751772	3.039235	0.000000																																																																																																															
5 Co	2.071692	3.595865	3.985291	2.011080	0.000000																																																																																																														
6 B	2.910727	2.130214	3.039076	2.879288	2.011163																																																																																																														
7 B	3.522694	2.112550	1.812307	2.925415	3.294108																																																																																																														
8 B	2.962637	3.216358	2.916320	1.770084	2.043200																																																																																																														
9 B	3.074512	3.211739	1.812307	1.863033	3.294117																																																																																																														
10 Se	2.089026	3.312406	2.030901	2.130184	3.595767																																																																																																														
11 B	1.673781	2.088917	3.156802	2.910785	2.071747																																																																																																														
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6 B	0.000000																																																																																																																		
7 B	1.862803	0.000000																																																																																																																	
8 B	1.770073	1.752452	0.000000																																																																																																																
9 B	2.925235	1.766777	1.752370	0.000000																																																																																																															
10 Se	3.751592	3.211685	3.216193	2.112523	0.000000																																																																																																														
11 B	1.911295	3.074343	2.962619	3.522674	3.147709																																																																																																														

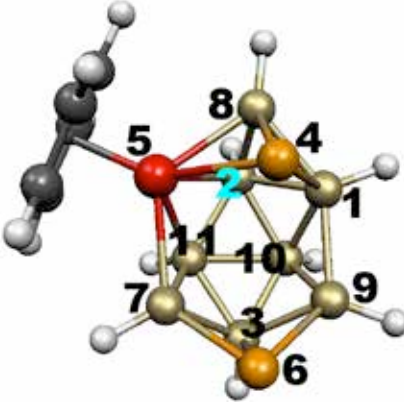
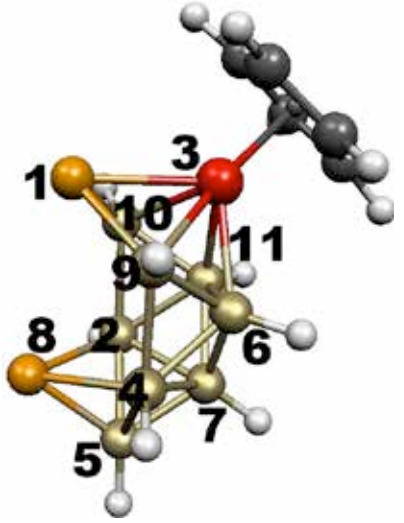
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Table S4C. Energy ranking for all of the CpCoSe₂B₈H₈ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	3-TricapCubeB-Co3Se2Se7	-6578.6152600	0.00
2	2-TricapCubeA-Co1Se1Se5	-6578.6152533	0.00
3	4-Icos-1vx-Co5Se1Se7	-6578.6151960	0.04
4	4-Icos-1vx-Co3Se1Se1	-6578.6151798	0.05
5	1-PentaCapTriPri-Co1Se1Se2	-6578.6151728	0.05
6	4-Icos-1vx-Co3Se1Se5	-6578.6151643	0.06
7	3-TricapCubeB-Co2Se1Se7	-6578.6151616	0.06
8	2-TricapCubeA-Co3Se7Se1	-6578.6151585	0.06
9	4-Icos-1vx-Co2Se1Se4	-6578.6151344	0.08
10	3-TricapCubeB-Co3Se4Se1	-6578.6018117	8.44
11	4-Icos-1vx-Co3Se1Se2	-6578.6017671	8.47
12	3-TricapCubeB-Co3Se2Se3	-6578.6017631	8.47
13	2-TricapCubeA-Co3Se3Se3	-6578.6017628	8.47
14	3-TricapCubeB-Co2Se3Se1	-6578.6017588	8.47
15	4-Icos-1vx-Co2Se2Se3	-6578.6017474	8.48
16	4-Icos-1vx-Co2Se1Se2	-6578.6017446	8.48
17	2-TricapCubeA-Co4Se2Se1	-6578.6017350	8.49
18	2-TricapCubeA-Co3Se4Se3	-6578.6017267	8.49
19	3-TricapCubeB-Co1Se1Se2	-6578.6017245	8.49
20	4-Icos-1vx-Co1Se1Se5	-6578.6017217	8.50
21	4-Icos-1vx-Co3Se1Se4	-6578.6017209	8.50
22	4-Icos-1vx-Co2Se1Se5	-6578.6017181	8.50
23	2-TricapCubeA-Co3Se9Se1	-6578.6017172	8.50
24	1-PentaCapTriPri-Co1Se1Se8	-6578.6017151	8.50
25	4-Icos-1vx-Co4Se3Se3	-6578.6017102	8.50
26	2-TricapCubeA-Co4Se3Se2	-6578.6017076	8.50
27	3-TricapCubeB-Co2Se1Se3	-6578.6016959	8.51
28	4-Icos-1vx-Co1Se3Se7	-6578.6016955	8.51
29	2-TricapCubeA-Co2Se1Se5	-6578.6016943	8.51
30	2-TricapCubeA-Co2Se2Se4	-6578.6016936	8.51
31	3-TricapCubeB-Co2Se5Se1	-6578.5968817	11.53
32	2-TricapCubeA-Co3Se7Se2	-6578.5968776	11.54
33	4-Icos-1vx-Co5Se3Se4	-6578.5968729	11.54
34	2-TricapCubeA-Co3Se2Se4	-6578.5968692	11.54
35	3-TricapCubeB-Co4Se1Se4	-6578.5968596	11.55
36	2-TricapCubeA-Co1Se2Se3	-6578.5968567	11.55
37	4-Icos-1vx-Co5Se1Se9	-6578.5968508	11.55
38	2-TricapCubeA-Co2Se4Se2	-6578.5968480	11.55
39	4-Icos-1vx-Co4Se1Se4	-6578.5968478	11.55

40	3-TricapCubeB-Co1Se2Se1	-6578.5968468	11.55
41	4-Icos-1vx-Co5Se4Se4	-6578.5968459	11.56
42	4-Icos-1vx-Co5Se2Se7	-6578.5968415	11.56
43	2-TricapCubeA-Co2Se1Se7	-6578.5968301	11.57
44	3-TricapCubeB-Co4Se2Se3	-6578.5968283	11.57
45	1-PentaCapTriPri-Co1Se1Se5	-6578.5968133	11.58
46	2-TricapCubeA-Co4Se5Se2	-6578.5968088	11.58
47	2-TricapCubeA-Co2Se2Se3	-6578.5968078	11.58
48	2-TricapCubeA-Co1Se2Se1	-6578.5968011	11.58
49	4-Icos-1vx-Co3Se5Se5	-6578.5967930	11.59
50	2-TricapCubeA-Co4Se2Se2	-6578.5967928	11.59
51	2-TricapCubeA-Co2Se1Se3	-6578.5967918	11.59
52	2-TricapCubeA-Co1Se3Se4	-6578.5967898	11.59
53	2-TricapCubeA-Co1Se2Se2	-6578.5967751	11.60
54	4-Icos-1vx-Co2Se2Se1	-6578.5967743	11.60
55	3-TricapCubeB-Co1Se2Se6	-6578.5967624	11.61
56	2-TricapCubeA-Co1Se1Se9	-6578.5967563	11.61
57	4-Icos-1vx-Co4Se2Se2	-6578.5967554	11.61
58	3-TricapCubeB-Co4Se2Se7	-6578.5967476	11.62
59	2-TricapCubeA-Co2Se1Se9	-6578.5962402	11.94
60	3-TricapCubeB-Co1Se1Se4	-6578.5962331	11.94
61	3-TricapCubeB-Co1Se4Se3	-6578.5962059	11.96
62	4-Icos-1vx-Co5Se1Se4	-6578.5962057	11.96
63	4-Icos-1vx-Co4Se1Se6	-6578.5962029	11.96
64	3-TricapCubeB-Co3Se5Se2	-6578.5961938	11.96
65	3-TricapCubeB-Co3Se3Se3	-6578.5961861	11.97
66	3-TricapCubeB-Co4Se1Se2	-6578.5961846	11.97
67	2-TricapCubeA-Co4Se6Se2	-6578.5961793	11.97
68	3-TricapCubeB-Co4Se5Se2	-6578.5961783	11.97
69	4-Icos-1vx-Co2Se1Se6	-6578.5961759	11.98
70	2-TricapCubeA-Co4Se6Se4	-6578.5961739	11.98
71	3-TricapCubeB-Co2Se5Se2	-6578.5961724	11.98
72	2-TricapCubeA-Co2Se3Se7	-6578.5961682	11.98
73	2-TricapCubeA-Co1Se1Se3	-6578.5961615	11.98
74	2-TricapCubeA-Co4Se4Se4	-6578.5961599	11.99
75	2-TricapCubeA-Co4Se1Se7	-6578.5961585	11.99
76	4-Icos-1vx-Co3Se7Se2	-6578.5961570	11.99
77	4-Icos-1vx-Co1Se3Se4	-6578.5961551	11.99
78	4-Icos-1vx-Co5Se4Se2	-6578.5961545	11.99
79	2-TricapCubeA-Co2Se4Se3	-6578.5961502	11.99
80	2-TricapCubeA-Co1Se1Se8	-6578.5961496	11.99
81	2-TricapCubeA-Co3Se4Se5	-6578.5961489	11.99
82	2-TricapCubeA-Co4Se2Se6	-6578.5961478	11.99

83	3-TricapCubeB-Co2Se1Se6	-6578.5961446	12.00
84	4-Icos-1vx-Co3Se5Se4	-6578.5961418	12.00
85	2-TricapCubeA-Co3Se2Se2	-6578.5961414	12.00
86	3-TricapCubeB-Co1Se3Se3	-6578.5961414	12.00
87	3-TricapCubeB-Co3Se2Se1	-6578.5961383	12.00
88	4-Icos-1vx-Co4Se2Se5	-6578.5961342	12.00
89	2-TricapCubeA-Co3Se6Se2	-6578.5961283	12.01
90	2-TricapCubeA-Co4Se8Se1	-6578.5961269	12.01
91	4-Icos-1vx-Co2Se2Se5	-6578.5961149	12.01
92	4-Icos-1vx-Co3Se9Se1	-6578.5961148	12.01
93	2-TricapCubeA-Co3Se6Se4	-6578.5961082	12.02
94	2-TricapCubeA-Co1Se3Se7	-6578.5960983	12.02
95	3-TricapCubeB-Co4Se6Se1	-6578.5960968	12.03
96	4-Icos-1vx-Co3Se6Se3	-6578.5960950	12.03
97	2-TricapCubeA-Co3Se1Se6	-6578.5826795	20.44
98	2-TricapCubeA-Co4Se7Se1	-6578.5826725	20.45
99	4-Icos-1vx-Co3Se3Se7	-6578.5826600	20.46
100	2-TricapCubeA-Co3Se5Se3	-6578.5826582	20.46
101	4-Icos-1vx-Co5Se4Se6	-6578.5826582	20.46
102	4-Icos-1vx-Co5Se4Se1	-6578.5826567	20.46
103	4-Icos-1vx-Co5Se3Se7	-6578.5826469	20.47
104	2-TricapCubeA-Co4Se8Se2	-6578.5826276	20.48
105	3-TricapCubeB-Co3Se3Se7	-6578.5826096	20.49
106	3-TricapCubeB-Co4Se1Se6	-6578.5826016	20.49
107	1-PentaCapTriPri-Co1Se3Se2	-6578.5825730	20.51
108	4-Icos-1vx-Co3Se8Se1	-6578.5825724	20.51
109	2-TricapCubeA-Co1Se3Se1	-6578.5825679	20.51
110	2-TricapCubeA-Co4Se7Se3	-6578.5722247	27.01
111	4-Icos-1vx-Co3Se8Se2	-6578.5721897	27.03
112	3-TricapCubeB-Co2Se2Se8	-6578.5721831	27.03
113	1-PentaCapTriPri-Co2Se5Se1	-6578.5721712	27.04
114	3-TricapCubeB-Co2Se2Se4	-6578.5721665	27.04
115	4-Icos-1vx-Co4Se2Se3	-6578.5721642	27.04
116	2-TricapCubeA-Co3Se2Se5_r-17	-6578.5721616	27.05
117	2-TricapCubeA-Co4Se5Se4	-6578.5721601	27.05
118	2-TricapCubeA-Co3Se2Se5_i-17	-6578.5721539	27.05
119	2-TricapCubeA-Co3Se2Se1	-6578.5721538	27.05
120	2-TricapCubeA-Co2Se4Se1	-6578.5721453	27.06
121	1-PentaCapTriPri-Co2Se4Se2	-6578.5721417	27.06
122	4-Icos-1vx-Co3Se4Se6	-6578.5721366	27.06
123	3-TricapCubeB-Co4Se1Se1	-6578.5712398	27.62
124	3-TricapCubeB-Co1Se3Se2	-6578.5712282	27.63
125	4-Icos-1vx-Co4Se1Se1	-6578.5712252	27.63

126	3-TricapCubeB-Co3Se1Se1	-6578.5712221	27.63
127	2-TricapCubeA-Co4Se6Se1	-6578.5712065	27.64
128	4-Icos-1vx-Co1Se3Se5	-6578.5711991	27.65
129	3-TricapCubeB-Co1Se1Se3	-6578.5711769	27.66
130	2-TricapCubeA-Co4Se1Se2	-6578.5711694	27.67
131	1-PentaCapTriPri-Co2Se3Se3	-6578.5711339	27.69
132	3-TricapCubeB-Co4Se2Se4	-6578.5711311	27.69
133	2-TricapCubeA-Co3Se4Se6	-6578.5711248	27.70
134	4-Icos-1vx-Co3Se4Se1	-6578.5711095	27.71
135	3-TricapCubeB-Co1Se5Se1	-6578.5646360	31.77
136	4-Icos-1vx-Co4Se4Se1	-6578.5646337	31.77
137	1-PentaCapTriPri-Co2Se1Se3	-6578.5646190	31.78
138	2-TricapCubeA-Co2Se1Se8	-6578.5646093	31.78
139	3-TricapCubeB-Co3Se1Se3	-6578.5611536	33.95
140	4-Icos-1vx-Co5Se2Se4	-6578.5611480	33.96
141	4-Icos-1vx-Co2Se1Se1	-6578.5611408	33.96
142	4-Icos-1vx-Co1Se1Se4	-6578.5611304	33.97
143	2-TricapCubeA-Co4Se4Se2	-6578.5611276	33.97
144	3-TricapCubeB-Co3Se2Se4	-6578.5611256	33.97
145	4-Icos-1vx-Co3Se5Se1	-6578.5611222	33.97
146	2-TricapCubeA-Co1Se1Se7	-6578.5611140	33.98
147	4-Icos-1vx-Co5Se1Se6	-6578.5611043	33.98
148	2-TricapCubeA-Co3Se3Se1	-6578.5610610	34.01
149	2-TricapCubeA-Co2Se1Se6	-6578.5577108	36.11
150	2-TricapCubeA-Co3Se1Se5	-6578.5576936	36.12
151	4-Icos-1vx-Co4Se1Se3	-6578.5576637	36.14
152	2-TricapCubeA-Co2Se3Se1	-6578.5576526	36.15
153	2-TricapCubeA-Co4Se1Se3	-6578.5558071	37.31
154	3-TricapCubeB-Co3Se2Se2	-6578.5557964	37.31
155	1-PentaCapTriPri-Co2Se1Se4	-6578.5557765	37.33
156	3-TricapCubeB-Co4Se1Se5	-6578.5557733	37.33
157	4-Icos-1vx-Co2Se1Se3	-6578.5557683	37.33
158	4-Icos-1vx-Co3Se6Se1	-6578.5557542	37.34
159	2-TricapCubeA-Co3Se4Se2	-6578.5557491	37.34
160	4-Icos-1vx-Co5Se1Se1	-6578.5557194	37.36
161	2-TricapCubeA-Co3Se1Se9	-6578.5557127	37.37
162	2-TricapCubeA-Co3Se8Se1	-6578.5557113	37.37
163	1-PentaCapTriPri-Co2Se6Se1	-6578.5536008	38.69
164	3-TricapCubeB-Co3Se1Se4	-6578.5535696	38.71
165	3-TricapCubeB-Co2Se1Se1	-6578.5535568	38.72
166	4-Icos-1vx-Co3Se2Se1	-6578.5535490	38.72
167	4-Icos-1vx-Co2Se6Se1	-6578.5535204	38.74
168	4-Icos-1vx-Co5Se2Se5	-6578.5521330	39.61

169	4-Icos-1vx-Co3Se5Se2	-6578.5521200	39.62
170	4-Icos-1vx-Co2Se1Se7	-6578.5519341	39.74
171	3-TricapCubeB-Co3Se4Se2	-6578.5519104	39.75
172	3-TricapCubeB-Co4Se4Se2	-6578.5519070	39.76
173	2-TricapCubeA-Co4Se1Se5	-6578.5518927	39.76
174	4-Icos-1vx-Co2Se4Se1	-6578.5518867	39.77
175	4-Icos-1vx-Co4Se1Se2	-6578.5516742	39.90
176	2-TricapCubeA-Co3Se1Se7	-6578.5516640	39.91
177	3-TricapCubeB-Co1Se1Se1	-6578.5516168	39.94
178	2-TricapCubeA-Co4Se3Se1	-6578.5515753	39.96
179	1-PentaCapTriPri-Co2Se1Se2	-6578.5491284	41.50
180	4-Icos-1vx-Co5Se1Se8	-6578.5490929	41.52
181	3-TricapCubeB-Co4Se4Se3	-6578.5490860	41.53
182	4-Icos-1vx-Co5Se4Se3	-6578.5490845	41.53
183	3-TricapCubeB-Co4Se5Se1	-6578.5490612	41.54
184	2-TricapCubeA-Co4Se1Se6	-6578.5482421	42.06
185	2-TricapCubeA-Co3Se8Se2	-6578.5482273	42.06
186	4-Icos-1vx-Co1Se3Se2	-6578.5481780	42.10
187	4-Icos-1vx-Co3Se4Se3	-6578.5481607	42.11
188	2-TricapCubeA-Co2Se1Se1	-6578.5472803	42.66
189	3-TricapCubeB-Co1Se1Se5	-6578.5472771	42.66
190	4-Icos-1vx-Co4Se3Se1	-6578.5472710	42.66
191	4-Icos-1vx-Co4Se3Se5	-6578.5472679	42.67
192	2-TricapCubeA-Co2Se3Se4	-6578.5472633	42.67
193	2-TricapCubeA-Co3Se1Se4	-6578.5472536	42.68
194	3-TricapCubeB-Co1Se1Se7	-6578.5472467	42.68
195	2-TricapCubeA-Co2Se1Se4 i-16	-6578.5472305	42.69
196	2-TricapCubeA-Co3Se3Se2	-6578.5472241	42.69
197	2-TricapCubeA-Co2Se1Se4 r-16	-6578.5471855	42.72
198	1-PentaCapTriPri-Co2Se5Se5	-6578.5450205	44.08
199	3-TricapCubeB-Co1Se4Se1	-6578.5444877	44.41
200	2-TricapCubeA-Co3Se2Se8	-6578.5444636	44.43
201	2-TricapCubeA-Co4Se4Se1	-6578.5444611	44.43
202	4-Icos-1vx-Co4Se1Se9	-6578.5444469	44.44
203	2-TricapCubeA-Co1Se1Se6	-6578.5444436	44.44
204	2-TricapCubeA-Co2Se1Se2	-6578.5444412	44.44
205	1-PentaCapTriPri-Co2Se1Se1	-6578.5444274	44.45
206	4-Icos-1vx-Co3Se5Se3	-6578.5444234	44.45
207	4-Icos-1vx-Co3Se3Se3	-6578.5444140	44.46
208	4-Icos-1vx-Co4Se2Se6	-6578.5444131	44.46
209	4-Icos-1vx-Co4Se4Se2	-6578.5443897	44.47
210	2-TricapCubeA-Co3Se1Se8	-6578.5443837	44.48
211	2-TricapCubeA-Co1Se3Se6	-6578.5443618	44.49

212	3-TricapCubeB-Co1Se1Se9	-6578.5443419	44.50
213	3-TricapCubeB-Co3Se2Se6	-6578.5443333	44.51
214	2-TricapCubeA-Co4Se2Se4	-6578.5441801	44.60
215	4-Icos-1vx-Co1Se1Se3	-6578.5441669	44.61
216	4-Icos-1vx-Co2Se1Se9	-6578.5441642	44.61
217	4-Icos-1vx-Co3Se1Se9	-6578.5441406	44.63
218	4-Icos-1vx-Co2Se2Se6	-6578.5441255	44.64
219	4-Icos-1vx-Co1Se2Se5	-6578.5441229	44.64
220	4-Icos-1vx-Co2Se3Se2	-6578.5441052	44.65
221	4-Icos-1vx-Co3Se6Se4	-6578.5410026	46.60
222	4-Icos-1vx-Co5Se1Se2	-6578.5409513	46.63
223	2-TricapCubeA-Co2Se3Se3	-6578.5408872	46.67
224	2-TricapCubeA-Co1Se1Se4	-6578.5408828	46.67
225	3-TricapCubeB-Co3Se6Se1	-6578.5408569	46.69
226	2-TricapCubeA-Co3Se1Se2	-6578.5408233	46.71
227	2-TricapCubeA-Co3Se4Se1	-6578.5393597	47.63
228	4-Icos-1vx-Co4Se1Se8	-6578.5393315	47.65
229	4-Icos-1vx-Co5Se1Se5	-6578.5393002	47.67
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232	3-TricapCubeB-Co1Se1Se8	-6578.5392018	47.73
233	3-TricapCubeB-Co4Se4Se1	-6578.5389047	47.91
234	4-Icos-1vx-Co1Se1Se6	-6578.5384148	48.22
235	2-TricapCubeA-Co4Se3Se4	-6578.5378997	48.55
236	4-Icos-1vx-Co5Se4Se5	-6578.5369700	49.13
237	2-TricapCubeA-Co4Se9Se1	-6578.5369320	49.15
238	2-TricapCubeA-Co3Se1Se1	-6578.5369120	49.16
239	3-TricapCubeB-Co4Se2Se1	-6578.5368918	49.18
240	3-TricapCubeB-Co2Se3Se6	-6578.5366790	49.31
241	4-Icos-1vx-Co1Se3Se1	-6578.5366579	49.32
242	2-TricapCubeA-Co3Se2Se6	-6578.5366526	49.33
243	3-TricapCubeB-Co1Se2Se4	-6578.5360376	49.71
244	3-TricapCubeB-Co4Se3Se2	-6578.5360224	49.72
245	3-TricapCubeB-Co3Se3Se2	-6578.5360146	49.73
246	3-TricapCubeB-Co4Se2Se5	-6578.5360130	49.73
247	4-Icos-1vx-Co1Se2Se2_r-22	-6578.5360107	49.73
248	3-TricapCubeB-Co1Se2Se5	-6578.5360096	49.73
249	4-Icos-1vx-Co5Se3Se2	-6578.5359613	49.76
250	2-TricapCubeA-Co4Se5Se5	-6578.5359552	49.77
251	1-PentaCapTriPri-Co2Se4Se3	-6578.5359523	49.77
252	3-TricapCubeB-Co3Se1Se2	-6578.5359326	49.78
253	4-Icos-1vx-Co4Se3Se2	-6578.5355889	50.00
254	1-PentaCapTriPri-Co1Se2Se5	-6578.5355738	50.00

255	2-TricapCubeA-Co1Se2Se4	-6578.5355475	50.02
256	2-TricapCubeA-Co3Se3Se4	-6578.5355382	50.03
257	4-Icos-1vx-Co3Se2Se4	-6578.5344415	50.72
258	2-TricapCubeA-Co1Se1Se1	-6578.5344294	50.72
259	3-TricapCubeB-Co4Se2Se2	-6578.5343869	50.75
260	4-Icos-1vx-Co3Se1Se6	-6578.5343180	50.79
261	4-Icos-1vx-Co3Se4Se2	-6578.5342950	50.81
262	2-TricapCubeA-Co4Se4Se3	-6578.5342836	50.81
263	3-TricapCubeB-Co3Se1Se5	-6578.5342362	50.84
264	4-Icos-1vx-Co3Se2Se5	-6578.5338972	51.06
265	3-TricapCubeB-Co2Se1Se2	-6578.5336916	51.19
266	1-PentaCapTriPri-Co1Se1Se9	-6578.5333188	51.42
267	3-TricapCubeB-Co1Se3Se5	-6578.5313080	52.68
268	3-TricapCubeB-Co3Se1Se8	-6578.5313001	52.69
269	4-Icos-1vx-Co5Se1Se3	-6578.5312486	52.72
270	2-TricapCubeA-Co4Se1Se4	-6578.5312053	52.75
271	2-TricapCubeA-Co1Se3Se5	-6578.5311508	52.78
272	4-Icos-1vx-Co3Se3Se2	-6578.5311373	52.79
273	2-TricapCubeA-Co1Se1Se2	-6578.5310342	52.85
274	2-TricapCubeA-Co3Se5Se4	-6578.5302813	53.33
275	4-Icos-1vx-Co4Se5Se2	-6578.5302397	53.35
276	1-PentaCapTriPri-Co2Se2Se2	-6578.5302198	53.36
277	2-TricapCubeA-Co4Se7Se2	-6578.5301903	53.38
278	4-Icos-1vx-Co5Se2Se2	-6578.5292798	53.95
279	4-Icos-1vx-Co2Se2Se2	-6578.5291640	54.03
280	4-Icos-1vx-Co3Se4Se5	-6578.5290952	54.07
281	4-Icos-1vx-Co3Se6Se2	-6578.5290584	54.09
282	2-TricapCubeA-Co4Se4Se6 r-22	-6578.5289696	54.15
283	2-TricapCubeA-Co3Se3Se5	-6578.5289451	54.16
284	2-TricapCubeA-Co4Se3Se6	-6578.5289314	54.17
285	3-TricapCubeB-Co3Se3Se1	-6578.5289128	54.18
286	4-Icos-1vx-Co3Se1Se8	-6578.5288370	54.23
287	1-PentaCapTriPri-Co2Se3Se2	-6578.5287588	54.28
288	2-TricapCubeA-Co3Se1Se3	-6578.5287404	54.29
289	2-TricapCubeA-Co4Se2Se3	-6578.5286633	54.34
290	2-TricapCubeA-Co3Se7Se3	-6578.5286435	54.35
291	4-Icos-1vx-Co4Se2Se4	-6578.5286403	54.36
292	3-TricapCubeB-Co1Se2Se3	-6578.5286127	54.37
293	1-PentaCapTriPri-Co1Se2Se2	-6578.5285953	54.38
294	3-TricapCubeB-Co1Se2Se2	-6578.5285701	54.40
295	3-TricapCubeB-Co3Se2Se5	-6578.5285584	54.41
296	2-TricapCubeA-Co4Se4Se5	-6578.5285569	54.41
297	2-TricapCubeA-Co3Se5Se2	-6578.5285476	54.41

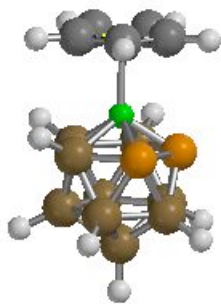
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311	4-Icos-1vx-Co2Se3Se5	-6578.5249161	56.69
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313	2-TricapCubeA-Co3Se2Se3	-6578.5245681	56.91
314	2-TricapCubeA-Co3Se6Se1	-6578.5240545	57.23
315	3-TricapCubeB-Co4Se3Se1	-6578.5240405	57.24
316	3-TricapCubeB-Co4Se3Se3	-6578.5240383	57.24
317	3-TricapCubeB-Co1Se3Se1	-6578.5239896	57.27
318	2-TricapCubeA-Co3Se4Se4	-6578.5239688	57.29
319	4-Icos-1vx-Co1Se1Se2	-6578.5230352	57.87
320	4-Icos-1vx-Co3Se1Se7	-6578.5230224	57.88
321	1-PentaCapTriPri-Co2Se2Se5	-6578.5219466	58.56
322	2-TricapCubeA-Co4Se1Se9	-6578.5219136	58.58
323	4-Icos-1vx-Co2Se2Se4	-6578.5212678	58.98
324	4-Icos-1vx-Co1Se3Se6	-6578.5210596	59.11
325	3-TricapCubeB-Co3Se1Se9	-6578.5209797	59.16
326	3-TricapCubeB-Co3Se3Se5	-6578.5209312	59.19
327	3-TricapCubeB-Co4Se3Se6	-6578.5209030	59.21
328	3-TricapCubeB-Co4Se2Se8	-6578.5208892	59.22
329	4-Icos-1vx-Co5Se3Se6	-6578.5208627	59.24
330	3-TricapCubeB-Co4Se1Se9	-6578.5205302	59.44
331	3-TricapCubeB-Co4Se2Se6	-6578.5205255	59.45
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334	4-Icos-1vx-Co5Se3Se5	-6578.5204553	59.49
335	3-TricapCubeB-Co4Se1Se8	-6578.5204425	59.50
336	1-PentaCapTriPri-Co1Se1Se7	-6578.5204331	59.51
337	4-Icos-1vx-Co5Se2Se6	-6578.5204303	59.51
338	3-TricapCubeB-Co2Se4Se3	-6578.5203439	59.56
339	3-TricapCubeB-Co2Se3Se4	-6578.5203426	59.56
340	2-TricapCubeA-Co3Se6Se3	-6578.5203282	59.57

341	4-Icos-1vx-Co4Se6Se1	-6578.5202910	59.59
342	4-Icos-1vx-Co2Se2Se8	-6578.5197683	59.92
343	2-TricapCubeA-Co4Se1Se8	-6578.5197626	59.93
344	4-Icos-1vx-Co2Se5Se1	-6578.5197389	59.94
345	2-TricapCubeA-Co2Se3Se6	-6578.5189349	60.45
346	4-Icos-1vx-Co4Se1Se7	-6578.5188625	60.49
347	2-TricapCubeA-Co4Se3Se3	-6578.5187882	60.54
348	3-TricapCubeB-Co4Se1Se3	-6578.5187822	60.54
349	3-TricapCubeB-Co2Se2Se2	-6578.5185775	60.67
350	2-TricapCubeA-Co4Se6Se3	-6578.5185538	60.69
351	4-Icos-1vx-Co3Se3Se1	-6578.5184976	60.72
352	4-Icos-1vx-Co5Se3Se3	-6578.5184923	60.72
353	3-TricapCubeB-Co2Se3Se3	-6578.5184796	60.73
354	3-TricapCubeB-Co2Se2Se1	-6578.5184756	60.73
355	1-PentaCapTriPri-Co2Se1Se6	-6578.5183271	60.83
356	2-TricapCubeA-Co4Se4Se6_i-22	-6578.5178132	61.15
357	2-TricapCubeA-Co2Se5Se1	-6578.5174932	61.35
358	3-TricapCubeB-Co1Se3Se7	-6578.5158281	62.40
359	4-Icos-1vx-Co4Se1Se5	-6578.5157794	62.43
360	3-TricapCubeB-Co1Se2Se7	-6578.5157515	62.44
361	2-TricapCubeA-Co3Se5Se1	-6578.5156755	62.49
362	4-Icos-1vx-Co5Se2Se3	-6578.5156489	62.51
363	4-Icos-1vx-Co3Se2Se6	-6578.5152969	62.73
364	2-TricapCubeA-Co4Se3Se7	-6578.5147939	63.04
365	2-TricapCubeA-Co4Se2Se7	-6578.5145670	63.19
366	1-PentaCapTriPri-Co2Se2Se3	-6578.5145376	63.21
367	4-Icos-1vx-Co3Se7Se1	-6578.5137294	63.71
368	2-TricapCubeA-Co4Se5Se3	-6578.5136896	63.74
369	4-Icos-1vx-Co4Se3Se7	-6578.5134885	63.86
370	4-Icos-1vx-Co3Se2Se8	-6578.5134582	63.88
371	4-Icos-1vx-Co4Se2Se7	-6578.5133698	63.94
372	2-TricapCubeA-Co3Se2Se7	-6578.5131649	64.07
373	4-Icos-1vx-Co3Se4Se4	-6578.5131490	64.08
374	3-TricapCubeB-Co1Se4Se2	-6578.5131437	64.08
375	4-Icos-1vx-Co1Se4Se2	-6578.5131351	64.09
376	4-Icos-1vx-Co1Se3Se3	-6578.5131223	64.09
377	3-TricapCubeB-Co1Se5Se2	-6578.5130853	64.12
378	4-Icos-1vx-Co4Se2Se8	-6578.5130650	64.13
379	1-PentaCapTriPri-Co2Se2Se4	-6578.5125183	64.47
380	2-TricapCubeA-Co2Se2Se2	-6578.5121722	64.69
381	4-Icos-1vx-Co2Se3Se1	-6578.5121211	64.72
382	4-Icos-1vx-Co2Se3Se3	-6578.5120968	64.74
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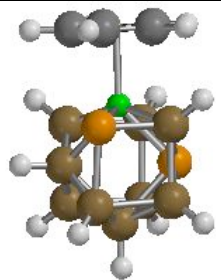
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386	4-Icos-1vx-Co4Se4Se3	-6578.5108401	65.53
387	1-PentaCapTriPri-Co1Se2Se3	-6578.5108103	65.54
388	4-Icos-1vx-Co5Se2Se1	-6578.5093104	66.49
389	4-Icos-1vx-Co2Se4Se2	-6578.5086391	66.91
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394	3-TricapCubeB-Co3Se3Se4	-6578.5082226	67.17
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403	4-Icos-1vx-Co2Se3Se7	-6578.5060734	68.52
404	4-Icos-1vx-Co2Se2Se7	-6578.5060528	68.53
405	2-TricapCubeA-Co4Se2Se5	-6578.5059129	68.62
406	4-Icos-1vx-Co3Se2Se2	-6578.5059111	68.62
407	3-TricapCubeB-Co3Se1Se7	-6578.5058209	68.68
408	2-TricapCubeA-Co2Se2Se5	-6578.5056458	68.79
409	1-PentaCapTriPri-Co2Se1Se5	-6578.5055817	68.83
410	4-Icos-1vx-Co2Se3Se4	-6578.5052453	69.04
411	4-Icos-1vx-Co4Se5Se1	-6578.5049239	69.24
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413	3-TricapCubeB-Co4Se3Se4	-6578.5040992	69.76
414	3-TricapCubeB-Co3Se2Se8	-6578.5039294	69.86
415	3-TricapCubeB-Co3Se5Se1	-6578.5039285	69.86
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419	1-PentaCapTriPri-Co1Se1Se3	-6578.5023908	70.83
420	4-Icos-1vx-Co5Se5Se1	-6578.5017324	71.24
421	3-TricapCubeB-Co2Se1Se5	-6578.5006861	71.90
422	3-TricapCubeB-Co1Se3Se4	-6578.5006634	71.91
423	3-TricapCubeB-Co2Se2Se6	-6578.5006151	71.94
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425	3-TricapCubeB-Co2Se4Se1	-6578.4994174	72.69
426	3-TricapCubeB-Co2Se3Se5	-6578.4993814	72.72

427	3-TricapCubeB-Co2Se1Se8	-6578.4993723	72.72
428	2-TricapCubeA-Co2Se2Se6	-6578.4988514	73.05
429	2-TricapCubeA-Co4Se2Se8	-6578.4977537	73.74
430	1-PentaCapTriPri-Co2Se5Se2	-6578.4962233	74.70
431	3-TricapCubeB-Co4Se1Se7	-6578.4952153	75.33
432	4-Icos-1vx-Co2Se3Se6	-6578.4940977	76.03
433	4-Icos-1vx-Co2Se5Se2	-6578.4939754	76.11
434	1-PentaCapTriPri-Co1Se2Se1	-6578.4931064	76.65
435	4-Icos-1vx-Co1Se2Se3	-6578.4928647	76.81
436	4-Icos-1vx-Co3Se3Se4	-6578.4925194	77.02
437	2-TricapCubeA-Co4Se1Se1	-6578.4912131	77.84
438	3-TricapCubeB-Co3Se4Se3	-6578.4903219	78.40
439	3-TricapCubeB-Co3Se1Se6	-6578.4888494	79.33
440	4-Icos-1vx-Co3Se3Se5	-6578.4887466	79.39
441	1-PentaCapTriPri-Co1Se1Se1	-6578.4871154	80.41
442	1-PentaCapTriPri-Co2Se4Se1	-6578.4863892	80.87
443	3-TricapCubeB-Co2Se2Se7	-6578.4842224	82.23
444	3-TricapCubeB-Co2Se4Se2	-6578.4841846	82.25
445	3-TricapCubeB-Co2Se3Se7	-6578.4841832	82.25
446	2-TricapCubeA-Co1Se3Se2	-6578.4837260	82.54
447	3-TricapCubeB-Co2Se2Se3	-6578.4819245	83.67
448	3-TricapCubeB-Co2Se1Se9	-6578.4818555	83.71
449	1-PentaCapTriPri-Co1Se2Se4	-6578.4815315	83.92
450	4-Icos-1vx-Co1Se4Se1	-6578.4808428	84.35
451	1-PentaCapTriPri-Co1Se3Se4	-6578.4803481	84.66
452	3-TricapCubeB-Co1Se1Se6	-6578.4702036	91.03
453	1-PentaCapTriPri-Co2Se5Se3	-6578.4691782	91.67
454	3-TricapCubeB-Co1Se2Se8	-6578.4681788	92.30
455	1-PentaCapTriPri-Co2Se4Se4	-6578.4680835	92.36
456	1-PentaCapTriPri-Co2Se3Se1	-6578.4680503	92.38
457	1-PentaCapTriPri-Co2Se4Se6	-6578.4672363	92.89
458	1-PentaCapTriPri-Co2Se2Se1	-6578.4666185	93.28
459	2-TricapCubeA-Co4Se3Se5	-6578.4659254	93.71
460	3-TricapCubeB-Co2Se2Se5	-6578.4630171	95.54
461	3-TricapCubeB-Co2Se6Se1	-6578.4629362	95.59
462	2-TricapCubeA-Co4Se5Se1	-6578.4593344	97.85
463	2-TricapCubeA-Co1Se3Se3	-6578.4544629	100.90
464	4-Icos-1vx-Co1Se2Se1	-6578.4511233	103.00
465	1-PentaCapTriPri-Co2Se3Se4	-6578.4471603	105.49
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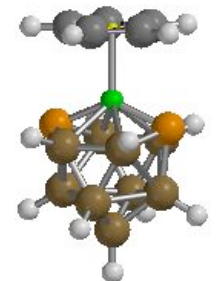
Table S5A. Initial CpCoSe₂B₉H₉ structures, 150 structures.



1. Icosahedron 9 structures

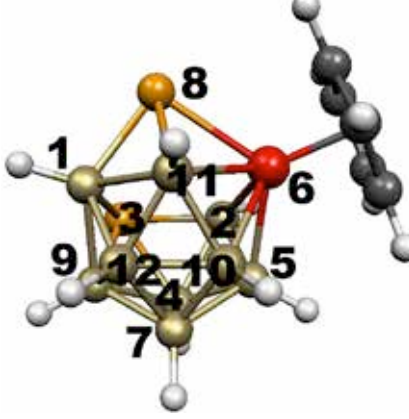
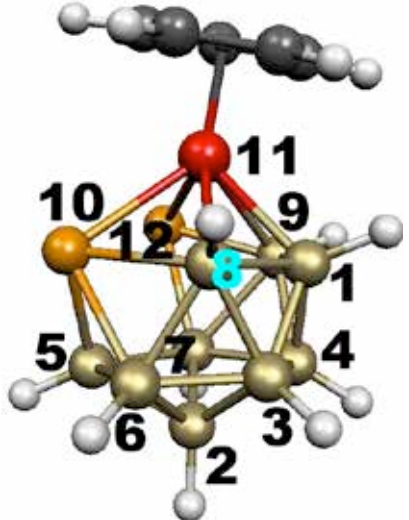


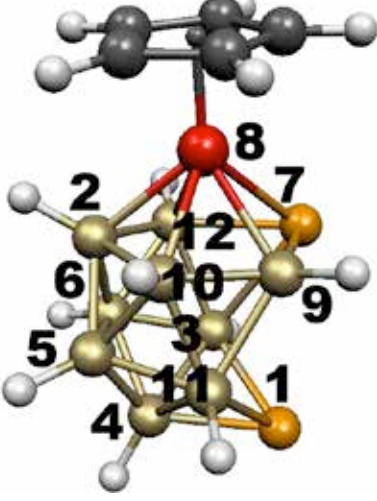
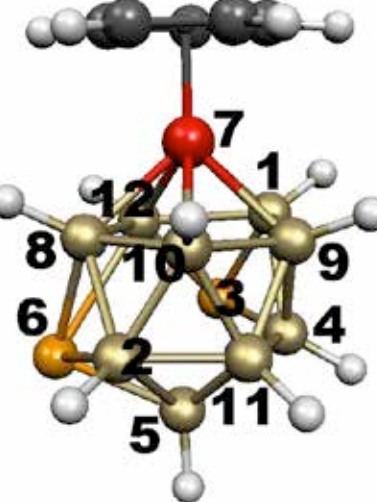
2. Cubeoctahedron 53 structures

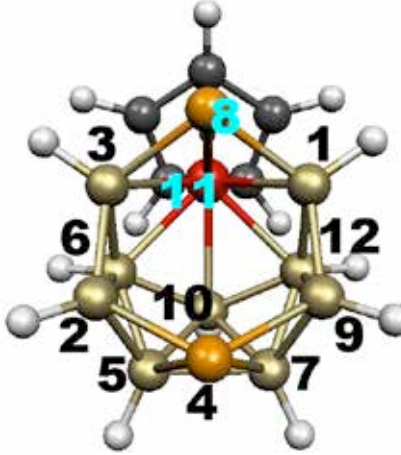
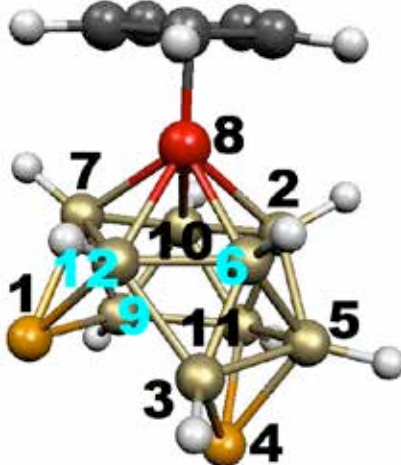


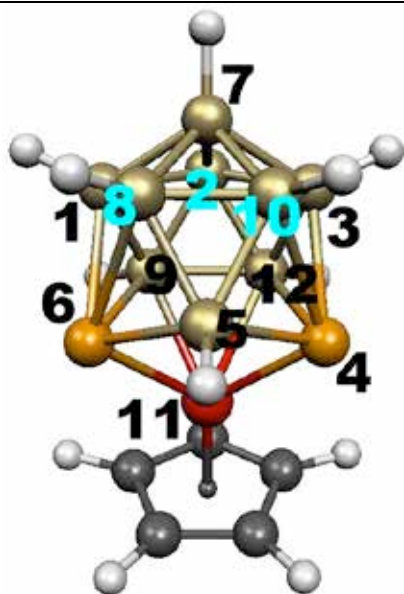
3. Anticubeoctahedron 88 structures

Table S5B. Distance table for the lowest-lying CpCoSe₂B₉H₉ structures after M06L/6-311G(d,p) optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry.

 <p>1. -6608.2722608 0.0 C₁</p>	<table border="1"> <thead> <tr> <th></th> <th>1</th> <th>2</th> <th>3</th> <th>4</th> <th>5</th> </tr> </thead> <tbody> <tr><td>1 B</td><td>0.000000</td><td></td><td></td><td></td><td></td></tr> <tr><td>2 B</td><td>3.173086</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>3 Se</td><td>2.445628</td><td>2.033443</td><td>0.000000</td><td></td><td></td></tr> <tr><td>4 B</td><td>3.214985</td><td>1.858278</td><td>2.045929</td><td>0.000000</td><td></td></tr> <tr><td>5 B</td><td>3.474298</td><td>1.717378</td><td>3.151615</td><td>1.763457</td><td>0.000000</td></tr> <tr><td>6 Co</td><td>3.218468</td><td>2.161084</td><td>3.644937</td><td>3.401980</td><td>2.118279</td></tr> <tr><td>7 B</td><td>2.954267</td><td>2.887485</td><td>3.203926</td><td>1.756087</td><td>1.779424</td></tr> <tr><td>8 Se</td><td>2.034479</td><td>3.127516</td><td>3.257663</td><td>4.183145</td><td>3.794754</td></tr> <tr><td>9 B</td><td>1.898684</td><td>2.931980</td><td>2.070987</td><td>1.874788</td><td>2.844965</td></tr> <tr><td>10 B</td><td>2.917814</td><td>2.957370</td><td>3.869872</td><td>2.914024</td><td>1.770505</td></tr> <tr><td>11 B</td><td>2.009127</td><td>3.416247</td><td>3.840728</td><td>3.825513</td><td>3.074116</td></tr> <tr><td>12 B</td><td>1.759454</td><td>3.477391</td><td>3.356154</td><td>2.958397</td><td>2.861313</td></tr> <tr> <td></td> <td>6</td> <td>7</td> <td>8</td> <td>9</td> <td>10</td> </tr> <tr><td>7 B</td><td>3.283234</td><td>0.000000</td><td></td><td></td><td></td></tr> <tr><td>8 Se</td><td>2.371821</td><td>4.154895</td><td>0.000000</td><td></td><td></td></tr> <tr><td>9 B</td><td>3.780240</td><td>1.750963</td><td>3.629346</td><td>0.000000</td><td></td></tr> <tr><td>10 B</td><td>2.098140</td><td>1.738781</td><td>3.346698</td><td>2.845046</td><td>0.000000</td></tr> <tr><td>11 B</td><td>2.167809</td><td>2.971924</td><td>2.013877</td><td>3.098326</td><td>1.776495</td></tr> <tr><td>12 B</td><td>3.215358</td><td>1.757822</td><td>3.181180</td><td>1.750357</td><td>1.773048</td></tr> <tr> <td></td> <td>11</td> <td>12</td> <td></td> <td></td> <td></td> </tr> <tr><td>12 B</td><td>1.777108</td><td>0.000000</td><td></td><td></td><td></td></tr> </tbody> </table>		1	2	3	4	5	1 B	0.000000					2 B	3.173086	0.000000				3 Se	2.445628	2.033443	0.000000			4 B	3.214985	1.858278	2.045929	0.000000		5 B	3.474298	1.717378	3.151615	1.763457	0.000000	6 Co	3.218468	2.161084	3.644937	3.401980	2.118279	7 B	2.954267	2.887485	3.203926	1.756087	1.779424	8 Se	2.034479	3.127516	3.257663	4.183145	3.794754	9 B	1.898684	2.931980	2.070987	1.874788	2.844965	10 B	2.917814	2.957370	3.869872	2.914024	1.770505	11 B	2.009127	3.416247	3.840728	3.825513	3.074116	12 B	1.759454	3.477391	3.356154	2.958397	2.861313		6	7	8	9	10	7 B	3.283234	0.000000				8 Se	2.371821	4.154895	0.000000			9 B	3.780240	1.750963	3.629346	0.000000		10 B	2.098140	1.738781	3.346698	2.845046	0.000000	11 B	2.167809	2.971924	2.013877	3.098326	1.776495	12 B	3.215358	1.757822	3.181180	1.750357	1.773048		11	12				12 B	1.777108	0.000000			
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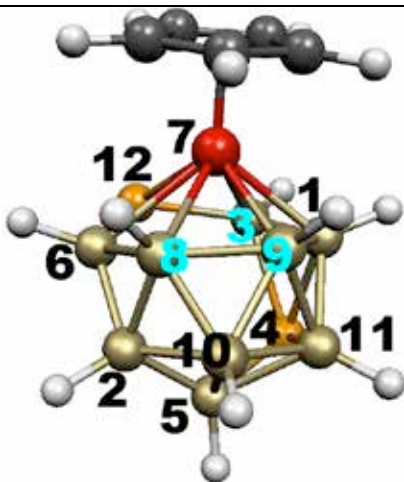
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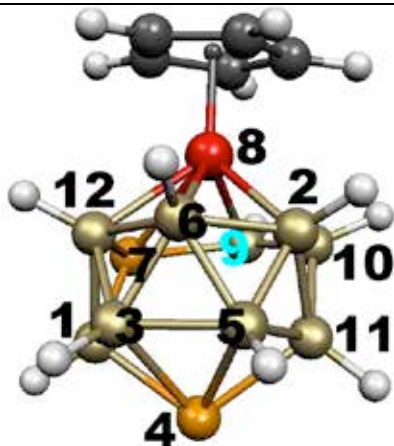
7. -6608.2386318 +21.1 C_S

	1	2	3	4	5
1 B	0.000000				
2 B	1.776927	0.000000			
3 B	2.851065	1.776907	0.000000		
4 Se	3.679535	3.235639	2.152603	0.000000	
5 B	2.938989	3.540102	2.939081	2.061295	0.000000
6 Se	2.152511	3.235569	3.679544	3.123572	2.061307
7 B	1.792365	1.787638	1.792405	3.324575	2.886216
8 B	1.839796	2.914657	2.853106	3.288391	1.819625
9 B	1.859044	1.713189	2.894521	3.202845	3.364170
10 B	2.852977	2.914631	1.839884	2.367228	1.819550
11 Co	3.488277	3.327055	3.488258	2.358558	3.065328
12 B	2.894530	1.713187	1.858979	2.205758	3.364171
	6	7	8	9	10
6 Se	0.000000				
7 B	3.324545	0.000000			
8 B	2.367288	1.692213	0.000000		
9 B	2.205691	2.974523	3.229286	0.000000	
10 B	3.288298	1.692210	1.667739	3.647904	0.000000
11 Co	2.358563	4.215637	4.013450	2.107124	4.013356
12 B	3.202796	2.974505	3.647964	1.726497	3.229220
	11	12			
12 B	2.107117	0.000000			



8. -6608.2365415 +22.4 C₁

	1	2	3	4	5
1 B	0.000000				
2 B	3.579888	0.000000			
3 B	1.852125	3.688167	0.000000		
4 Se	2.115300	3.342412	2.082459	0.000000	
5 B	3.013914	1.687584	3.330482	2.074766	0.000000
6 B	3.537521	1.735290	3.032403	3.698705	2.929157
7 Co	2.148112	3.335352	2.138473	3.556448	3.782404
8 B	3.016492	1.721736	3.530871	3.826065	2.782294
9 B	1.727914	2.845249	3.104367	3.184635	2.863129
10 B	2.924643	1.732174	3.894136	3.232266	1.788541
11 B	1.835012	2.910386	3.167053	2.079524	1.898972
12 Se	3.427732	3.328383	1.964325	3.399148	3.743070
	6	7	8	9	10
6 B	0.000000				
7 Co	2.374511	0.000000			
8 B	1.820897	2.237512	0.000000		
9 B	3.119596	2.151732	1.771235	0.000000	
10 B	2.965718	3.360258	1.722351	1.768052	0.000000
11 B	3.759470	3.370775	2.876462	1.764512	1.741651
12 Se	1.971854	2.397300	3.382661	3.926518	4.302032
	11	12			
12 Se	4.336200	0.000000			



9. -6608.2351257 +23.3 C₁

	1	2	3	4	5	
1 B	0.000000					
2 B	3.673280	0.000000				
3 B	1.788935	2.938755	0.000000			
4 Se	2.038687	3.177131	2.162709	0.000000		
5 B	3.064835	1.733576	1.844306	2.148246	0.000000	
6 B	2.897243	1.782323	1.736611	3.179152	1.758818	
7 Se	2.051612	3.791536	3.339166	3.431906	4.110738	
8 Co	3.384867	2.156072	3.337137	4.035878	3.310098	
9 B	3.305779	3.011420	4.086158	3.597977	3.940667	
10 B	3.764182	1.754906	3.856008	3.351851	3.006955	
11 B	3.333696	1.719561	3.064200	2.061329	1.815067	
12 B	1.783709	3.039094	1.717379	3.170761	2.920314	
	6	7	8	9	10	
6 B	0.000000					
7 Se	3.449486	0.000000				
8 Co	2.144271	2.520254	0.000000			
9 B	3.650462	1.973780	2.214016	0.000000		
10 B	3.083565	3.172541	2.184074	1.616800	0.000000	
11 B	2.870775	3.745556	3.221043	2.852358	1.759646	
12 B	1.737384	2.198384	2.221977	3.305335	3.552445	
	11	12				
11 B	0.000000					
12 B	3.591198	0.000000				

Table S5C. Energy ranking for all of the CpCoSe₂B₉H₉ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	3-AnticubeOh-Co3Se1Se7	-6604.0433368	0.00
2	2-CubeOh-Co1Se1Se2	-6604.0433283	0.01
3	2-CubeOh-Co2Se1Se2	-6604.0433283	0.01
4	3-AnticubeOh-Co3Se3Se3	-6604.0433283	0.01
5	1-Icos-Co1Se1Se1	-6604.0433280	0.01
6	3-AnticubeOh-Co3Se1Se5_i-31	-6604.0433212	0.01
7	3-AnticubeOh-Co2Se2Se6	-6604.0433119	0.02
8	3-AnticubeOh-Co3Se1Se5_r-31	-6604.0433075	0.02
9	3-AnticubeOh-Co2Se1Se2	-6604.0432749	0.04
10	3-AnticubeOh-Co3Se1Se2	-6604.0432527	0.05
11	3-AnticubeOh-Co2Se1Se6	-6604.0432338	0.06
12	3-AnticubeOh-Co1Se2Se4_i-24	-6604.0382534	3.19
13	3-AnticubeOh-Co1Se1Se5	-6604.0382524	3.19
14	2-CubeOh-Co2Se1Se1	-6604.0382523	3.19
15	3-AnticubeOh-Co3Se2Se1	-6604.0382523	3.19
16	3-AnticubeOh-Co1Se2Se4_r-24	-6604.0382521	3.19
17	2-CubeOh-Co2Se3Se3	-6604.0382514	3.19
18	3-AnticubeOh-Co3Se1Se1	-6604.0382408	3.20
19	3-AnticubeOh-Co2Se2Se5	-6604.0359992	4.60
20	3-AnticubeOh-Co3Se3Se4	-6604.0359451	4.64
21	2-CubeOh-Co1Se2Se3	-6604.0359412	4.64
22	3-AnticubeOh-Co3Se2Se3	-6604.0358554	4.69
23	2-CubeOh-Co1Se1Se7	-6604.0339762	5.87
24	2-CubeOh-Co1Se3Se2	-6604.0339762	5.87
25	2-CubeOh-Co2Se3Se1	-6604.0339757	5.87
26	1-Icos-Co1Se1Se3	-6604.0339751	5.87
27	3-AnticubeOh-Co1Se2Se5	-6604.0339690	5.88
28	2-CubeOh-Co2Se1Se3	-6604.0339651	5.88
29	3-AnticubeOh-Co2Se3Se5	-6604.0339639	5.88
30	3-AnticubeOh-Co3Se3Se1	-6604.0339521	5.89
31	3-AnticubeOh-Co3Se1Se4	-6604.0339418	5.90
32	3-AnticubeOh-Co3Se4Se2	-6604.0264903	10.57
33	3-AnticubeOh-Co2Se1Se4	-6604.0264036	10.63
34	2-CubeOh-Co2Se4Se2	-6604.0193365	15.06
35	1-Icos-Co1Se2Se1	-6604.0193345	15.06
36	2-CubeOh-Co2Se2Se2	-6604.0193345	15.06
37	2-CubeOh-Co2Se2Se3	-6604.0193345	15.06
38	3-AnticubeOh-Co1Se2Se9	-6604.0193301	15.06
39	1-Icos-Co1Se1Se2	-6604.0189145	15.33

40	2-CubeOh-Co1Se1Se1	-6604.0189145	15.33
41	2-CubeOh-Co1Se2Se1	-6604.0189145	15.33
42	2-CubeOh-Co2Se1Se9	-6604.0135849	18.67
43	2-CubeOh-Co2Se3Se5	-6604.0135847	18.67
44	2-CubeOh-Co2Se3Se8	-6604.0092697	21.38
45	2-CubeOh-Co2Se4Se6	-6604.0092692	21.38
46	3-AnticubeOh-Co2Se1Se3	-6604.0070290	22.78
47	2-CubeOh-Co1Se1Se6	-6604.0056268	23.66
48	2-CubeOh-Co1Se3Se4	-6604.0046571	24.27
49	2-CubeOh-Co2Se2Se5	-6604.0046571	24.27
50	2-CubeOh-Co2Se4Se3	-6604.0046570	24.27
51	3-AnticubeOh-Co3Se4Se7	-6604.0046559	24.27
52	3-AnticubeOh-Co3Se4Se1	-6604.0046553	24.27
53	1-Icos-Co1Se2Se3_i-42	-6604.0046535	24.27
54	3-AnticubeOh-Co1Se3Se5	-6604.0042062	24.56
55	3-AnticubeOh-Co3Se2Se2	-6604.0042058	24.56
56	1-Icos-Co1Se2Se3_r-42	-6604.0041275	24.60
57	2-CubeOh-Co2Se5Se2	-6604.0041272	24.60
58	3-AnticubeOh-Co3Se4Se3	-6604.0041260	24.61
59	3-AnticubeOh-Co3Se2Se5	-6604.0037964	24.81
60	3-AnticubeOh-Co2Se2Se3	-6604.0037791	24.82
61	3-AnticubeOh-Co2Se4Se1	-6604.0037672	24.83
62	3-AnticubeOh-Co3Se4Se6	-6604.0037401	24.85
63	3-AnticubeOh-Co3Se3Se8_i-42	-6604.0037376	24.85
64	3-AnticubeOh-Co3Se3Se8_r-42	-6604.0037323	24.85
65	3-AnticubeOh-Co3Se3Se7_i-25	-6604.0033504	25.09
66	3-AnticubeOh-Co3Se3Se7_r-25	-6604.0033382	25.10
67	2-CubeOh-Co2Se2Se6	-6604.0025851	25.57
68	2-CubeOh-Co2Se1Se8	-6604.0025834	25.57
69	3-AnticubeOh-Co2Se3Se1	-6604.0003051	27.00
70	3-AnticubeOh-Co2Se2Se2	-6604.0002892	27.01
71	2-CubeOh-Co1Se1Se4	-6604.0002786	27.02
72	2-CubeOh-Co2Se3Se6	-6604.0002784	27.02
73	2-CubeOh-Co2Se2Se8	-6604.0002783	27.02
74	3-AnticubeOh-Co2Se1Se5	-6604.0002751	27.02
75	3-AnticubeOh-Co2Se2Se1	-6603.9995351	27.49
76	2-CubeOh-Co2Se1Se5	-6603.9994048	27.57
77	3-AnticubeOh-Co1Se2Se1	-6603.9994047	27.57
78	1-Icos-Co1Se1Se6	-6603.9969952	29.08
79	3-AnticubeOh-Co3Se3Se2	-6603.9964518	29.42
80	3-AnticubeOh-Co3Se1Se6	-6603.9964453	29.43
81	3-AnticubeOh-Co1Se4Se2	-6603.9924753	31.92
82	3-AnticubeOh-Co3Se1Se3	-6603.9901723	33.36

83	3-AnticubeOh-Co1Se1Se7	-6603.9901656	33.37
84	2-CubeOh-Co2Se1Se4	-6603.9901644	33.37
85	3-AnticubeOh-Co3Se1Se9	-6603.9895433	33.76
86	3-AnticubeOh-Co3Se3Se5	-6603.9895207	33.77
87	3-AnticubeOh-Co1Se2Se8	-6603.9876946	34.92
88	1-Icos-Co1Se1Se4	-6603.9875126	35.03
89	2-CubeOh-Co2Se4Se1	-6603.9875122	35.03
90	2-CubeOh-Co2Se3Se2	-6603.9871268	35.27
91	3-AnticubeOh-Co2Se3Se4	-6603.9870719	35.31
92	2-CubeOh-Co2Se3Se7	-6603.9859111	36.04
93	2-CubeOh-Co2Se2Se1	-6603.9857324	36.15
94	3-AnticubeOh-Co1Se2Se6	-6603.9856050	36.23
95	3-AnticubeOh-Co1Se1Se6_r-36	-6603.9856021	36.23
96	2-CubeOh-Co2Se1Se7	-6603.9856013	36.23
97	3-AnticubeOh-Co1Se1Se6_i-36	-6603.9855947	36.23
98	2-CubeOh-Co1Se1Se3	-6603.9838627	37.32
99	3-AnticubeOh-Co3Se6Se1	-6603.9826082	38.11
100	2-CubeOh-Co2Se4Se5	-6603.9824565	38.20
101	2-CubeOh-Co1Se2Se5	-6603.9824553	38.20
102	3-AnticubeOh-Co3Se4Se5	-6603.9824553	38.20
103	3-AnticubeOh-Co3Se2Se9	-6603.9824420	38.21
104	3-AnticubeOh-Co2Se2Se4	-6603.9804009	39.49
105	2-CubeOh-Co2Se2Se9	-6603.9796806	39.95
106	3-AnticubeOh-Co3Se2Se6	-6603.9793102	40.18
107	3-AnticubeOh-Co3Se1Se8	-6603.9781870	40.88
108	2-CubeOh-Co1Se3Se1	-6603.9769013	41.69
109	3-AnticubeOh-Co1Se3Se2	-6603.9768903	41.70
110	2-CubeOh-Co2Se4Se7	-6603.9756118	42.50
111	3-AnticubeOh-Co1Se2Se7	-6603.9748807	42.96
112	3-AnticubeOh-Co1Se3Se1	-6603.9748804	42.96
113	1-Icos-Co1Se2Se2	-6603.9748802	42.96
114	2-CubeOh-Co2Se2Se4	-6603.9748790	42.96
115	3-AnticubeOh-Co2Se2Se8	-6603.9748207	43.00
116	2-CubeOh-Co2Se4Se4	-6603.9737714	43.65
117	2-CubeOh-Co2Se1Se10	-6603.9737702	43.65
118	2-CubeOh-Co2Se3Se4	-6603.9723633	44.54
119	2-CubeOh-Co2Se2Se7	-6603.9722612	44.60
120	2-CubeOh-Co1Se1Se5	-6603.9700658	45.98
121	1-Icos-Co1Se1Se5	-6603.9700649	45.98
122	2-CubeOh-Co1Se2Se4	-6603.9700649	45.98
123	3-AnticubeOh-Co1Se2Se2	-6603.9667637	48.05
124	3-AnticubeOh-Co2Se2Se7	-6603.9608607	51.76
125	3-AnticubeOh-Co3Se2Se4	-6603.9607882	51.80

126	2-CubeOh-Co2Se5Se1	-6603.9597828	52.43
127	3-AnticubeOh-Co1Se1Se1	-6603.9541910	55.94
128	3-AnticubeOh-Co1Se1Se3	-6603.9519635	57.34
129	3-AnticubeOh-Co3Se2Se7	-6603.9515720	57.58
130	2-CubeOh-Co2Se6Se1	-6603.9510483	57.91
131	3-AnticubeOh-Co2Se3Se3	-6603.9495772	58.84
132	3-AnticubeOh-Co2Se4Se2	-6603.9494566	58.91
133	3-AnticubeOh-Co2Se3Se2_i-24	-6603.9492072	59.07
134	3-AnticubeOh-Co2Se3Se2_r-24	-6603.9491919	59.08
135	3-AnticubeOh-Co2Se1Se1_r-10	-6603.9491652	59.09
136	3-AnticubeOh-Co2Se1Se1_i-10	-6603.9491469	59.11
137	3-AnticubeOh-Co3Se3Se6	-6603.9473997	60.20
138	3-AnticubeOh-Co1Se2Se3	-6603.9473996	60.20
139	3-AnticubeOh-Co3Se2Se8	-6603.9473462	60.24
140	2-CubeOh-Co1Se3Se3	-6603.9303708	70.89
141	3-AnticubeOh-Co3Se4Se4	-6603.9291181	71.67
142	3-AnticubeOh-Co3Se1Se10	-6603.9290682	71.71
143	3-AnticubeOh-Co3Se5Se2	-6603.9288770	71.83
144	3-AnticubeOh-Co1Se3Se4	-6603.9265698	73.27
145	3-AnticubeOh-Co1Se4Se1	-6603.9264851	73.33
146	3-AnticubeOh-Co2Se4Se4	-6603.9264452	73.35
147	3-AnticubeOh-Co1Se1Se4	-6603.9252284	74.12
148	3-AnticubeOh-Co3Se5Se1	-6603.9241087	74.82
149	3-AnticubeOh-Co2Se2Se9	-6603.9191689	77.92
150	2-CubeOh-Co2Se1Se6	-6603.9125747	82.06
151	3-AnticubeOh-Co2Se4Se3_r-11	-6603.9062104	86.05
152	3-AnticubeOh-Co2Se4Se3_i-11	-6603.9062076	86.05
153	3-AnticubeOh-Co1Se1Se2	-6603.9047812	86.95
154	3-AnticubeOh-Co1Se3Se3	-6603.9047645	86.96
155	2-CubeOh-Co1Se2Se2	-6603.9007182	89.50

Table S6. Orbital energies and HOMO/LUMO gaps:

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO Gap (eV)
CoSe2B5-1	-0.207703	-0.123366	2.294928
CoSe2B5-2	-0.202609	-0.115067	2.382140
CoSe2B5-3	-0.190934	-0.118471	1.971820
CoSe2B5-4	-0.197226	-0.141080	1.527811
CoSe2B5-5	-0.198927	-0.135388	1.728985
CoSe2B5-6	-0.213043	-0.106927	2.887565
CoSe2B5-7	-0.190944	-0.115449	2.054325
CoSe2B5-8	-0.182151	-0.098794	2.268261
CoSe2B5-9	-0.202180	-0.108189	2.557627
CoSe2B5-10	-0.183508	-0.109032	2.026596
CoSe2B6-1	-0.199706	-0.114847	2.309132
CoSe2B6-2	-0.194602	-0.109244	2.322711
CoSe2B6-3	-0.202580	-0.118173	2.296833
CoSe2B6-4	-0.200471	-0.132398	1.852362
CoSe2B6-5	-0.190255	-0.075874	3.112467
CoSe2B6-6	-0.202695	-0.129903	1.980772
CoSe2B6-7	-0.180960	-0.107646	1.994977
CoSe2B6-8	-0.194234	-0.124046	1.909914
CoSe2B6-9	-0.192161	-0.123966	1.855681
CoSe2B6-10	-0.191537	-0.118976	1.974486
CoSe2B6-11	-0.185259	-0.120009	1.775544
CoSe2B6-12	-0.190777	-0.112938	2.118108
CoSe2B6-13	-0.186662	-0.108521	2.126326
CoSe2B7-1	-0.215829	-0.125439	2.459638
CoSe2B7-2	-0.209763	-0.151553	1.583976
CoSe2B7-3	-0.186634	-0.122791	1.737257
CoSe2B7-4	-0.199457	-0.124463	2.040692
CoSe2B7-5	-0.207802	-0.142188	1.785449
CoSe2B7-6	-0.201751	-0.123288	2.135088
CoSe2B7-7	-0.194659	-0.116894	2.116095
CoSe2B7-8	-0.192861	-0.121290	1.947547
CoSe2B7-9	-0.186950	-0.119201	1.843545
CoSe2B7-10	-0.179862	-0.143056	1.001543
CoSe2B8-1	-0.211559	-0.130002	2.219280
CoSe2B8-2	-0.197889	-0.109928	2.393542
CoSe2B8-3	-0.200179	-0.120124	2.178409
CoSe2B8-4	-0.202527	-0.125717	2.090108
CoSe2B8-5	-0.209418	-0.102703	2.903865

CoSe2B8-6	-0.193355	-0.113083	2.184314
CoSe2B8-7	-0.214349	-0.123077	2.483639
CoSe2B8-8	-0.210269	-0.118291	2.502850
CoSe2B9-1	-0.203283	-0.123955	2.158626
CoSe2B9-2	-0.186029	-0.144097	1.141028
CoSe2B9-3	-0.198906	-0.122144	2.088801
CoSe2B9-4	-0.202275	-0.110322	2.502170
CoSe2B9-5	-0.206947	-0.136695	1.911655
CoSe2B9-6	-0.200818	-0.132675	1.854266
CoSe2B9-7	-0.167636	-0.123400	1.203723
CoSe2B9-8	-0.200326	-0.144544	1.517906
CoSe2B9-9	-0.202835	-0.135969	1.819517

Cartesian coordinates of all optimized structures (M06-L/6-311G(d,p)).

CoSe2B5-1

B	1.71149700	-0.75865200	1.40605600
H	2.41590800	-1.20347100	2.24610900
B	0.23361600	0.64529700	1.62830100
B	0.72509300	-1.45847000	-0.00889200
H	0.63360300	-2.54247700	-0.47769200
Se	2.55720400	-0.54591300	-0.37212000
B	0.08947300	-1.03916300	1.52476400
H	-0.36215100	-1.66608000	2.42114000
H	-0.11808100	1.20302600	2.61442500
B	0.75139200	0.11622100	-1.06587400
H	0.64943300	0.14324100	-2.24574400
Se	0.25329100	1.76213900	0.00502700
Co	-0.99549100	-0.20337100	0.05683500
H	-2.43470300	0.86386900	-2.11205700
C	-2.51936100	0.18605100	-1.27442500
C	-2.90771800	0.53987300	0.05581200
H	-1.79717300	-1.74797400	-2.11623500
H	-3.16456500	1.53405600	0.39443500
C	-2.83169500	-0.61796900	0.86553800
H	-3.01464500	-0.66622300	1.92929800
C	-2.36628700	-1.68816000	0.04763900
H	-2.15382200	-2.69509200	0.37789700
C	-2.18956000	-1.18807700	-1.27901900

CoSe2B5-2

Se	0.73180100	1.69953500	-0.60790300
B	2.32806000	-1.06586900	0.33006600
Co	-0.71816300	0.00001700	0.10211500
B	2.32809000	1.06578900	0.33005800
Se	0.73175100	-1.69953600	-0.60791600
H	3.25518500	1.79508900	0.24598400
H	3.25512800	-1.79520200	0.24599200
B	0.74494200	0.92931000	1.33285900
H	0.31511600	1.64170000	2.17521000
B	2.17378300	-0.00003700	1.58825100
H	2.91930600	-0.00004600	2.50368300
B	0.74492000	-0.92935200	1.33285800
H	0.31502300	-1.64168500	2.17522000
H	-2.23534900	2.17475300	0.89326700
C	-2.31495200	1.14761800	0.56562800
C	-2.26875400	0.00040500	1.40261500
H	-2.45450700	1.34193800	-1.66342300
H	-2.13543600	0.00076900	2.47493800
C	-2.31491000	-1.14735400	0.56637700
H	-2.23525200	-2.17427800	0.89466300
C	-2.42685300	-0.70587500	-0.78980300

H	-2.45443900	-1.34309800	-1.66255200
C	-2.42688800	0.70527900	-0.79026600

CoSe2B5-3

B	-2.20136800	0.14160800	-0.38919200
B	-0.58398600	0.21316800	1.81586200
B	-1.93871900	-0.70503300	1.23114900
Co	0.76148800	-0.04061000	0.09945700
Se	-0.83340600	1.65018600	-0.40533300
B	-1.95275600	1.00679400	1.13988800
Se	-0.96799000	-1.53493500	-0.59533600
B	-0.26657100	-1.33596000	1.29758100
H	0.21657700	-2.27745900	1.81853200
H	-2.82667400	1.66225100	1.58576200
H	-3.17549800	0.16238300	-1.05002500
H	-0.13941600	0.48038200	2.88182200
H	-2.82261000	-1.31488200	1.72369300
H	2.49605500	-2.22630100	0.12693500
C	2.46542300	-1.14816000	0.05271500
C	2.48996800	-0.23859300	1.14504100
H	2.34891300	-0.79654500	-2.16013600
H	2.50307200	-0.50466100	2.19209300
C	2.36192900	1.07371100	0.61812400
H	2.30212100	1.98758000	1.19222100
C	2.33250000	0.97048600	-0.81422900
H	2.22964000	1.79719100	-1.50396900
C	2.39553700	-0.38993000	-1.15930800

CoSe2B5-4

B	-1.69424900	-0.62031900	1.40277000
B	-0.73177900	-1.55984400	0.09039500
Co	1.03277000	-0.20068200	0.11413800
B	-0.39248500	0.67252300	1.54956600
B	-1.90519700	0.95972400	0.48547900
B	-0.02375500	-1.02571000	1.52865000
Se	-0.18355200	1.74346900	-0.17457700
Se	-2.41533000	-0.71853800	-0.54097200
H	-2.77124300	1.70920900	0.76937000
H	-0.21946300	1.28204100	2.54981500
H	-0.67631900	-2.72259500	-0.14321200
H	-2.45893900	-0.93624200	2.24432500
H	0.45863700	-1.69913400	2.37286300
H	3.23329300	1.56520700	0.24343800
C	2.93904700	0.56271000	-0.03408900
C	2.48102400	0.15184500	-1.31760200
H	3.14711400	-0.57873600	1.87832800
H	2.34751800	0.79309600	-2.17795500
C	2.13625000	-1.22011100	-1.25116300
H	1.71308400	-1.81356600	-2.04922600

C	2.40756400	-1.67281500	0.08040400
H	2.22186300	-2.66662000	0.46172700
C	2.90595000	-0.57058500	0.82464700

CoSe2B5-5

B	1.97395000	-0.85576400	1.04340400
H	2.86686200	-1.52043800	1.45154800
B	0.68223000	0.00003900	1.89071900
Se	0.95902100	-1.61709900	-0.62750600
B	1.97412000	0.85551700	1.04334500
B	0.35464100	-1.56192700	1.22657700
H	-0.21115500	-2.41403900	1.81428200
H	2.86718600	1.52003400	1.45140400
H	0.44039700	0.00006100	3.05737900
Se	0.95927500	1.61697600	-0.62753700
B	0.35493500	1.56204300	1.22655000
H	-0.21030500	2.41447800	1.81429600
Co	-0.65154300	0.00006600	0.14185700
H	-2.06554000	1.34518900	-1.92109800
C	-2.19647100	0.70735000	-1.05792400
C	-2.32942900	1.15023200	0.29173600
H	-2.06478700	-1.33840500	-1.92590000
H	-2.33243700	2.17703700	0.62536000
C	-2.41765900	-0.00211300	1.12264900
H	-2.47926200	-0.00411900	2.20166300
C	-2.32873800	-1.15137500	0.28762300
H	-2.33092300	-2.17932700	0.61771700
C	-2.19600300	-0.70369700	-1.06046800

CoSe2B5-6

Se	1.80606800	1.66098600	-0.14717700
B	0.00571600	1.20573500	-0.81822900
H	-0.38838600	2.00754100	-1.59973600
B	1.80284600	0.00032700	1.04781600
H	2.54172800	0.00063800	1.96626600
B	0.21921000	-0.87733800	1.03143400
H	-0.04106200	-1.55348700	1.96764500
Se	1.80725000	-1.66026700	-0.14722800
B	0.21855100	0.87681600	1.03127500
H	-0.04241300	1.55277600	1.96743300
Co	-1.24946400	-0.00076400	-0.02990600
B	0.00611600	-1.20714500	-0.81757200
H	-0.38821400	-2.01050800	-1.59738800
H	-2.77847300	-0.00566200	2.30819100
C	-2.86934300	-0.00278900	1.23144200
C	-2.90794300	-1.14963300	0.39080500
H	-2.84716200	2.17449800	0.73065000
H	-2.85048000	-2.17761700	0.71986000
C	-2.96453900	-0.70614900	-0.95785000

H	-2.95802800	-1.33958900	-1.83297400
C	-2.96350400	0.71140800	-0.95430100
H	-2.95600800	1.34912900	-1.82630700
C	-2.90650100	1.14824200	0.39656400

CoSe2B5-7

B	-0.21584000	0.57213700	-1.54339500
Se	-0.04849000	1.88527000	-0.09025000
Co	0.97898100	-0.23727400	0.00921400
B	-0.75292900	-1.03329600	0.80581400
B	-0.28264300	0.54260300	1.43115900
B	-0.72706600	-0.91734800	-1.02704500
Se	-2.61952100	-0.71880500	-0.16834500
B	-1.95868900	0.22265900	1.35475900
H	0.13448400	0.96812600	-2.60628600
H	0.17281400	0.85430300	2.47955200
H	-0.66340100	-1.92634500	-1.65396000
H	-0.68688000	-2.04644300	1.41657800
H	-2.66907200	0.57970000	2.22578500
H	1.60409000	-2.91276900	-0.11341900
C	2.06011100	-1.93571700	-0.03842800
C	2.33071600	-1.23006200	1.17204600
H	2.31243200	-1.34015500	-2.18174800
H	2.11274300	-1.58207800	2.17029100
C	2.83857000	0.04527000	0.82529700
H	3.07789900	0.84372100	1.51377000
C	2.90056200	0.12191400	-0.59855800
H	3.18868200	0.99286400	-1.17061300
C	2.43369600	-1.10442400	-1.13418500

CoSe2B5-8

Se	0.31558000	1.67816500	-0.12470700
Se	2.44241500	-0.74779000	-0.40825900
Co	-1.09065400	-0.18181000	0.03121600
B	1.90395700	0.84325900	0.91644000
B	0.51231900	-0.15575600	-1.09905800
H	0.48750600	-0.22944600	-2.28039600
H	2.72189600	1.61331400	1.27423400
B	0.25681000	0.03765400	1.50463200
H	-0.14990500	0.29148100	2.58795700
B	1.74539500	-0.74326700	1.50411900
H	2.37674100	-1.23762700	2.36396100
B	0.47038600	-1.35966300	0.44825100
H	0.30743700	-2.53058600	0.38132600
H	-3.05304700	0.30827900	2.02015800
C	-2.90790400	-0.08539000	1.02457600
C	-2.55581000	-1.41612000	0.68837900
H	-3.14775300	1.72247000	-0.25713600
H	-2.39393900	-2.22996500	1.38091500

C	-2.41201600	-1.49053600	-0.73738800
H	-2.12130400	-2.37003900	-1.29448100
C	-2.68692400	-0.20707800	-1.28003600
H	-2.65086300	0.06956500	-2.32363400
C	-2.96156100	0.65871500	-0.18667200

CoSe2B5-9

B	1.60595000	1.75455300	0.57682600
H	2.22249200	2.75319000	0.70843100
B	0.55444900	-1.18596200	-0.82683900
H	0.39926500	-2.00027700	-1.67444900
B	0.30256000	0.68424800	1.36083400
H	-0.15881200	1.07130000	2.38109200
Co	-0.92519000	-0.29118000	0.03110800
B	1.99369000	0.27573600	1.29010800
H	2.74545100	0.17295000	2.19538700
B	0.73735900	-0.97859100	0.99622900
H	0.69476800	-1.91201200	1.72373500
Se	2.42363200	-0.92300300	-0.31344800
Se	-0.04611300	1.85451400	-0.40343400
H	-1.75438800	-2.92065900	-0.00129400
C	-2.12541000	-1.90548800	0.01141700
C	-2.41866500	-1.10623100	-1.13051700
H	-2.21451700	-1.44499400	2.20279700
H	-2.31381500	-1.40420300	-2.16341000
C	-2.82055900	0.16712100	-0.65836200
H	-3.05698000	1.02319100	-1.27610300
C	-2.81373200	0.15484500	0.76753000
H	-3.03331400	0.99542600	1.41026800
C	-2.38091600	-1.12580200	1.18357300

CoSe2B6-1

Se	-0.75446000	1.57285200	-0.58885800
Co	0.85794400	-0.00005900	0.09081000
B	-0.51422900	0.91524300	1.42273200
H	0.00239000	1.75032100	2.08416700
B	-2.31638500	-0.87916300	0.70907300
H	-3.19529700	-1.66630400	0.68571900
Se	-0.75473700	-1.57270000	-0.58893000
B	-1.79264800	-0.00002600	2.04008000
H	-2.18721800	-0.00008000	3.14937700
B	-2.31672000	0.87916700	0.70921700
H	-3.19603000	1.66588500	0.68609900
B	-2.05869900	0.00015000	-0.84798400
H	-2.80072100	0.00021700	-1.76061300
B	-0.51429600	-0.91524700	1.42270800
H	0.00231100	-1.75056500	2.08385900
H	2.40127400	-0.00225300	2.39215700
C	2.47148100	-0.00121600	1.31396200

C	2.47052300	1.14591400	0.47541800
H	2.41495700	-2.17501100	0.80288800
H	2.41516200	2.17352700	0.80690100
C	2.52741000	0.70464100	-0.88838900
H	2.52650700	1.34323700	-1.76074100
C	2.52737300	-0.70306700	-0.88973400
H	2.52652800	-1.34004200	-1.76326000
C	2.47041600	-1.14679500	0.47327900

CoSe2B6-2

H	0.11029100	-0.18351900	2.95330400
B	-0.19381500	0.03388700	1.82579800
B	-1.88923800	-0.23844800	1.37690800
H	-2.72406500	-0.43808500	2.18579900
Se	-0.34399000	1.64560000	-0.63534700
B	-2.16309400	0.77530200	-0.12593200
H	-3.12744700	1.37057700	-0.44945800
Se	-2.13332600	-1.20465900	-0.41816200
B	-1.24848900	1.39986000	1.30356800
H	-1.75218800	2.33406800	1.81886400
B	0.53837000	1.45654300	1.21638900
H	1.15254900	2.34170000	1.69607300
B	-0.47634900	-1.29176900	0.74296300
H	-0.29559500	-2.39872600	1.12978300
Co	1.08522000	-0.10511600	0.17347600
H	3.53807100	0.44383300	1.41155500
C	3.08797700	-0.11789000	0.60576100
C	2.87990800	0.33475900	-0.71761200
H	2.45353400	-2.01442500	1.61079100
H	3.15447200	1.30367500	-1.11209200
C	2.21109800	-0.70700600	-1.44483900
H	1.89153600	-0.65074900	-2.47666300
C	2.00465900	-1.79473200	-0.57430100
H	1.51587100	-2.72748700	-0.81413200
C	2.51199800	-1.41706500	0.71151600

CoSe2B6-3

B	-0.60209000	-1.38649800	-0.51798600
B	-0.28446400	0.53909800	1.56801800
B	-0.58190600	0.36785700	-1.16008300
Se	-2.48233600	-0.30044700	-0.47532900
B	-1.83558400	-0.32410000	1.53624400
B	-1.82445700	-1.81871200	0.70661300
B	-0.34867300	-1.20971500	1.24638500
Co	1.02770000	-0.21646700	-0.00108900
Se	-0.04312900	1.84114000	0.07468000
H	0.22994200	0.88066000	2.58308300
H	-0.45879700	-2.17160500	-1.39411700
H	-2.37864500	-2.85393000	0.76406800

H	-2.60973000	-0.05019600	2.38702500
H	-0.53868400	0.54067000	-2.33145400
H	0.18281700	-1.92077700	2.03567300
H	2.69758500	-1.18567700	2.01317900
C	2.69056300	-0.92759500	0.96431600
C	2.94819400	0.34922000	0.41713700
H	1.98634500	-2.81616500	-0.00900300
H	3.19783100	1.23913400	0.97747600
C	2.75047500	0.27886700	-1.00112900
H	2.83129100	1.10559500	-1.69266700
C	2.36127300	-1.03949100	-1.32172400
H	2.07729400	-1.40208700	-2.29952600
C	2.29725000	-1.78504400	-0.10497200

CoSe2B6-4

Co	-1.06367500	-0.16776200	0.09226200
Se	0.33005400	1.64946000	-0.60204000
Se	2.46332100	-0.91091700	-0.31338000
B	0.66277600	-1.24533600	0.64910200
B	-0.56782900	1.42795700	1.26566500
B	0.18390200	-0.01632100	1.79715300
B	1.90519300	-0.11043500	1.45103300
B	1.14060600	1.42784900	1.37816200
B	0.68420400	-0.35539800	-1.02446100
H	2.59738400	-0.46281000	2.34601400
H	-1.40337300	2.17179200	1.63989100
H	0.44239300	-0.70993000	-2.12917100
H	-0.17947200	-0.31806500	2.88946200
H	1.58449100	2.40133800	1.88590000
H	0.45495900	-2.39382700	0.84520400
H	-2.10476800	-2.35927800	1.39266600
C	-2.35265300	-1.62031000	0.64374800
C	-2.09903800	-1.73103000	-0.75518200
H	-3.20190100	0.05575100	1.85948700
H	-1.61454100	-2.56329500	-1.24483000
C	-2.48254000	-0.51390100	-1.36081400
H	-2.34944200	-0.25373400	-2.40201500
C	-2.99843600	0.34695200	-0.34376600
H	-3.32129900	1.36967600	-0.48282500
C	-2.93470100	-0.34172600	0.89103800

CoSe2B6-5

B	-0.03332200	0.87569900	0.98397800
B	-0.03339800	0.87557800	-0.98501700
Se	-1.84730500	1.56194900	0.00011200
Co	1.41701700	-0.00143400	-0.00061400
B	-0.03336700	-0.87900200	-0.98549800
B	-0.03319600	-0.87889600	0.98462300
Se	-1.84639300	-1.56369400	0.00003400

B	-1.56631100	-0.00083400	1.33652900
B	-1.56667200	-0.00078100	-1.33660100
H	0.17504900	1.68501100	-1.82615300
H	0.17675500	1.68455700	1.82526800
H	0.16989700	-1.68313300	1.83212700
H	0.16814900	-1.68375700	-1.83290100
H	-2.16128300	-0.00140800	-2.35166600
H	-2.16020500	-0.00157600	2.35201500
H	3.05776400	-1.82611200	-1.37462400
C	3.08467000	-0.96152900	-0.72671600
C	3.08291100	-0.98540400	0.69547000
H	3.03353400	0.74619000	-2.16721200
H	3.05467200	-1.87099500	1.31423500
C	3.06577200	0.35750500	1.15917800
H	3.02886200	0.67333600	2.19197900
C	3.04998600	1.21398100	0.02074500
H	3.00243500	2.29364300	0.03902200
C	3.06865600	0.39603000	-1.14543300

CoSe2B6-6

H	-2.89224700	0.55932700	2.29242200
B	-2.19148700	0.26163800	1.38533500
B	-1.97733600	1.47904400	0.12607000
H	-2.62241500	2.46385600	0.26272700
Co	0.81096900	-0.12711300	0.09820600
Se	-1.05898400	-1.36687400	-0.70767400
B	-2.65560200	-0.07145800	-0.29194400
H	-3.60548900	-0.05199900	-0.99610500
Se	-0.12670000	1.92681400	-0.42596800
B	-0.54570100	0.97896200	1.32787600
H	-0.13994500	1.51538800	2.30266700
B	-2.39094300	-1.31460000	0.84432500
H	-2.95414800	-2.26534700	1.24393600
B	-0.75319500	-0.81129400	1.35771800
H	-0.27443000	-1.50905500	2.18517600
H	2.22970300	-0.61562800	2.42453700
C	2.34315700	-0.59057700	1.35026400
C	2.65118300	0.55565600	0.57147100
H	1.76099500	-2.65789100	0.74144300
H	2.84417000	1.54870100	0.95228100
C	2.61740900	0.17628300	-0.80962800
H	2.78426000	0.83294700	-1.65205500
C	2.26506800	-1.18937200	-0.87728600
H	2.11225500	-1.76412900	-1.78048200
C	2.08079900	-1.66425100	0.45998300

CoSe2B6-7

B	0.54670800	-0.03437700	-1.20240200
Se	0.37485700	1.65027300	-0.03480300

B	1.49515200	-0.97363000	1.42026400
Se	2.42660800	-0.61263700	-0.50301900
Co	-1.09028500	-0.21353000	0.04310800
B	0.52321000	-1.55016700	-0.14857200
B	-0.13665400	-1.35750000	1.40606900
B	0.29874600	0.23081100	1.74433700
B	1.87373000	0.72518700	1.01361700
H	-0.68101500	-2.19811700	2.03346600
H	2.28731500	-1.51165200	2.11194200
H	0.41715500	-0.01154100	-2.37655000
H	2.70852800	1.36356200	1.54468600
H	0.53235300	-2.57443100	-0.74556100
H	0.06538800	0.90579100	2.68766500
H	-2.49539200	-2.57864300	-0.09470500
C	-2.61022000	-1.50761900	-0.17919600
C	-2.46107500	-0.73981700	-1.37409600
H	-3.02469600	-0.88103400	1.92986000
H	-2.19746600	-1.13017300	-2.34679700
C	-2.62807700	0.62403900	-1.03969800
H	-2.52522700	1.46305700	-1.71439400
C	-2.88448600	0.70403200	0.36596500
H	-3.00075500	1.61493700	0.93715900
C	-2.89993200	-0.61025300	0.89180800

CoSe2B7-1

B	-0.12293500	0.36440200	1.43778800
B	-0.12275000	0.36416000	-1.43763900
Se	-3.00800300	-0.14201600	-0.00009500
B	-0.22925100	-1.30475700	0.90287200
B	-1.68347400	-1.74361800	0.00011200
B	-0.22912900	-1.30492800	-0.90247000
Se	0.00434300	1.73345100	-0.00002800
B	-1.70610900	-0.59430400	-1.43343200
B	-1.70634600	-0.59411600	1.43351100
Co	1.29196200	-0.20315100	0.00020700
H	-2.20469900	-0.78840100	-2.48596700
H	-2.20511400	-0.78807100	2.48598900
H	0.22944200	0.72397100	2.51106700
H	0.22987500	0.72351400	-2.51090900
H	-2.15261200	-2.82415300	0.00016000
H	0.20988000	-2.12889600	-1.63701800
H	0.20969300	-2.12851700	1.63769900
H	2.41495800	-2.72542700	0.00093300
C	2.68197100	-1.67821500	0.00040500
C	2.85882800	-0.86145800	1.15607900
H	2.73608500	-1.18241700	-2.18090800
H	2.73777900	-1.18061600	2.18127400
C	3.10270000	0.45828300	0.71449300
H	3.20730200	1.32946000	1.34619500
C	3.10222300	0.45768700	-0.71578600

H	3.20632300	1.32834900	-1.34827500
C	2.85803400	-0.86241600	-1.15608400

CoSe2B7-2

Se	-0.18649800	1.72970400	-0.64638300
B	-0.12546200	1.18555900	1.38038600
B	2.58922700	0.59030200	0.41429300
B	0.59791200	-1.50842100	0.28997500
B	1.96910700	-0.87919900	1.32842300
B	0.26886700	-0.51680900	1.66361700
B	1.35248400	1.94065100	0.54601900
B	1.53940500	0.75898900	1.79285600
Se	2.22984200	-0.98858300	-0.73822700
Co	-1.08315800	-0.22496800	0.11326100
H	1.74761300	3.04865300	0.64675200
H	1.99825400	1.17174300	2.80263100
H	3.70036600	0.98508900	0.34326400
H	-0.80817600	1.81319400	2.11358300
H	2.64345700	-1.57843200	1.99442200
H	-0.18297500	-1.00053900	2.64978400
H	0.35579000	-2.66393700	0.19565300
H	-1.99248500	-2.58347900	1.22043200
C	-2.30647700	-1.76364500	0.59079100
C	-2.14463100	-1.69085800	-0.82719400
H	-3.05302300	-0.26512300	2.06645600
H	-1.70871700	-2.45521400	-1.45420400
C	-2.60827800	-0.42112600	-1.24950400
H	-2.57910700	-0.03901000	-2.26057000
C	-3.05248900	0.29493700	-0.09962500
H	-3.41622900	1.31282300	-0.08824500
C	-2.86994000	-0.54016100	1.03734600

CoSe2B8-1

B	0.37681300	0.89440500	1.41743400
Se	0.46437300	1.69880000	-0.54399700
B	1.82574000	0.00011300	1.79566100
Se	0.46473400	-1.69882500	-0.54396700
B	2.28774200	0.86650900	-0.92700100
B	2.05933000	-1.43587900	0.80313500
B	2.28791600	-0.86606400	-0.92703400
Co	-1.00254400	-0.00013900	0.09697000
B	0.37700200	-0.89444600	1.41740800
B	2.05898400	1.43621000	0.80320600
H	2.48986700	2.45248700	1.21450100
H	-0.15866400	1.57516500	2.22180600
H	2.49047200	-2.45207700	1.21435400
H	2.91519300	-1.55625900	-1.65385800
H	2.91485900	1.55690300	-1.65377400
H	2.19977800	0.00014200	2.91541700

B	2.96709300	0.00027100	0.42883600
H	-0.15834700	-1.57546700	2.22165200
H	4.13995500	0.00040100	0.56861300
H	-2.57979600	2.17098400	0.80762700
C	-2.63488400	1.14392900	0.47387600
C	-2.64919000	-0.00241100	1.30862000
H	-2.65097700	1.34594600	-1.76224800
H	-2.57643800	-0.00459300	2.38663400
C	-2.63488200	-1.14549000	0.46934500
H	-2.57985000	-2.17383700	0.79912200
C	-2.66711400	-0.70246000	-0.89383600
H	-2.65126000	-1.33886700	-1.76758600
C	-2.66706900	0.70611000	-0.89098800

CoSe2B8-2

Se	-0.06227500	1.64497000	-0.51177600
B	-1.54123600	1.59865500	1.00139100
Se	-2.08361100	-1.01505500	-0.79063700
B	-0.01086600	-0.83256100	1.62558500
B	0.15178500	0.93021500	1.48959200
B	-1.65618200	-1.30065900	1.27305200
B	-1.36611000	0.24005100	2.07186400
Co	1.21146700	-0.20145600	0.10557000
B	-0.28239200	-1.56577500	0.08367400
B	-1.99573900	1.02277500	-0.64947600
H	-2.70683500	1.62332200	-1.37221500
H	-1.91308800	2.66937400	1.32112500
H	-2.26672500	-2.19413600	1.73928600
H	0.52127100	-1.43313000	2.49998700
H	-1.69825600	0.37000300	3.19725100
H	0.78425600	1.65587900	2.17689600
B	-2.61638700	0.23591700	0.85682800
H	-0.07513700	-2.69339400	-0.22512000
H	-3.77443400	0.29512400	1.06003100
H	2.60314600	0.57438200	-2.22001300
C	2.71218400	0.05111600	-1.27894200
C	2.46226300	-1.32435800	-1.06688800
H	3.33567300	1.69079600	0.12157700
H	2.13952000	-2.04212200	-1.80634800
C	2.66047300	-1.57594100	0.32442100
H	2.49603300	-2.51914200	0.82571100
C	3.07998600	-0.36157600	0.94875400
H	3.26356000	-0.22968200	2.00577100
C	3.10628900	0.64606500	-0.03648400

CoSe2B8-3

B	-0.06871000	1.45164200	0.96013900
Se	-0.12182600	-1.63567800	-0.17548500
B	-1.64210100	-0.99993200	1.02757200

B	-1.54075500	0.71784100	1.53576200
B	-0.03693600	1.51510400	-0.81616900
B	-0.07589800	-0.11361600	-1.54564200
B	-1.50700100	0.87798100	-1.48866800
B	-1.51252800	1.86277300	0.03199800
Se	-2.83884500	0.19963800	-0.10317800
B	-0.08719200	-0.21210300	1.52068800
Co	1.33266800	0.20282000	0.01020400
H	-2.18762000	-1.81891700	1.67712800
H	-2.11741300	1.02014300	2.51783600
H	-2.06777900	1.31562300	-2.43393600
H	-2.07453900	2.89370100	0.13041900
H	0.47006000	-0.43076900	-2.55176800
H	0.45302600	2.39386100	-1.44695200
H	0.38703000	2.31626200	1.63140700
H	0.37484400	-0.65549500	2.51517200
H	2.71316500	2.57558500	0.16306300
C	2.86575400	1.50757600	0.09913800
C	2.94887900	0.74755800	-1.10374500
H	2.86819700	0.87983300	2.24751800
H	2.85717800	1.13811100	-2.10670500
C	3.04622100	-0.61699100	-0.74090000
H	3.05892600	-1.45533000	-1.42406800
C	3.05638600	-0.69919900	0.68796500
H	3.06186600	-1.61213200	1.26742200
C	2.95599700	0.60943700	1.20489600

CoSe2B8-4

Co	1.19551800	-0.21260400	0.08037000
B	-0.38835800	-0.28526800	-1.24889500
B	-0.06159300	-0.69718100	1.65492500
B	-1.49368900	1.73249500	0.90493700
Se	-2.26868100	-0.89244800	-0.68254300
B	-1.36441900	0.43724900	2.06596600
B	-2.61905100	0.45605900	0.83503900
Se	-0.13550600	1.62294800	-0.63190000
B	0.11944500	1.06739100	1.46016000
B	-0.39003300	-1.51734100	0.15273500
H	-0.19120300	-2.65507000	-0.10703400
H	-0.11984500	-0.57104900	-2.36726900
H	-1.67655900	0.65783500	3.18477600
H	-1.70541200	2.85987300	1.19531100
H	-3.77550600	0.48444400	1.08385400
H	0.46607600	-1.30872000	2.52331500
B	-1.75573000	-1.11090600	1.34502300
H	0.88585600	1.74379900	2.05510500
H	-2.31418500	-2.00847000	1.86534700
H	2.40292300	-2.52277800	0.98272400
C	2.61610800	-1.59106400	0.47820100
C	2.95564900	-0.35759000	1.10963100

H	2.25354700	-2.09411400	-1.66996700
H	3.02366400	-0.18982200	2.17485500
C	3.06484800	0.62713300	0.10128500
H	3.23549100	1.68256600	0.26314300
C	2.81186900	0.00500100	-1.16088100
H	2.77641700	0.50552400	-2.11896900
C	2.54639600	-1.36567900	-0.92716600

CoSe2B8-5

Se	-1.79520200	-1.65543900	-0.17920900
Co	1.39637900	-0.00046100	-0.00312300
B	-0.02341900	0.87836300	-1.11415600
B	-1.58301900	0.00023100	-1.35265300
B	-1.31373200	-0.85784400	1.65730100
B	0.21199700	-0.00058300	1.67862600
B	0.13803700	1.45361300	0.71075200
B	-1.31311700	0.85805900	1.65741200
Se	-1.79422900	1.65597100	-0.17912100
B	-0.02379300	-0.87853100	-1.11436800
B	0.13713100	-1.45432500	0.71006900
H	0.28021600	1.55800000	-2.03539100
H	-2.15514300	0.00051900	-2.38427300
H	0.59313100	2.52662100	0.91915800
H	-1.68461400	1.58333900	2.51623000
H	0.76819400	-0.00077400	2.72894200
H	-1.68561100	-1.58296800	2.51607900
H	0.59179200	-2.52741200	0.91903100
H	0.27914100	-1.55865900	-2.03548000
H	2.91735000	2.16990300	-0.86095800
C	3.00948600	1.14599700	-0.52710800
C	2.94311000	-0.01050500	-1.35107000
H	3.13452600	1.36091600	1.69345400
H	2.80304600	-0.02024400	-2.42262700
C	3.01217300	-1.15236900	-0.50699100
H	2.92257300	-2.18213600	-0.82306500
C	3.12571900	-0.70213600	0.83664600
H	3.13788800	-1.32876500	1.71665500
C	3.12376100	0.71919600	0.82433800

CoSe2B9-1

B	-1.54511500	1.15038900	0.98366600
B	-0.53480400	-0.96608300	-1.15369100
Se	-2.33849600	-0.03981300	-1.00003300
B	-1.84167200	-1.83887700	-0.16196400
B	-0.12015200	-1.92260500	0.21104900
Co	1.16724600	-0.25726700	-0.02635400
B	-1.32082400	-1.74747300	1.51261200
Se	0.10138300	1.86099900	0.02284300
B	-2.45840700	-0.51396500	1.01237600

B	0.25403100	-1.03356900	1.69573400
B	0.29228700	0.74249100	1.68663300
B	-1.19223900	-0.11566400	2.15339500
H	-1.65705800	-2.63545200	2.21310000
H	-2.28064000	2.03619000	1.25466200
H	-3.58420900	-0.45886400	1.35706500
H	0.42398700	-2.96038200	0.02118700
H	-1.57131300	0.07164800	3.25908000
H	0.97722200	-1.48819600	2.51846500
H	0.92958200	1.24599700	2.54791500
H	-2.50352800	-2.74255900	-0.52813900
H	-0.30133000	-1.22463300	-2.28666300
H	2.78922000	-2.35675400	0.79268400
C	2.80578300	-1.45617000	0.19685500
C	3.12909800	-0.15363900	0.65647200
H	2.08286900	-2.18018800	-1.78924800
H	3.39453400	0.11668200	1.66826600
C	2.93666700	0.74080500	-0.42391200
H	3.04741000	1.81564200	-0.37338400
C	2.50802600	-0.00110700	-1.56575200
H	2.25656700	0.40340600	-2.53567500
C	2.43331900	-1.36153100	-1.17738500

CoSe2B9-2

B	0.29646800	-0.20743700	1.93543900
B	2.84619800	0.15788500	0.72709400
B	1.90692700	-0.88911200	1.81546000
B	1.69573600	0.85399000	1.88417400
B	2.31890700	0.02829000	-0.87109200
B	2.33304600	-1.45801900	0.22170000
B	1.84755500	1.53035000	0.22297800
B	0.61221700	-1.60681500	0.91864600
B	0.19462000	1.45173900	1.24638700
Se	0.78965800	-1.25642100	-1.15583400
Co	-0.93270100	-0.14451800	0.19240900
Se	0.01898100	1.86795300	-0.72418400
H	2.44884500	2.54422800	0.10841300
H	-0.32285600	-0.35913000	2.93574000
H	-0.33039100	2.27778000	1.91229100
H	2.96317100	0.19683900	-1.84435500
H	0.16422000	-2.68442500	1.11061900
H	2.99567600	-2.41622900	0.04708100
H	2.09216700	1.42807100	2.83764200
H	3.98744100	0.43047000	0.86525600
H	2.37517500	-1.46794500	2.73147800
H	-2.59152900	-0.39656800	-2.08115400
C	-2.58635600	-0.43070300	-1.00079200
C	-2.77827200	0.67060800	-0.12387400
H	-2.09431900	-2.56710000	-0.55027400
H	-2.93710100	1.69866000	-0.41954400

C	-2.64595000	0.21097500	1.21718300
H	-2.68487300	0.82374500	2.10575600
C	-2.38967700	-1.18748600	1.17258900
H	-2.18674600	-1.82358200	2.02119900
C	-2.34108400	-1.57660900	-0.19152800

CoSe2B9-3

Se	2.95987900	-0.33560200	-0.41208600
B	-0.41375500	1.70786200	0.73485700
B	1.80657600	-0.17423800	1.31241600
B	2.49055500	1.42107200	0.44680100
B	1.05172700	2.26419700	-0.00917600
B	1.12212700	1.42931900	1.55729600
Se	0.10342000	-1.47653000	0.29697900
Co	-1.50440900	0.12085200	-0.05370300
B	0.16659900	-0.26561800	-1.31065100
B	-0.12405600	1.38936000	-0.98826600
B	1.61324200	1.04196400	-1.21785200
B	-0.08833500	0.15534900	1.55938300
H	0.05413400	-0.82406200	-2.34948900
H	1.30280600	1.94947400	2.60366300
H	3.43192400	2.08413400	0.70523700
H	-0.48273400	-0.20539000	2.61605000
H	2.26862900	-0.78499400	2.21049000
H	-0.55314700	1.99541000	-1.91616600
H	-1.13227600	2.53119600	1.19113400
H	2.06462500	1.43366400	-2.23827100
H	1.21103700	3.42768300	-0.13272000
H	-3.36239600	1.18222000	1.76031700
C	-3.29585000	0.64667100	0.82422900
C	-3.21848200	-0.75654700	0.66998800
H	-3.09469000	2.29458000	-0.67420300
H	-3.22763400	-1.48446200	1.46973200
C	-3.05360100	-1.04341100	-0.72194300
H	-2.93049700	-2.02540300	-1.15711700
C	-3.01454600	0.18632900	-1.42095700
H	-2.83912300	0.31419700	-2.47957700
C	-3.14538000	1.23610900	-0.46290600

CoSe2B9-4

B	-0.31820700	1.56651300	0.51058900
B	1.15356600	-1.92513900	1.00720600
Se	1.48490700	1.84584400	-0.35932900
B	1.17296200	1.08703500	1.54820200
B	2.28005600	-0.41834100	1.07310000
Se	2.00547600	-1.29823800	-0.74674800
Co	-1.43308200	-0.06583700	0.03018900
B	-0.02190800	-1.46711900	-0.36847300
B	-0.47141500	0.39844400	1.79807100

B	-0.44918300	-1.30726600	1.33848500
B	0.96925000	-0.57848800	2.13512500
B	0.18235500	0.38573600	-1.03983000
H	-1.13260100	0.73906400	2.72142500
H	-0.41016800	-2.31830000	-1.09751500
H	1.61028300	1.85211000	2.33495700
H	-0.90808400	2.58561400	0.64073400
H	0.04865800	0.49079400	-2.21454500
H	-1.12525600	-2.08991200	1.91769100
H	1.43071000	-3.02852700	1.31399400
H	1.25660400	-0.69278300	3.27677200
H	3.41455400	-0.36262600	1.38861100
H	-2.46459300	-0.83199400	-2.46759700
C	-2.77516300	-0.47573700	-1.49558800
C	-2.86472100	0.88411800	-1.09443300
H	-3.00729300	-2.36171600	-0.32648300
H	-2.65771800	1.74637400	-1.71228700
C	-3.22789400	0.91154200	0.28362900
H	-3.30999400	1.79515700	0.90009300
C	-3.34783400	-0.42556500	0.73174800
H	-3.53830600	-0.73822700	1.74851000
C	-3.06338600	-1.28317400	-0.36622300

CoSe2B9-5

B	0.06156400	0.78799700	-1.53180700
B	1.62522100	-0.00848200	1.66952200
B	0.06141500	0.78813900	1.53178400
Se	2.78187000	0.01592500	0.00002800
B	1.73889200	-1.62892500	0.94209000
B	0.24027200	-0.99769400	1.49638300
B	1.73891100	-1.62904400	-0.94181600
Se	-0.33727000	1.95041300	-0.00007900
B	1.62524800	-0.00871400	-1.66951500
B	0.29245800	-1.90976600	0.00013400
Co	-1.17151800	-0.29142800	-0.00001500
B	0.24028800	-0.99791700	-1.49622600
H	2.38863600	-2.47804200	-1.43670800
H	-0.44940200	1.22737300	-2.50935400
H	2.25871400	0.21829200	-2.64324200
H	2.38858500	-2.47787500	1.43710700
H	-0.25172000	-1.44109400	2.48150400
H	-0.25170200	-1.44140600	-2.48130600
H	-0.17587400	-2.99996200	0.00026400
H	2.25861500	0.21878400	2.64323600
H	-0.44954300	1.22759800	2.50929200
H	-2.26660000	-2.43580000	1.34294400
C	-2.54309200	-1.60158800	0.71526100
C	-2.54298900	-1.60188700	-0.71490500
H	-2.91309100	0.03910600	2.18171300
H	-2.26641200	-2.43636200	-1.34219900

C	-2.88217800	-0.29864300	-1.15603100
H	-2.91279600	0.03818400	-2.18210800
C	-3.09027500	0.50312700	-0.00031100
H	-3.31901900	1.55923100	-0.00054800
C	-2.88232500	-0.29815800	1.15578300

CoSe2B9-6

Se	1.26475600	1.96601500	-0.15472300
B	-0.34511400	-1.64301600	0.56945400
B	1.39370000	-0.53145000	-1.46533200
Se	2.74739800	-0.94475600	-0.04883700
B	1.08437500	-2.04944300	-0.35701800
B	-0.18753000	-1.09067600	-1.14631300
B	-0.45866500	1.33695100	0.74096300
Co	-1.60206800	-0.16029500	0.01681800
B	1.17031500	0.77040800	1.46637000
B	-0.25149100	-0.18359900	1.59812600
B	1.21965500	-1.17172300	1.31495700
B	-0.07979600	0.69283100	-1.10405700
H	1.77042000	1.16919500	2.40209800
H	-0.70245300	-1.54227500	-2.11811600
H	-1.10285300	2.24511900	1.14580000
H	-0.47071900	1.27203500	-2.06448300
H	1.85885300	-0.47356600	-2.54908700
H	-0.64705100	-0.32559200	2.70999700
H	-0.89598700	-2.62097600	0.95044100
H	1.63410600	-1.76620000	2.24746700
H	1.27681400	-3.19914500	-0.53782200
H	-3.11180800	-2.30867700	-0.89567000
C	-3.21709300	-1.29861800	-0.52575100
C	-3.15786800	-0.11237200	-1.31326000
H	-3.32533200	-1.58702400	1.68421700
H	-3.00406000	-0.06939400	-2.38211600
C	-3.23585300	0.99890100	-0.43632500
H	-3.15992300	2.03910200	-0.71930700
C	-3.33551100	0.50086300	0.89241500
H	-3.33745000	1.09824100	1.79296600
C	-3.33154400	-0.91828900	0.83539000